Chapter 1

A Brief Review of Quantum Mechanics

1. (a) We know that $p = -i\hbar d/dx$. To find $[x, p]$, let it act on an arbitrary differentiable function $f(x)$,

$$[x, p]f = [x, -i\hbar d/dx]f = -i\hbar x(d/dx)f + i\hbar(d/dx)xf$$

We should understand the meaning of $(d/dx)xf$: both d/dx and x are operators, so x acts first on f giving the new function xf on which d/dx acts. Therefore

$$[x, p]f = -i\hbar xf' + i\hbar f + i\hbar xf' = i\hbar f$$

Since f is arbitrary, $[x, p] = i\hbar$.
To find $[x^2, p] = [xx, p]$, we use $[AB, C] = A[B, C] + [A, C]B$ along with $[x, p] = i\hbar$. We find $[x^2, p] = 2i\hbar x$.
To find $[p, V(x)]$, let $f(x)$ be an arbitrary differentiable function,

$$\begin{aligned}[p, V]f &= pVf - Vpf = -i\hbar(d/dx)Vf + i\hbar V(d/dx)f \\ &= -i\hbar(dV/dx)f - i\hbar Vf' + i\hbar Vf' = -i\hbar(dV/dx)f \\ &\Longrightarrow [p, V] = -i\hbar(dV/dx)\end{aligned}$$

(b) Consider any orthonormal basis $\{|1\rangle, |2\rangle, \dots\}$. By definition of the adjoint of an operator,

$$\begin{aligned}\langle n|(AB)^\dagger|m\rangle &= \langle m|AB|n\rangle^* = \left(\sum_k \langle m|A|k\rangle\langle k|B|n\rangle\right)^* \\ &= \sum_k \langle m|A|k\rangle^*\langle k|B|n\rangle^* = \sum_k \langle k|A^\dagger|m\rangle\langle n|B^\dagger|k\rangle = \sum_k \langle n|B^\dagger|k\rangle\langle k|A^\dagger|m\rangle \\ &= \langle n|B^\dagger A^\dagger|m\rangle\end{aligned}$$

It follows that $(AB)^\dagger = B^\dagger A^\dagger$.

(c) To show that $Tr(ABC) = Tr(CAB)$, it is sufficient to show that $Tr(AB) = Tr(BA)$.

$$\begin{aligned}Tr(AB) &= \sum_n \langle n|AB|n\rangle = \sum_{nm} \langle n|A|m\rangle\langle m|B|n\rangle = \sum_{nm} \langle m|B|n\rangle\langle n|A|m\rangle = \sum_m \langle m|BA|m\rangle \\ &= Tr(BA)\end{aligned}$$

The first equality results from the definition of the trace of an operator: it is the sum of the diagonal elements. The second equality is valid because $\sum_m |m\rangle\langle m| = 1$. The third equality holds true because $\langle n|A|m\rangle$ and $\langle m|B|n\rangle$ are simply numbers.

(d) Writing $S_x = (\hbar/2)\sigma_x$, $S_y = (\hbar/2)\sigma_y$, and $S_z = (\hbar/2)\sigma_z$, it is straightforward to check that $[S_x, S_y] = i\hbar S_z$, $[S_y, S_z] = i\hbar S_x$, and $[S_z, S_x] = i\hbar S_y$. These are the commutation relations for spin operators; hence, the representation of $\mathbf{S}$ as $(\hbar/2)\boldsymbol{\sigma}$ is a valid one.
Note that this representation is obtained if we take $|\uparrow\rangle$ and $|\downarrow\rangle$ as the basis states of the 2-dimensional spin vector space. In this case, $|\uparrow\rangle$ is represented by $\begin{pmatrix}1\\0\end{pmatrix}$, $|\downarrow\rangle$ by $\begin{pmatrix}0\\1\end{pmatrix}$, and S_z by

$$S_z = \begin{bmatrix}\langle\uparrow|S_z|\uparrow\rangle & \langle\uparrow|S_z|\downarrow\rangle \\ \langle\downarrow|S_z|\uparrow\rangle & \langle\downarrow|S_z|\downarrow\rangle\end{bmatrix} = \begin{bmatrix}\hbar/2 & 0 \\ 0 & -\hbar/2\end{bmatrix} = (\hbar/2)\sigma_z$$

(e)

$$S_x|\uparrow\rangle = \frac{\hbar}{2}\begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix}\begin{pmatrix}1\\0\end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix}0\\1\end{pmatrix} = \frac{\hbar}{2}|\downarrow\rangle$$

$$S_x|\downarrow\rangle = \frac{\hbar}{2}\begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix}\begin{pmatrix}0\\1\end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix}1\\0\end{pmatrix} = \frac{\hbar}{2}|\uparrow\rangle$$

$$S_y|\uparrow\rangle = \frac{\hbar}{2}\begin{bmatrix}0 & -i\\ i & 0\end{bmatrix}\begin{pmatrix}1\\0\end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix}0\\i\end{pmatrix} = i\frac{\hbar}{2}|\downarrow\rangle$$

$$S_y|\downarrow\rangle = \frac{\hbar}{2}\begin{bmatrix}0 & -i\\ i & 0\end{bmatrix}\begin{pmatrix}0\\1\end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix}-i\\0\end{pmatrix} = -i\frac{\hbar}{2}|\uparrow\rangle$$

2. Dirac-delta function

$$I = \int_{-\infty}^{\infty} e^{ikx}dk = \int_{-\infty}^{0} e^{ikx}dk + \int_{0}^{\infty} e^{ikx}dk = \lim_{\eta\to 0^+}\left[\int_{-\infty}^{0} e^{ikx}e^{\eta k}dk + \int_{0}^{\infty} e^{ikx}e^{-\eta k}dk\right]$$
$$= \lim_{\eta\to 0^+}\left[\frac{e^{(ix+\eta)k}}{ix+\eta}\bigg|_{-\infty}^{0} + \frac{e^{(ix-\eta)k}}{ix-\eta}\bigg|_{0}^{\infty}\right] = \lim_{\eta\to 0^+}\left[\frac{1}{x+i\eta} - \frac{1}{ix-\eta}\right]$$
$$= \lim_{\eta\to 0^+}\frac{2\eta}{x^2+\eta^2}$$

We note the following:

- If $x \neq 0$ then $I = 0$.
- If $x = 0$ then $I = \infty$.
- Integrating I over x, we find

$$J = \int_{-\infty}^{\infty}\frac{2\eta}{x^2+\eta^2} = 2\int_{-\infty}^{\infty}\frac{dy}{y^2+1}$$

where $y = x/\eta$. We thus find,

$$J = 2tan^{-1}y\big|_{-\infty}^{\infty} = 2[\pi/2 - (-\pi/2)] = 2\pi$$

Therefore,

$$\int_{-\infty}^{\infty} e^{ikx}dk = 2\pi\delta(x)$$

3. Another representation of the Dirac-delta function.

$$A(x) = \lim_{\alpha\to\infty}\frac{sin^2(\alpha x}{\alpha x^2}$$

We note the following:

- $x \neq 0 \Longrightarrow A(x) = 0$.
- $x \to 0 \Longrightarrow A(x) \to \alpha \to \infty$.
- Define I as:

$$I = \int_{-\infty}^{\infty}\frac{sin^2(\alpha x}{\alpha x^2}dx$$

Setting $y = \alpha x$,

$$I = \int_{-\infty}^{\infty}\frac{sin^2 y}{y^2}dy = 2\int_{0}^{\infty}\frac{sin^2 y}{y^2}dy \equiv 2J$$

Integrate by parts: $u = sin^2 y,\ dv = dy/y^2 \Rightarrow v = -1/y$.

$$J = -\frac{sin^2 y}{y}\bigg|_{0}^{\infty} + \int_{0}^{\infty}\frac{sin(2y)}{y}dy = \int_{0}^{\infty}\frac{sinx}{x}dx$$

Evaluation of $J = \int_0^\infty \frac{sinx}{x}dx$:

– First method:

$$\int_0^\infty e^{-sx} ds = \left. \frac{e^{-sx}}{-x} \right|_0^\infty = \frac{1}{x}$$

$$\Longrightarrow J = \int_0^\infty dx \int_0^\infty dse^{-sx} sinx = \int_0^\infty ds \left[\int_0^\infty e^{-sx} sinxdx \right] = \int_0^\infty f(s)ds$$

where

$$f(s) = \int_0^\infty e^{-sx} sinxdx$$

Integrate by parts: $u = sinx,\ dv = e^{-sx}dx \Rightarrow v = -\frac{1}{s}e^{-sx}$. We find

$$f(s) = -\frac{1}{s}e^{-sx} sinx \Big|_0^\infty + \frac{1}{s}\int_0^\infty e^{-sx} cosxdx = \frac{1}{s}\int_0^\infty e^{-sx} cosxdx$$

Integrate by parts again: $u = cosx,\ dv = e^{-sx}dx$. We find

$$f(s) = -\frac{1}{s^2}e^{-sx} cosx \Big|_0^\infty - \frac{1}{s^2}\int_0^\infty e^{-sx} sinxdx = \frac{1}{s^2} - \frac{1}{s^2}f(s)$$

Therefore,

$$f(s) = \frac{1/s^2}{1 + 1/s^2} = \frac{1}{s^2 + 1}$$

Hence,

$$J = \int_0^\infty \frac{ds}{s^2 + 1} = \pi/2$$

$$\Longrightarrow \int_{-\infty}^\infty \frac{sin^2(\alpha x)}{\alpha x^2} dx = \pi$$

$$\Longrightarrow \lim_{\alpha \to \infty} \frac{1}{\pi} \frac{sin^2(\alpha x)}{\alpha x^2} = \delta(x)$$

Second method:

$$I = \int_{-\infty}^\infty \frac{sinx}{x} dx = Im \int_{-\infty}^\infty \frac{e^{ix}}{x} dx$$

Consider

$$A = \int_C \frac{e^{iz}}{z} dz$$

where C is a closed contour in the complex plane which consists of four segments: two segments along the real axis, one of which extending from $-\infty$ to $x = -\epsilon$ ($\epsilon \to 0$) and the other segment running from $x = \epsilon$ to ∞, a semicircle C_1 of radius ϵ in the upper half-plane, and a semicircle C_2 at ∞ also in the upper half-plane.

$$A = \lim_{\epsilon \to 0} \left[\int_{-\infty}^{\epsilon} \frac{e^{ix}}{x} dx + \int_\epsilon^\infty \frac{e^{ix}}{x} dx + \int_{C_1} \frac{e^{iz}}{z} dz + \int_{C_1} \frac{e^{iz}}{z} dz \right]$$

The integral over C_2 vanishes (Jordan's lemma). Thus,

$$P \int_{-\infty}^\infty \frac{eix}{x} = -\int_{C_1} \frac{e^{iz}}{z} dz$$

Here, P stands for the principal value. The principal value of the integral is the value of the integral from $-\infty$ to ∞ excluding the value $x = 0$. To evaluate the integral over C_1, let $z = \epsilon e^{i\theta}$, then $dz/z = id\theta$. Furthermore, $e^{iz} \to 1$. Therefore,

$$P \int_{-\infty}^\infty \frac{e^{ix}}{x} = -i \int_\pi^0 d\theta = i\pi$$

Since the integrand $sinx/x$ is finite at $x = 0$ (it is equal to 1) the principal value of the integral of $sinx/x$ is equal to the integral itself (they differ only by $\lim_{\epsilon \to 0} \int_{-\epsilon}^{\epsilon} [sinx/x] dx$). Hence $I = \pi$.

4. Periodic boundary conditions.

The eigenvalue equation is

$$-(\hbar^2/2m)\nabla^2\phi = \epsilon\phi$$

The normalized eigenfunctions are $\phi_{\mathbf{k}} = \frac{1}{\sqrt{V}}e^{i\mathbf{k}.\mathbf{r}}$, where $\mathbf{k}$ is a real vector, and the eigenvalues are $\epsilon_{\mathbf{k}} = \hbar^2 k^2/2m$. Note that $\int \phi^*_{\mathbf{k}}\phi_{\mathbf{k}} d^3r = 1$.

The boundary condition $e^{ik_x(x+L)} = e^{ik_x x}$ implies that

$$e^{ik_x L} = 1 \Longrightarrow k_x = 0, \pm 2\pi/L, \pm 4\pi/L, \cdots = 2n\pi/L, \quad n \in \mathcal{Z}$$

Taking into account the electron's spin, the states are given by $|\mathbf{k}\sigma\rangle$, where $\sigma =\uparrow$ or $\downarrow$, and

$$\phi_{\mathbf{k}\sigma}(\mathbf{r}) = \langle \mathbf{r}|\mathbf{k}\sigma\rangle = \frac{1}{\sqrt{V}}e^{i\mathbf{k}.\mathbf{r}}|\sigma\rangle$$

To show that the states are orthonormal, consider

$$\langle \mathbf{k}'\sigma'|\mathbf{k}\sigma\rangle = \frac{1}{V}\int d^3r e^{i(\mathbf{k}-\mathbf{k}').\mathbf{r}}\langle\sigma'|\sigma\rangle = \delta_{\sigma\sigma'}\frac{1}{V}\int e^{i(\mathbf{k}-\mathbf{k}').\mathbf{r}}d^3r$$

where the integration is over the volume of the cube. the integral may be written as

$$I = \frac{1}{V}\int e^{i(\mathbf{k}-\mathbf{k}').\mathbf{r}}d^3r = I_x I_y I_z$$

where

$$I_x = \frac{1}{L}\int_0^L e^{i(k_x-k'_x)x}dx$$

and I_y and I_z are the same as I_x with x replaced by y and z, respectively. If $k_x \neq k'_x$, then

$$I_x = \frac{1}{L}\frac{e^{i(k_x-k'_x)L} - 1}{i(k_x - k'_x)}$$

Since $k_x, k'_x = 2n\pi/L, n \in \mathcal{Z}$, and $k_x \neq k'_x$, it follows that $k_x - k'_x = 2m\pi/L, m \in \mathcal{Z}$, and the numerator in the above expression for I_x vanishes. If $k_x = k'_x$, then $I_x = 1$. Therefore, $I_x = \delta_{k_x,k'_x}$. Similarly, $I_y = \delta_{k_y,k'_y}$ and $I_z = \delta_{k_z,k'_z}$. Hence $I = \delta_{\mathbf{k}\mathbf{k}'}$ and $\langle \mathbf{k}'\sigma'|\mathbf{k}\sigma\rangle = \delta_{\mathbf{k}\mathbf{k}'}\delta_{\sigma\sigma'}$; the states are orthonormal.

To establish the completeness property, we evaluate

$$\sum_{\mathbf{k}\sigma}\phi_{\mathbf{k}\sigma}(\mathbf{r})\phi^*_{\mathbf{k}\sigma}(\mathbf{r}') = \sum_{\mathbf{k}}\phi_{\mathbf{k}}(\mathbf{r})\phi_{\mathbf{k}}(\mathbf{r}')\sum_{\sigma}|\sigma\rangle\langle\sigma|$$

First, consider the spin part. for an arbitrary state $|\chi\rangle = a|\uparrow\rangle + b|\downarrow\rangle$,

$$\sum_{\sigma}|\sigma\rangle\langle\sigma|\chi\rangle = |\uparrow\rangle\langle\uparrow|\chi\rangle + |\downarrow\rangle\langle\downarrow|\chi\rangle = |\uparrow\rangle a + |\downarrow\rangle b = |\chi\rangle$$

$$\Longrightarrow \sum_{\sigma}|\sigma\rangle\langle\sigma| = 1$$

Now consider the spatial part,

$$A = \sum_{\mathbf{k}}\phi_{\mathbf{k}}(\mathbf{r})\phi_k v^*(\mathbf{r}') = \frac{1}{V}\sum_{\mathbf{k}}e^{i\mathbf{k}.(\mathbf{r}-\mathbf{r}')} = A_x A_y A_z$$

where

$$A_x = \frac{1}{L}\sum_{k_x}e^{ik_x(x-x')}$$

Similar expressions can be written for A_y and A_z with x replaced by y and z, respectively. We note the following:

(a) If $x = x'$, then $A_x = \frac{1}{L}\sum 1 = \infty$ since there is an infinite number of terms in the sum.

(b) Suppose that $x \neq x'$. We can write

$$A_x = \cdots + e^{-i4\pi(x-x')/L} + e^{-i2\pi(x-x')/L} + 1 + e^{i2\pi(x-x')/L} + e^{i4\pi(x-x')/L} + \cdots$$

We make the crucial observation that if we multiply the above infinite series by $e^{i2n\pi(x-x')/L}$, for any integer n, the value of the series remains unchanged, because we are still summing exactly the same terms, the 1 being simply shifted n spaces. Therefore,

$$A_x = e^{i2n\pi(x-x')/L} A_x, \quad n \in \mathcal{Z}$$

Since $-L < x - x' < L$, and $x \neq x'$, the only way the above equation is satisfied is by setting $A_x = 0$. We conclude that: $x \neq x' \Longrightarrow A_x = 0$.

(c) Consider

$$\int_0^L A_x dx = \frac{1}{L}\int_0^L \sum_{k_x} e^{ik_x(x-x')} dx = \frac{1}{L}\sum_{k_x}\int_{-x'}^{L-x'} e^{ik_x u} du$$
$$= \frac{1}{L}\sum_{k_x} \frac{e^{ik_x L}e^{-ik_x x'} - e^{-ik_x x'}}{ik_x} = \frac{1}{L}\sum_{k_x} e^{-ik_x x'}\frac{e^{ik_x L} - 1}{ik_x}$$

Since $k_x L = 2n\pi,\ n \in \mathcal{Z}$, it follows that $e^{ik_x L} = e^{2in\pi} = 1$, and the above integral vanishes if $k_x \neq 0$. If $k_x = 0$, the integral is equal to 1. Therefore, $\int A(x)dx = 1$.

To summarize, $A_x(x - x')$ is equal to zero if $x \neq x'$, is equal to ∞ if $x = x'$, and its integral over x is 1 $\Rightarrow A_x = \delta(x - x')$.

Similarly, $A_y = \delta(y - y')$ and $A_z = \delta(z - z')$. Therefore,

$$\sum_{\mathbf{k}\sigma} \phi_{\mathbf{k}\sigma}(\mathbf{r})\phi^*_{\mathbf{k}\sigma}(\mathbf{r}') = \delta(\mathbf{r} - \mathbf{r}')$$

The completeness property is thus established.

5. Singlets and triplets.

$$S^2 = (\mathbf{S}_1 + \mathbf{S}_2)^2 = S_1^2 + S_2^2 + 2\mathbf{S}_1.\mathbf{S}_2 = S_1^2 + S_2^2 + 2S_{1x}S_{2x} + 2S_{1y}S_{2y} + 2S_{1z}S_{2z}$$

S_1^2 acts only on states of electron 1 and S_2^2 acts only on states of electron 2.

$$(S_1^2 + S_2^2)\alpha(1)\alpha(2) = \hbar^2 s_1(s_1+1)\alpha(1)\alpha(2) + \hbar^2 s_2(s_2+1)\alpha(1)\alpha(2)$$
$$= \hbar^2\left[\frac{1}{2}(\frac{1}{2}+1) + \frac{1}{2}(\frac{1}{2}+1)\right]\alpha(1)\alpha(2) = \frac{3\hbar^2}{2}\alpha(1)\alpha(2)$$

$$S_{1z}S_{2z}\alpha(1)\alpha(2) = \frac{\hbar}{2}\frac{\hbar}{2}\alpha(1)\alpha(2) = (\hbar^2/4)\alpha(1)\alpha(2)$$
$$S_{1x}S_{2x}\alpha(1)\alpha(2) = (\hbar^2/4)\beta(1)\beta(2)$$
$$S_{1y}S_{2y}\alpha(1)\alpha(2) = (-i\hbar/2)^2\beta(1)\beta(2) = -(\hbar^2/4)\beta(1)\beta(2)$$

We have used the results of problem 1 in writing the last two equations. Collecting terms, we find

$$S^2\alpha(1)\alpha(2) = 2\hbar^2\alpha(1)\alpha(2) = \hbar^2 s(s+1)\alpha(1)\alpha(2)$$

$$S_z\alpha(1)\alpha(2) = (S_{1z} + S_{2z})\alpha(1)\alpha(2) = \frac{\hbar}{2}\alpha(1)\alpha(2) + \frac{\hbar}{2}\alpha(1)\alpha(2) = \hbar\alpha(1)\alpha(2)$$

where $s = 1$. We conclude that $\alpha(1)\alpha(2)$ is an eigenstate of S^2 and S_z with $s = 1$ and $m_s = 1$.

Following the same steps as above, we find

$$S^2\frac{1}{\sqrt{2}}\left[\alpha(1)\beta(2) + \beta(1)\alpha(2)\right] = 2\hbar^2\frac{1}{\sqrt{2}}\left[\alpha(1)\beta(2) + \beta(1)\alpha(2)\right]$$
$$S_z\frac{1}{\sqrt{2}}\left[\alpha(1)\beta(2) + \beta(1)\alpha(2)\right] = 0$$
$$S^2\beta(1)\beta(2) = 2\hbar^2\beta(1)\beta(2)$$
$$S_z\beta(1)\beta(2) = -\hbar\beta(1)\beta(2)$$

As for the singlet state, we obtain

$$S^2 \frac{1}{\sqrt{2}} [\alpha(1)\beta(2) - \beta(1)\alpha(2)] = 0$$
$$S_z \frac{1}{\sqrt{2}} [\alpha(1)\beta(2) - \beta(1)\alpha(2)] = 0$$

To summarize:

$$\text{Triplet}: \begin{cases} \alpha(1)\alpha(2) & s = 1,\ m_s = 1 \\ \frac{1}{\sqrt{2}} [\alpha(1)\beta(2) + \beta(1)\alpha(2)] & s = 1,\ m_s = 0 \\ \beta(1)\beta(2) & s = 1,\ m_s = -1 \end{cases}$$

$$\text{Singlet}: \ \frac{1}{\sqrt{2}} [\alpha(1)\beta(2) - \beta(1)\alpha(2)] \quad s = 0,\ m_s = 0$$

We conclude with the following remarks:

- The four states given above are normalized and orthogonal to each other.
- The triplet states are symmetic under the interchange of electrons 1 and 2, while the singlet state is antisymmetric under such an interchange.

6. Particle bound by a delta-function potential.

(a) The potential energy is $V(x) = -\lambda\delta(x)$. The wave function $\phi(x)$ satisfies the Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\phi(x) - \lambda\delta(x)\phi(x) = E\phi(x)$$

For a bound state the energy E must be negative (if $E > 0$, the wave function for $x < 0$ and for $x > 0$ will be plane waves extending to $\pm\infty$; the particle will not be bound).
Writing $E = -|E|$, and noting that $V(x) = 0$ for $x < 0$ and for $x > 0$, and that the wave function must vanish at $\pm\infty$, we obtain

$$\phi(x) = \begin{cases} Ae^{\kappa x} & x < 0 \\ Be^{-\kappa x} & x > 0 \end{cases}$$

where $\kappa = \sqrt{2m|E|}/\hbar$. The continuity of $\phi(x)$ at $x = 0$ implies that $A = B$. Thus we can write $\phi(x) = Ae^{-\kappa|x|}$ for all values of x. The constant A is determined by requiring that $\phi(x)$ be normalized: $\int_{-\infty}^{\infty} |\phi(x)|^2 dx = 1$. This readily gives $A = \sqrt{\kappa}$. To determine κ, we integrate the Schrödinger equation from $-\epsilon$ to ϵ, and take the limit as $\epsilon \to 0$,

$$-\frac{\hbar^2}{2m}\lim_{\epsilon\to 0}\int_{-\epsilon}^{\epsilon}\frac{d^2\phi}{dx^2}dx - \lambda\lim_{\epsilon\to 0}\int_{-\epsilon}^{\epsilon}\delta(x)\phi(x)dx = E\lim_{\epsilon\to 0}\int_{-\epsilon}^{\epsilon}\phi(x)dx$$

Continuity of $\phi(x)$ implies that the right hand side (RHS) vanishes. Using the sifting property of $\delta(x)$, we find

$$-\frac{\hbar^2}{2m}\left[\phi'(0^+) - \phi'(0^-)\right] = \lambda\phi(0) \Rightarrow -\frac{\hbar^2}{2m}[-\kappa A - \kappa A] = \lambda A \Rightarrow \kappa = m\lambda/\hbar^2$$
$$\Longrightarrow E = -\frac{m\lambda^2}{2\hbar^2}$$

Thus, we find that there is only one bound state with energy E as given above.

(b) Now $V(x) = -b\lambda\delta(x)$, where b is a dimensionless positive constant. We want to determine the probability that the particle remains bound.
With the new potential energy, the bound state wave function $\psi(x)$ is obtained from $\phi(x)$ by replacing λ with $b\lambda$. Since $\kappa = m\lambda/\hbar^2$, it follows that $\psi(x) = \sqrt{b\kappa}e^{-b\kappa|x|}$. The particle is initially in the state with wave function $\phi(x)$, so the probability amplitude of finding it in the state with wave function $\psi 9x)$ is $\langle\psi|\phi\rangle = \int_{-\infty}^{\infty}\psi^*(x)\phi(x)dx$. The integral is easily evaluated; it yields $2\sqrt{b}/(b+1)$. The probability that the particle remains bound is thus given by

$$P = |\langle\psi|\phi\rangle|^2 = \frac{4b}{(b+1)^2}$$

Note that $P \leq 1$, as it should; it is equal to 1 only if $b = 1$, which corresponds to no change in the delta-function potential.

7. Harmonic oscillator. We want to show that in the ground state of a harmonic oscillator, $\langle p^2/2m\rangle = \langle (1/2)m\omega^2x^2\rangle = \hbar\omega/4$.

One way to obtain this result is by using the wave function of the ground state, which is a gaussian, and carrying out the integrals $\int_{-\infty}^{\infty}\psi_0^*(p^2/2m)psi_0dx$ and $\int_{-\infty}^{\infty}\psi_0^*(1/2)m\omega^2x^2psi_0dx$. Another way is to use the expressions for x and p in terms of creation and annihilation operators. Starting from

$$a = b\left(x + \frac{i}{m\omega}p\right)$$
$$a^\dagger = b\left(x - \frac{i}{m\omega}p\right), \qquad b = \left(\frac{m\omega}{2\hbar}\right)^{1/2},$$

we solve for x. We find

$$x = \left(\frac{\hbar}{2m\omega}\right)^{1/2}(a + a^\dagger)$$
$$\Longrightarrow \frac{1}{2}m\omega^2x^2 = \frac{\hbar\omega}{4}\left(a + a^\dagger\right)^2 = \frac{\hbar\omega}{4}\left(a^2 + aa^\dagger + a^\dagger a + a^{\dagger 2}\right)$$

Using $aa^\dagger = a^\dagger a - 1$, we find

$$\frac{1}{2}m\omega^2x^2 = \frac{\hbar\omega}{4} + \frac{\hbar\omega}{4}\left(a^2 + 2a^\dagger a + a^{\dagger 2}\right)$$

Therefore,

$$\langle 0|\frac{1}{2}m\omega^2x^2|0\rangle = \frac{\hbar\omega}{4} + \frac{\hbar\omega}{4}\langle 0|a^2 + 2a^\dagger a + a^{\dagger 2}|0\rangle = \frac{\hbar\omega}{4}$$

Since

$$\langle 0|H|0\rangle = \frac{\hbar\omega}{2}$$

and $H = p^2/2m + (1/2)m\omega^2x^2$, it follows that

$$\langle 0|p^2/2m|0\rangle = \hbar\omega/2 - \hbar\omega/4 = \hbar\omega/4$$

8. Harmonic oscillator coherent states.

(a) Since any state $|\psi\rangle$ can be expanded as $\psi\rangle = \sum_n c_n|n\rangle$, where the states $|n\rangle$ are the harmonic oscillator eigenstates, it follows that $a^\dagger$ does not have an eigenstate. To show this, suppose that in the expansion $\psi\rangle = \sum_n c_n|n\rangle$, the lowest value of n is m. Then, in $a^\dagger|\psi\rangle = \sum_n c_n\sqrt{n+1}|n+1\rangle$, the lowest energy state that occurs in the expansion is $|m+1\rangle$; hence $a^\dagger|\psi\rangle$ cannot be equal to a constant times $|\psi\rangle$. We conclude that no state $|\psi\rangle$ could be an eigenstate of $a^\dagger$.

(b) For any complex number z, consider the state

$$|z\rangle = e^{-z^*z/2}e^{za^\dagger}|0\rangle$$

To show that this is an eigenstate of the annihilation operator a, let us first prove that $[a, a^{\dagger n}] = na^{\dagger n-1}$. This is proved by mathematical induction. It is clearly true for $n = 1$ since $[a, a^\dagger] = 1$. We assume that the formula is true for n and show that it is true for $n+1$. That is, we assume that $[a, a^{\dagger n}] = na^{\dagger n-1}$, and show that $[a, a^{\dagger n+1}] = (n+1)a^{\dagger n}$. Using

$$[A, BC] = B[A, C] + [A, B]C,$$

which is easily checked, we can write

$$\left[a, a^{\dagger n+1}\right] = \left[a, a^{\dagger n}a^\dagger\right] = a^{\dagger n}\left[a, a^\dagger\right] + \left[a, a^{\dagger n}\right]a^\dagger = a^{\dagger n}(1) + \left(na^{\dagger n-1}\right)a^\dagger = a^{\dagger n} + na^{\dagger n} = (n+1)a^{\dagger n}$$

In the third equality, we used the assumption that the formula is true for n. The formula is thus verified. Now consider

$$\left[a, e^{za^\dagger}\right] = \sum_{n=0}^{\infty}\frac{z^n}{n!}\left[a, a^{\dagger n}\right] = \sum_{n=0}^{\infty}\frac{z^n}{n!}na^{\dagger n-1} = z\sum_{n=1}^{\infty}\frac{z^{n-1}}{(n-1)!}a^{\dagger n-1} = z\sum_{m=0}^{\infty}\frac{z^m}{m!}a^{\dagger m} = ze^{za^\dagger}$$

It follows that

$$ae^{za^\dagger}|0\rangle = e^{za^\dagger}a|0\rangle + ze^{za^\dagger}|0\rangle = ze^{za^\dagger}|0\rangle$$

This shows that $e^{za^\dagger}|0\rangle$ is indeed an eigenstate of a with eigenvalue z. We can write

$$|z\rangle = e^{-z^*z/2}e^{za^\dagger}|0\rangle = e^{-z^*z/2}\sum_{n=0}^{\infty}\frac{z^n}{n!}a^{\dagger n}|0\rangle = e^{-z^*z/2}\sum_{n=0}^{\infty}\frac{z^n}{n!}\sqrt{n!}\,|n\rangle$$

$$\langle z'| = e^{-z'^*z'/2}\sum_{n=0}^{\infty}\frac{z'^{*n}}{n!}\sqrt{n!}\,\langle n|$$

(recall that $9! = 1$). We thus obtain

$$\begin{aligned}\langle z'|z\rangle &= e^{-(z^*z+z'^*z')/2}\sum_{nm}\frac{z^n z'^{*m}}{n!m!}\sqrt{n!}\sqrt{m!}\langle m|n\rangle = e^{-(z^*z+z'^*z')/2}\sum_{n=0}^{\infty}\frac{(zz'^*)^n}{n!}\\ &= e^{-(z^*z+z'^*z'-2zz'^*)/2}\end{aligned}$$

This shows that $\langle z|z\rangle = 1$: the states are normalized. However, the above shows that $\langle z'|z\rangle \neq \delta(z-z')$, i.e., the states are not orthogonal.

9. Time-independent perturbation.

(a)

$$H = H_0 + V, \qquad H_0 = p^2/2m + (1/2)m\omega^2x^2, \qquad V = \lambda x$$

Treating V as a perturbation, the shift in energy of the ground state is given by

$$\Delta E_0 = \langle 0|V|0\rangle + \sum_{m\neq 0}\frac{|\langle m|V|0\rangle|^2}{E_0 - E_m} \equiv \Delta E_0^{(1)} + \Delta E_0^{(2)}$$

The perturbation can be written in terms of creation and annihilation operators:

$$V = \lambda x = \lambda\left(\frac{\hbar}{2m\omega}\right)^{1/2}(a + a^\dagger)$$

Since $\langle 0|a|0\rangle = \langle |a^\dagger|0\rangle = 0$, it follows that $\Delta E_0^{(1)} = 0$. Noting that $a|0\rangle = 0$ and $a^\dagger|0\rangle = |1\rangle$, we obtain

$$\langle m|V|0\rangle = \lambda\left(\frac{\hbar}{2m\omega}\right)^{1/2}\delta_{m,1}$$

Hence,

$$\begin{aligned}\Delta E_0^{(2)} &= \frac{\hbar\lambda^2}{2m\omega}\sum_{m\neq 0}\frac{\delta_{m,1}}{E_0 - E_m} = \frac{\hbar\lambda^2}{2m\omega}\frac{1}{E_0 - E_1} = \frac{\hbar\lambda^2}{2m\omega}\left(\frac{1}{-\hbar\omega}\right)\\ &= -\frac{\lambda^2}{2m\omega^2}\end{aligned}$$

(b)

$$\begin{aligned}H &= \frac{p^2}{2m} + \frac{1}{2}m\omega^2x^2 + \lambda x\\ &= \frac{p^2}{2m} + \frac{1}{2}m\omega^2\left(x^2 + \frac{2\lambda}{m\omega^2}x\right)\\ &= \frac{p^2}{2m} + \frac{1}{2}m\omega^2\left(x^2 + \frac{2\lambda}{m\omega^2}x + \frac{\lambda^2}{m^2\omega^4} - \frac{\lambda^2}{m^2\omega^4}\right)\\ &= \frac{p^2}{2m} + \frac{1}{2}m\omega^2\left(x + \frac{\lambda}{m\omega^2}\right)^2 - \frac{\lambda^2}{2m\omega^2}\end{aligned}$$

Except for the last term, which is a constant, this is the Hamiltonian for a harmonic oscillator whose center is at $x = -\lambda/m\omega^2$. Therefore,

$$E_n = (n + 1/2)\hbar\omega - \frac{\lambda^2}{2m\omega^2}$$

The perturbation shifts all states downward by $\lambda^2/2m\omega^2$. In this case, the second-order perturbation theory yields the exact answer.

10. Heisenberg picture of quantum mechanics.

    (a) Denoting an operator in the Schrödinger picture by A, the corresponding operator in the Heisenberg picture is given by
    $$A_H(t) = e^{iHt/\hbar} A e^{-iHt/\hbar}$$
    Taking the derivative with respect to time,
    $$\frac{d}{dt} A_H(t) = (iH/\hbar) e^{iHt/\hbar} A e^{-iHt/\hbar} + e^{iHt/\hbar} A(-iH/\hbar) e^{-iHt/\hbar} + e^{iHt/\hbar} \frac{\partial A}{\partial t} e^{-iHt/\hbar}$$
    Note that H commutes with $e^{\pm iHt/\hbar}$. Therefore,
    $$\frac{d}{dt} A_H(t) = \frac{i}{\hbar}\left(H A_H - A_H H\right) + e^{iHt/\hbar} \frac{\partial A}{\partial t} e^{-iHt/\hbar}$$
    The last term is simply $\partial A/\partial t$ in the Heisenberg picture. If A has no explicit time dependence, as is usually the case, then
    $$\frac{d}{dt} A_H = \frac{1}{\hbar}\left[H, A_H\right]$$

    (b) Let $a(t)$ be the annihilation operator in the Heisenberg picture. Then
    $$\frac{da}{dt} = \frac{i}{\hbar}[H, a]$$
    For the harmonic oscillator, $H = \hbar\omega\left(a^\dagger a + 1/2\right)$. Thus,
    $$[H, a] = \hbar\omega\left[a^\dagger a, a\right] + \hbar\omega[1/2, a]$$
    The last term on the RHS vanishes (a number commutes with an operator). To evaluate the first term, we use
    $$[AB, C] = A[B, C] + [A, C]B$$
    We thus find
    $$\left[a^\dagger a, a\right] = a^\dagger[a, a] + \left[a^\dagger, a\right] a = 0 - a = -a$$
    Hence
    $$\frac{da}{dt} = -i\omega a \Longrightarrow a(t) = a(0) e^{-i\omega t}$$
    For $a^\dagger(t)$, we can either repeat the same steps as above, or simply note that $a^\dagger(t)$ is the adjoint of $a(t)$. Therefore,
    $$a^\dagger(t) = a^\dagger(0) e^{i\omega t}$$

11. The interaction picture

    (a) Let A be an operator in the Schrödinger picture. The corresponding operator in the interaction picture is defined as
    $$A_I(t) = e^{iH_0 t/\hbar} A e^{-iH_0 t/\hbar}$$
    This has the same form as $A_H(t)$ except that $H \to H_0$. Thus
    $$\frac{d}{dt} A_I(t) = \frac{i}{\hbar}\left[H_0, A_I(t)\right]$$

    (b)
    $$|\psi_I(t)\rangle = e^{iH_0 t/\hbar}|\psi_S(t)\rangle \Rightarrow i\hbar\frac{\partial}{\partial t}|\psi_I(t)\rangle = -H_0 e^{iH_0 t/\hbar}|\psi_S(t)\rangle + e^{iH_0 t/\hbar} i\hbar\frac{\partial}{\partial t}|\psi_S(t)\rangle$$
    Using the Schrödinger equation
    $$i\hbar\frac{\partial}{\partial t}|\psi_S(t)\rangle = H|\psi_S(t)\rangle = H_0|\psi_S(t)\rangle + V|\psi_S(t)\rangle$$
    and noting that $H_0 e^{iH_0 t/\hbar} = e^{iH_0 t/\hbar} H_0$, we obtain
    $$i\hbar\frac{\partial}{\partial t}|\psi_I(t)\rangle = e^{iH_0 t/\hbar} V|\psi_S(t)\rangle + e^{iH_0 t/\hbar} V e^{-iH_0 t/\hbar}|\psi_I(t)\rangle$$
    Hence,
    $$i\hbar\frac{\partial}{\partial t}|\psi_I(t)\rangle = V_I(t)|\psi_I(t)\rangle$$

(c) For an arbitrary state $|\psi_I(t_0)\rangle$,

$$|\psi_I(t)\rangle = U_I(t,t_0)|\psi_I(t_0)\rangle \Rightarrow i\hbar\frac{\partial}{\partial t}|\psi_I(t)\rangle = i\hbar\frac{\partial}{\partial t}U_I(t,t_0)|\psi_I(t_0)\rangle$$

We also have

$$i\hbar\frac{\partial}{\partial t}|\psi_I(t)\rangle = V_I(t)|\psi_I(t)\rangle = V_I(t)U_I(t,t_0)|\psi_I(t_0)\rangle$$

Since $|\psi_I(t_0)\rangle$ is arbitrary, it follows that

$$i\hbar\frac{\partial}{\partial t}U_I(t,t_0) = V_I(t)U_I(t,t_0)$$

(d) Let us integrate the above equation from t_0 to t,

$$\begin{aligned}\int_{t_0}^{t}\frac{\partial}{\partial t_1}U_I(t_1,t_0)dt_1 &= -\frac{i}{\hbar}\int_{t_0}^{t}V_I(t_1)U_I(t_1,t_0)dt_1\\ \Longrightarrow U_I(t,t_0)-U_I(t_0,t_0) &= -\frac{i}{\hbar}\int_{t_0}^{t}V_I(t_1)U_I(t_1,t_0)dt_1\end{aligned}$$

Since $U_I(t_0,t_0)=1$, we obtain

$$U_I(t,t_0) = 1-\frac{i}{\hbar}\int_{t_0}^{t}V_I(t_1)U_I(t_1,t_0)dt_1$$

This is an integral equation. We solve it by iteration:

$$\begin{aligned}U_I(t,t_0) &= 1-\frac{i}{\hbar}\int_{t_0}^{t}dt_1V_I(t_1)\left[1-\frac{i}{\hbar}\int_{t_0}^{t_1}dt_2V_I(t_2)U_I(t_2,t_0)\right]\\ &= 1-\frac{i}{\hbar}\int_{t_0}^{t}dt_1V_I(t_1)+\left(\frac{-i}{\hbar}\right)^2\int_{t_0}^{t}dt_1\int_{t_0}^{t_1}dt_2V_I(t_1)V_I(t_2)U_I(t_2,t_0)\end{aligned}$$

We continue to iterate; we find

$$U_I(t,t_0) = 1-\frac{i}{\hbar}\int_{t_0}^{t}dt_1V_I(t_1)+\left(\frac{-i}{\hbar}\right)^2\int_{t_0}^{t}dt_1\int_{t_0}^{t_1}dt_2V_I(t_1)V_I(t_2)+\cdots$$

(e)

$$\begin{aligned}|\psi_I(t)\rangle &= e^{iH_0t/\hbar}|\psi_S(t)\rangle = e^{iH_0t/\hbar}U(t,t_0)|\psi_S(t_0)\rangle\\ &= e^{iH_0t/\hbar}U(t,t_0)e^{-iH_0t_0/\hbar}|\psi_I(t_0)\rangle\end{aligned}$$

Therefore,

$$U_I(t,t_0) = e^{iH_0t/\hbar}U(t,t_0)e^{-iH_0t_0/\hbar},$$

and

$$\begin{aligned}\langle f|U_I(t,t_0)|i\rangle &= \langle f|e^{iH_0t/\hbar}U(t,t_0)e^{-iH_0t_0/\hbar}|i\rangle\\ &= e^{iE_ft/\hbar}e^{-iE_it_0/\hbar}\langle f|U(t,t_0)|i\rangle\end{aligned}$$

Therefore,

$$|\langle f|U_I(t,t_0)|i\rangle|^2 = |\langle f|U(t,t_0)|i\rangle|^2 = P_{i\to f}$$

12. Fermi golden rule.

(a)

$$V(t) = \begin{cases}0 & t<0\\ V & t\geq 0\end{cases}$$

$$P_{i\to f} = |\langle f|U_I(t,t_0)|i\rangle|^2$$

Here, $t_0=0$, and

$$U_I(t,0) = 1-\frac{i}{\hbar}\int_0^t V_I(t_1)dt_1+\cdots$$

Suppose that $|f\rangle \neq |i\rangle$. Then to first order in the perturbation,

$$\langle f|U_I(t,0)|i\rangle = -\frac{i}{\hbar}\int_0^t dt_1 \langle f|V_I(t_1)|i\rangle$$

The matrix element is given by

$$\langle f|V_I(t_1)|i\rangle = \langle f|e^{iH_0t_1/\hbar}Ve^{-iH_0t_1/\hbar}|i\rangle = e^{i\omega_{fi}t_1}V_{fi}$$

where $\omega_{fi} = (E_f - E_i)/\hbar$ and $V_{fi} = \langle f|V|i\rangle$. Therefore,

$$\begin{aligned}\langle f|U_I(t,0)|i\rangle &= -\frac{i}{\hbar}V_{fi}\int_0^t dt_1 e^{i\omega_{fi}t_1} = -\frac{i}{\hbar}V_{fi}\frac{e^{i\omega_{fi}t}-1}{i\omega_{fi}} = -\frac{i}{\hbar\omega_{fi}}V_{fi}e^{i\omega_{fi}t/2}\left(\frac{e^{i\omega_{fi}t/2}-e^{-i\omega_{fi}t/2}}{i}\right)\\ &= \left(\frac{-2i}{\hbar\omega_{fi}}\right)V_{fi}e^{i\omega_{fi}t/2}sin\,(\omega_{fi}t/2)\end{aligned}$$

The transition probability is thus given by

$$P_{i\to f} = \frac{4}{\hbar^2}\left|V_{fi}\right|^2\frac{sin^2\,(\omega_{fi}t/2)}{\omega_{fi}^2}$$

(b) The above is rewritten as

$$P_{i\to f} = t\frac{\left|V_{fi}\right|^2}{\hbar^2}\frac{sin^2\,(t\omega_{fi}/2)}{t\,(\omega_{fi}/2)^2}$$

Using the result of problem 2.3, we can write

$$\lim_{t\to\infty}\frac{sin^2\,(t\omega_{fi}/2)}{t\,(\omega_{fi}/2)^2} = \pi\delta\,(\omega_{fi}/2) = \pi\delta\left(\frac{E_f-E_i}{2\hbar}\right) = 2\pi\hbar\delta\,(E_f - E_i)$$

where we used the formula $\delta(ax) = \delta(x)/|a|$. Hence,

$$\lim_{t\to\infty}P_{i\to f} = \frac{2\pi}{\hbar^2}\left|V_{fi}\right|^2 t\delta\,(E_f - E_i)$$

The transition rate is thus given by

$$wi\to f = \frac{d}{dt}\lim_{t\to\infty}P_{i\to f} = \frac{2\pi}{\hbar^2}\left|V_{fi}\right|^2\delta\,(E_f - E_i)$$

This is Fermi's golden rule.

13. Harmonic perturbation.

(a)

$$V(t) = Ae^{i\omega t} + A^\dagger e^{-i\omega t} \qquad t \geq 0$$

We assume that $\omega \neq 0$. If $\omega = 0$, then V is constant for $t \geq 0$, and the problem becomes identical to the previous one. To first order in the interaction, the evolution operator in the interaction picture is given by

$$U_I(t,0) = 1 - \frac{i}{\hbar}\int_0^t V_I(t')dt' + \cdots$$

The transition probability from state $|i\rangle$ to state $|f\rangle$ (these are eigenstates of H_0) is given by

$$P_{i\to f} = \left|\langle f|U_I(t,0)|i\rangle\right|^2$$

Assuming that $|f\rangle \neq |i\rangle$,

$$\begin{aligned}\langle f|U_I(t,0)|i\rangle &= -\frac{i}{\hbar}\int_0^t dt'\,\langle f|V_I(t')|i\rangle = -\frac{i}{\hbar}\int_0^t dt'\,\left\langle f|e^{iH_0t'/\hbar}Ve^{-iH_0t'/\hbar}|i\right\rangle\\ &= -\frac{i}{\hbar}\int_0^t dt'\left[e^{i(\omega_{fi}+\omega)t'}\langle f|A|i\rangle + e^{i(\omega_{fi}-\omega)t'}\langle f|A^\dagger|i\rangle\right]\\ &= -\frac{i}{\hbar}\left[\frac{e^{i(\omega_{fi}+\omega)t}-1}{i(\omega_{fi}+\omega)}\langle f|A|i\rangle + \frac{e^{i(\omega_{fi}-\omega)t}-1}{i(\omega_{fi}-\omega)}\langle f|A^\dagger|i\rangle\right]\end{aligned}$$

Hence,

$$P_{i\to f} = \frac{1}{\hbar^2}\left|\frac{1-e^{i(\omega_{fi}+\omega)t}}{\omega_{fi}+\omega}\langle f|A|i\rangle + \frac{1-e^{i(\omega_{fi}-\omega)t}}{\omega_{fi}-\omega}\langle f|A^\dagger|i\rangle\right|^2$$

(b) Writing

$$\begin{aligned} 1-e^{i(\omega_{fi}\pm\omega)t} &= e^{i(\omega_{fi}\pm\omega)t/2}\left[e^{-i(\omega_{fi}\pm\omega)t/2}-e^{i(\omega_{fi}\pm\omega)t/2}\right] \\ &= -2ie^{i(\omega_{fi}\pm\omega)t/2} sin\left[(\omega_{fi}\pm\omega)\,t/2\right], \end{aligned}$$

we obtain

$$\begin{aligned} P_{i\to f} &= \frac{1}{\hbar^2}\left|\frac{sin\left[(\omega_{fi}+\omega)\,t/2\right]}{(\omega_{fi}+\omega)\,/2}e^{i(\omega_{fi}+\omega)t/2}\langle f|A|i\rangle+\frac{sin\left[(\omega_{fi}-\omega)\,t/2\right]}{(\omega_{fi}-\omega)\,/2}e^{i(\omega_{fi}-\omega)t/2}\langle f|A^\dagger|i\rangle\right|^2 \\ &= \frac{1}{\hbar^2}\left|B(\omega)\langle f|A|i\rangle+B(-\omega)\langle f|A^\dagger|i\rangle\right|^2 \\ &= \frac{1}{\hbar^2}\left\{|\langle f|A|i\rangle|^2|B(\omega)|^2+|\langle f|A^\dagger|i\rangle|^2|B(-\omega)|^2+2Re\left[\langle f|A|i\rangle\langle f|A^\dagger|i\rangle^* B(\omega)B^*(-\omega)\right]\right\} \end{aligned}$$

The term $|B(\omega)|^2$ is given by

$$|B(\omega)|^2=\frac{sin^2\left[(\omega_{fi}+\omega)\,t/2\right]}{(\omega_{fi}+\omega)\,/2}=\frac{t\,sin^2\left[t\,(\omega_{fi}+\omega)\,/2\right]}{t\,(\omega_{fi}+\omega)\,/2}$$

Using the result of problem 1.3, we can write

$$\begin{aligned} \lim_{t\to\infty}|B(\omega)|^2 &= \lim_{t\to\infty}\pi\,t\,\delta\left(\frac{\omega_{fi}+\omega}{2}\right)=\lim_{t\to\infty}\pi\,t\,\delta\left(\frac{E_f-E_i+\hbar\omega}{2\hbar}\right) \\ &= \lim_{t\to\infty}2\pi\,\hbar\,t\;\delta\left(E_f-E_i+\hbar\omega\right) \end{aligned}$$

Therefore,

$$\frac{1}{\hbar^2}\frac{d}{dt}\lim_{t\to\infty}|B(\omega)|^2=\frac{2\pi}{\hbar}\delta\left(E_f-E_i+\hbar\omega\right)$$

Similarly,

$$\frac{1}{\hbar^2}\frac{d}{dt}\lim_{t\to\infty}|B(-\omega)|^2=\frac{2\pi}{\hbar}\delta\left(E_f-E_i-\hbar\omega\right)$$

The term in $P_{i\to f}$ containing $B(\omega)B^*(-\omega)$ vanishes as $t\to\infty$. To see this, note that

$$\lim_{t\to\infty}\frac{1}{\pi}\frac{sin\left[(\omega_{fi}+\omega)\,t/2\right]}{(\omega_{fi}+\omega)\,/2}=\delta\left(\frac{\omega_{fi}+\omega}{2}\right)=2\delta\left(\omega_{fi}+\omega\right)$$

We can prove this as follows:

$$\begin{aligned} \delta(\theta) &= \frac{1}{2\pi}\int_{-\infty}^{\infty}e^{i\theta t}dt=\frac{1}{2\pi}\lim_{R\to\infty}\int_{-R}^{R}e^{i\theta t}dt=\frac{1}{2\pi}\lim_{R\to\infty}\frac{e^{iR\theta}-e^{-iR\theta}}{i\theta} \\ &= \frac{1}{\pi}\lim_{R\to\infty}\frac{sin(R\theta)}{\theta} \end{aligned}$$

Thus, the product $B(\omega)B^*(-\omega)$ contains $\delta(\omega_{fi}+\omega)\,\delta(\omega_{fi}-\omega)$, which vanishes if $\omega\neq 0$. Therefore,

$$w_{i\to f}=\frac{2\pi}{\hbar}\left[|\langle f|A|i\rangle|^2\,\delta\left(E_f-E_i+\hbar\omega\right)+\left|\langle f|A^\dagger|i\rangle\right|^2\delta\left(E_f-E_i-\hbar\omega\right)\right]$$

1. *Important sums.*

(a)

$$\mathbf{k} = \frac{m_1}{N_1}\mathbf{b}_1 + \frac{m_2}{N_2}\mathbf{b}_2 + \frac{m_3}{N_3}\mathbf{b}_3$$

where $N_1,\ N_2,\ N_3$ are, respectively, the number of primitive cells along the directions of $\mathbf{a}_1,\ \mathbf{a}_2$, and $\mathbf{a}_3$. The vectors $\mathbf{b}_1,\ \mathbf{b}_2$, and $\mathbf{b}_3$ are primitive reciprocal lattice vectors, and $m_1,\ m_2, m_3 \in \mathbb{Z}$. Let I and I' be defined by

$$I = \sum_n e^{i\mathbf{k}.\mathbf{R}_n}, \qquad I' = Ie^{i\mathbf{k}.\mathbf{R}}$$

where

$$\mathbf{R} = u_1\mathbf{a}_1 + u_2\mathbf{a}_2 + u_3\mathbf{a}_3\,, \qquad u_1\,, u_2\,, u_3 \in \mathbb{Z}$$

Setting $\mathbf{R}_n = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3\,, n_1\,, n_2\,, n_3 \in \mathbb{Z}$, we can write

$$I = \sum_{n_1=1}^{N_1}\sum_{n_2=1}^{N_2}\sum_{n_3=1}^{N_3} exp\left[2\pi i\left(\frac{m_1n_1}{N_1} + \frac{m_2n_2}{N_2} + \frac{m_3n_3}{N_3}\right)\right]$$

where we used the formula $\mathbf{b}_i.\mathbf{a}_j = 2\pi\delta_{ij}$. On the other hand,

$$\begin{aligned}
I' &= \sum_{n_1=1}^{N_1}\sum_{n_2=1}^{N_2}\sum_{n_3=1}^{N_3} exp\left[2\pi i\left(\frac{m_1(n_1+u_1)}{N_1} + \frac{m_2(n_2+u_2)}{N_2} + \frac{m_3(n_3+u_3)}{N_3}\right)\right] \\
&= \sum_{n_1=u_1+1}^{N_1+u_1}\sum_{n_2=u_2+1}^{N_2+u_2}\sum_{n_3=u_3+1}^{N_3+u_3} exp\left[2\pi i\left(\frac{m_1n_1}{N_1} + \frac{m_2n_2}{N_2} + \frac{m_3n_3}{N_3}\right)\right] \\
&\Longrightarrow I' - I = \sum_{n_1=N_1+1}^{N_1+u_1}\sum_{n_2=N_2+1}^{N_2+u_2}\sum_{n_3=N_3+1}^{N_3+u_3} exp\left[2\pi i\left(\frac{m_1n_1}{N_1} + \frac{m_2n_2}{N_2} + \frac{m_3n_3}{N_3}\right)\right] \\
&- \sum_{n_1=1}^{u_1}\sum_{n_2=1}^{u_2}\sum_{n_3=1}^{u_3} exp\left[2\pi i\left(\frac{m_1n_1}{N_1} + \frac{m_2n_2}{N_2} + \frac{m_3n_3}{N_3}\right)\right] = 0
\end{aligned}$$

Therefore,

$$0 = I' - I = I\left(e^{i\mathbf{k}.\mathbf{R}} - 1\right)$$

This is true for every lattice vector $\mathbf{R}$. The only way to satisfy this for $I \neq 0$ is to set $\mathbf{k} = \mathbf{G}$, where $\mathbf{G}$ is a reciprocal lattice vector. However, the only reciprocal lattice vector within the FBZ is $\mathbf{G} = 0$. Hence, I must vanish unless $\mathbf{k} = 0$. When $\mathbf{k} = 0,\ I = N$. Therefore, $I = N\delta - \mathbf{k}, \mathbf{0}$.

(b)

$$\mathbf{k} = \frac{m_1}{N_1}\mathbf{b}_1 + \frac{m_2}{N_2}\mathbf{b}_2 + \frac{m_3}{N_3}\mathbf{b}_3$$

Since $\mathbf{k} \in$ FBZ, $-N_i/2 \leq m_i \leq N_i/2 - 1$, $i = 1, 2, 3$. Let $\mathbf{R} = u_1\mathbf{a}_1 + u_2\mathbf{a}_2 + u_3\mathbf{a}_3$, where $u_1, u_2, u_3 \in \mathbb{Z}$. Let $J = \sum_{\mathbf{k}\in\mathrm{FBZ}} exp(i\mathbf{k}.\mathbf{R})$. Then,

$$J = \sum_{m_1=-N_1/2}^{N_1/2-1} \sum_{m_2=-N_2/2}^{N_2/2-1} \sum_{m_3=-N_3/2}^{N_3/2-1} exp\left[2\pi i\left(\frac{m_1u_1}{N_1} + \frac{m_2u_2}{N_2} + \frac{m_3u_3}{N_3}\right)\right]$$

Let $\mathbf{k}_0 = \frac{p_1}{N_1}\mathbf{b}_1 + \frac{p_2}{N_2}\mathbf{b}_2 + \frac{p_3}{N_3}\mathbf{b}_3$, $p_1, p_2, p_3 \in \mathbb{Z}$. be any vector $\in$ FBZ. Define

$$J' = e^{i\mathbf{k}_0.\mathbf{R}}J = \sum_{\mathbf{k}\in\mathrm{FBZ}} e^{i(\mathbf{k}+\mathbf{k}_0).\mathbf{R}}$$

Then

$$J' = \sum_{m_1=-N_1/2}^{N_1/2-1} \sum_{m_2=-N_2/2}^{N_2/2-1} \sum_{m_3=-N_3/2}^{N_3/2-1} exp\left[2\pi i\left(\frac{(m_1+p_1)\,u_1}{N_1} + \frac{(m_2+p_2)\,u_2}{N_2} + \frac{(m_3+p_3)\,u_3}{N_3}\right)\right]$$
$$= \sum_{m_1=-N_1/2+p_1}^{N_1/2+p_1-1} \sum_{m_2=-N_2/2+p_2}^{N_2/2+p_2-1} + \sum_{m_3=-N_3/2+p_3}^{N_3/2+p_3-1} exp\left[2\pi i\left(\frac{m_1u_1}{N_1} + \frac{m_2u_2}{N_2} + \frac{m_3u_3}{N_3}\right)\right]$$

It is straightforward to show that $J' - J = 0 \Rightarrow J(e^{i\mathbf{k}_0.\mathbf{R}} - 1) = 0$. The only way for J to be nonzero is if $e^{i\mathbf{k}_0.\mathbf{R}} = 1$, which is satisfied if either k_0 is a reciprocal lattice vector or if $\mathbf{R} = \mathbf{0}$. But $\mathbf{k}_0 \in$ FBZ, and if it is nonzero, then it cannot be a reciprocal lattice vector. Therefore $J = 0$ unless $\mathbf{R} = \mathbf{0}$, and when $\mathbf{R} = \mathbf{0}$, J is equal to N, the number of $\mathbf{k}$-points in the FBZ. Hence, $J = N\delta_{\mathbf{R0}}$.

2. *Free electron model at zero temperature.*

(a) The mean energy per electron (in 3D) is $\bar{\epsilon} = 3\epsilon_F/5$, where $\epsilon_F = \hbar^2k_F^2/2m$ is the Fermi energy. The Fermi wave vector $k_F = (3\pi^2N/V)^{1/3}$.
The parameter r_s is defined by

$$\frac{4\pi}{3}(r_sa_0)^3 = \frac{V}{N} \Rightarrow (N/V)^{1/3} = \left(\frac{3}{4\pi}\right)^{1/3}(r_sa_0)^{-1} \Rightarrow k_F = \left(\frac{9\pi}{4}\right)^{1/3}(r_sa_0)^{-1}$$
$$\Longrightarrow \bar{\epsilon} = \frac{3\hbar^2}{10ma_0^2}\left(\frac{9\pi}{4}\right)^{2/3}\frac{1}{r_s^2} \backsimeq \frac{2.21}{r_s^2}\,\mathrm{Ry}$$

where 1 Ry $= \hbar^2/(2ma_0^2)$ is one Rydberg (1 Ry $\backsimeq 13.6eV$).

(b) Consider a spherical shell in $\mathbf{k}$-space bounded by the constant energy surfaces $\epsilon = h^2k^2/2m$ and $\epsilon + d\epsilon = h^2k^2/2m + (h^2k/m)dk$. The volume of the shell is $4\pi k^2dk$. Since each $\mathbf{k}$-point occupies a volume in $\mathbf{k}$-space given by $(2\pi)^3/V$, the number of $\mathbf{k}$-points in the shell is $4\pi k^2dk/(2\pi)^3/V = Vk^2dk/2\pi^2$. The number of states in the shell with one spin orientation (for example, the number of states with spin up) is equal to the number of $\mathbf{k}$-points in the shell. Thus,

$$N_\sigma(\epsilon, \epsilon + d\epsilon) = Vk^2dk/2\pi^2 = D_\sigma(\epsilon)d\epsilon = Vd_\sigma(\epsilon)d\epsilon$$

where $D_\sigma(\epsilon)$ is the density of states with one spin orientation, and $d_\sigma(\epsilon)$ is the density of states per unit volume per spin orientation. Thus,

$$d_\sigma(\epsilon) = \frac{k^2}{2\pi^2(d\epsilon/dk)} = \frac{k^2}{2\pi^2\hbar^2 k/m} = \frac{mk}{2\pi^2\hbar^2}$$
$$\Longrightarrow d_\sigma(\epsilon_F) = \frac{mk_F}{2\pi^2\hbar^2}$$

3. *Free electron model in lower dimensions.*

(a) For a two-dimensional system in the ground state at $T = 0$, the electrons fill states in $\mathbf{k}$-space within a circle of radius k_F. Since each $\mathbf{k}$-point occupies an area of $(2\pi)^2/A$, where A is the area of the crystal, the number of $\mathbf{k}$-points within the Fermi circle is $\pi k_F^2/(2\pi)^2/A = Ak_F^2/4\pi$. Each $\mathbf{k}$-point can accommodate two electrons, one with its spin up and another with its spin down. Thus, the number of electrons N is given by

$$N = 2\left(Ak_F^2/4\pi\right) = Ak_F^2/2\pi \Rightarrow k_F^2 = 2\pi N/A = 2\pi n$$
$$\Longrightarrow k_F = \sqrt{2\pi n}$$

In 1D, the Fermi surface consists of two k-points at $k = \pm k_F$. The points in $\mathbf{k}$-space are separated by $2\pi/L$. The number of $\mathbf{k}$-points between $-k_F$ and k_F is therefore $2k_F/2\pi/L = Lk_F/\pi$, and the number of electrons is

$$N = 2Lk_F/\pi \Rightarrow k_F = \pi N/2L$$
$$\Longrightarrow k_F = \pi n/2$$

(b) In 3D,

$$\bar{\epsilon} = 3\epsilon_F/5 = \epsilon_F d/(d+2), \quad d = 3$$

In 2D,

$$\bar{\epsilon} = \frac{1}{N}\sum_{\mathbf{k}\sigma}{}' \frac{\hbar^2k^2}{2m} = \frac{2}{N}\sum_{\mathbf{k}}{}' \frac{\hbar^2k^2}{2m}$$

The factor 2 arises from summing over σ ($\uparrow$ or $\downarrow$), and the prime on the summation symbol means that the sum is over all $\mathbf{k}$-points within the Fermi circle of radius k_F. Replacing the sum over $\mathbf{k}$ by an integral, we obtain

$$\bar{\epsilon} = \frac{2}{N}\frac{\hbar^2}{2m}\frac{A}{(2\pi)^2}\int_0^{k_F} k^2 2\pi k dk = \frac{\hbar^2 A}{8\pi Nm}k_F^4 = \frac{1}{4\pi n}\frac{\hbar^2k_F^2}{2m}k_F^2 = \frac{1}{4\pi n}\epsilon_F 2\pi n = \epsilon_F/2$$
$$= \epsilon_F d/(d+2), \quad d = 2$$

In 1D,

$$\bar{\epsilon} = \frac{1}{N}\sum_{\mathbf{k}\sigma}{}' \frac{\hbar^2k^2}{2m} = \frac{2}{N}\sum_{\mathbf{k}}{}' \frac{\hbar^2k^2}{2m} = \frac{\hbar^2}{Nm}\frac{L}{2\pi}\int_{-k_F}^{k_F} k^2 dk = \frac{\hbar^2}{Nm}\frac{L}{2\pi}\frac{2k_F^3}{3} = \frac{\hbar^2k_F^2}{2m}\frac{2k_F}{3\pi n}$$
$$= \epsilon_F\frac{\pi n}{3\pi n} = \epsilon_F/3 = \epsilon_F d/(d+2), \quad d = 1$$

In the above, $n = N/L$. The prime on Σ means that the sum is over $\mathbf{k}$-points between $-k_F$ and $+k_F$.

4. *Graphene bands.*

(a) The real lattice vectors are

$$\mathbf{a}_1 = a(\sqrt{3}/2, -1/2), \quad \mathbf{a}_2 = a(0, 1)$$

The formulas for the primitive lattice vectors $\mathbf{b}_1$ and $\mathbf{b}_2$ are written assuming that there are three primitive real lattice vectors. We imagine that there is a third primitive lattice vector $\mathbf{a}_3$ perpendicular to the x-y plane. Then

$$\mathbf{b}_1 = \frac{2\pi\mathbf{a}_2 \times \mathbf{a}_3}{\mathbf{a}_1.\mathbf{a}_2 \times \mathbf{a}_3} = \frac{4\pi}{\sqrt{3}a}\hat{\mathbf{x}}$$
$$\mathbf{b}_2 = \frac{2\pi\mathbf{a}_3 \times \mathbf{a}_1}{\mathbf{a}_1.\mathbf{a}_2 \times \mathbf{a}_3} = \frac{4\pi}{\sqrt{3}a}(\frac{1}{2}\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}\hat{\mathbf{y}})$$

where $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ are unit vectors in the x- and y-directions, respectively. The vectors $\mathbf{b}_1$ and $\mathbf{b}_2$ have the same magnitude $(4\pi/\sqrt{3}a)$ and the angle between them is 60°. The reciprocal lattice vectors are $\mathbf{G} = m_1\mathbf{b}_1 + m_2\mathbf{b}_2, m_1, m_2 \in \mathbb{Z}$. To draw the first Brillouin zone (FBZ), choose one reciprocal lattice point, draw all reciprocal lattice vectors starting from this point and draw the perpendicular bisectors of these vectors. The area enclosed by these perpendicular bisectors, and centered on the chosen point, is the FBZ. For the case of graphene, the FBZ is a regular hexagon. The center of the FBZ is called the Γ-point. The point M has coordinates $(2\pi/\sqrt{3}a, 0)$, the point K has coordinates $(2\pi/\sqrt{3}a, 2\pi/3a)$, and the point K′ has coordinates $(0, 4\pi/\sqrt{3}a)$.

(b)

$$\psi^A_{\mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{N}}\sum_n e^{i\mathbf{k}.\mathbf{R}_n}\phi(\mathbf{r} - \mathbf{R}_n), \quad \psi^B_{\mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{N}}\sum_n e^{i\mathbf{k}.\mathbf{R}_n}\phi(\mathbf{r} - \boldsymbol{\delta} - \mathbf{R}_n)$$

These are normalized Bloch functions; they satisfy Bloch's theorem:

$$\psi^{A,B}_{\mathbf{k}}(\mathbf{r} + \mathbf{R}_m) = e^{i\mathbf{k}.\mathbf{R}_m}\psi^{A,B}_{\mathbf{k}}(\mathbf{r})$$

Since we are neglecting the overlap between atomic orbitals on different sites, $\psi^A_{\mathbf{k}}(\mathbf{r})$ and $\psi^B_{\mathbf{k}}(\mathbf{r})$ are orthogonal:

$$\int \psi^{A*}_{\mathbf{k}}(\mathbf{r})\psi^B_{\mathbf{k}}(\mathbf{r})d^3r = 0$$

To solve the Schrödinger equation $H\Psi_{\mathbf{k}}(\mathbf{r}) = E_{\mathbf{k}}\Psi_{\mathbf{k}}(\mathbf{r})$, we consider a solution of the form

$$\Psi_{\mathbf{k}}(\mathbf{r}) = a\psi^A_{\mathbf{k}}(\mathbf{r}) + b\psi^B_{\mathbf{k}}(\mathbf{r})$$

Since $\psi^A_{\mathbf{k}}(\mathbf{r})$ and $\psi^B_{\mathbf{k}}(\mathbf{r})$ are orthogonal, $\Psi_{\mathbf{k}}(\mathbf{r})$ is normalized if $|a|^2 + |b|^2 = 1$. The Schrödinger equation becomes

$$\sum_n e^{i\mathbf{k}.\mathbf{R}_n}\left[aH\phi(\mathbf{r} - \mathbf{R}_n) + bH\phi(\mathbf{r} - \boldsymbol{\delta} - \mathbf{R}_n)\right]$$
$$= E_n\sum_n e^{i\mathbf{k}.\mathbf{R}_n}\left[aH\phi(\mathbf{r} - \mathbf{R}_n) + bH\phi(\mathbf{r} - \boldsymbol{\delta} - \mathbf{R}_n)\right]$$

We multiply the above equation by $\phi^*(\mathbf{r})$ and integrate over d^3r. First, we note that

$$\int \phi^*(\mathbf{r}) H \phi(\mathbf{r} - \mathbf{R}_n) d^3r = 0$$

This is because if $\mathbf{R}_n = \mathbf{0}$, the integral is equal to the orbital energy ϵ which we set equal to zer0, and if $\mathbf{R}_n \neq \mathbf{0}$, then $\phi(\mathbf{r})$ and $\phi(\mathbf{r} - \mathbf{R}_n)$ are atomic orbitals centered on atoms of type A, and such atoms are not nearest neighbors. Since we assume that interactions exist only between nearest neighbors, the integral vanishes. Since we also ignore the overlap between orbitals on different sites, we set $\int \phi^*(\mathbf{r})\phi(\mathbf{r} - \boldsymbol{\delta} - \mathbf{R}_n)$ equal to zero.

Taking account of these observations, the Schrödinger equation becomes

$$\sum_n e^{i\mathbf{k}.\mathbf{R}_n} b \int \phi^*(\mathbf{r}) H \phi(\mathbf{r} - \boldsymbol{\delta} - \mathbf{R}_n) d^3r = E_{\mathbf{k}} \sum_n e^{i\mathbf{k}.\mathbf{R}_n} a \int \phi^*(\mathbf{r}) \phi(\mathbf{r} - \mathbf{R}_n) d^3r$$

On the RHS, the integral vanishes unless $\mathbf{R}_n = \mathbf{0}$, in which case the integral is equal to 1 (we are neglecting the overlap between orbitals on different atoms and we are assuming that the atomic orbitals are normalized). Hence, $RHS = aE_{\mathbf{k}}$.

On the LHS, the integral vanishes unless $\phi(\mathbf{r} - \boldsymbol{\delta} - \mathbf{R}_n)$ is centered on one of the three nearest neighbors of atom A. Therefore, in summing over n, only three terms survive: $\mathbf{R}_1 = \mathbf{0}$, $\mathbf{R}_2 = a(-\sqrt{3}/2, 1/2)$, and $\mathbf{R}_3 = a(-\sqrt{3}/2, -1/2)$. For each of these values of $\mathbf{R}_n$, the integral on the LHS of the above equation is the matrix element of H between the p_z orbital on A and the p_z orbital on one of the nearest neighbors of A; it is thus $-t$. Hence, the above equation becomes

$$-btg_{\mathbf{k}} = aE_{\mathbf{k}}$$

where

$$g_{\mathbf{k}} = 1 + exp\left[i\left(-\frac{\sqrt{3}}{2}k_x a + \frac{1}{2}k_y a\right)\right] + exp\left[i\left(-\frac{\sqrt{3}}{2}k_x a - \frac{1}{2}k_y a\right)\right]$$

Next we multiply the Schrödinger equation by $\phi^*(\mathbf{r} - \boldsymbol{\delta})$ and integrate over d^3r. On the RHS we end up with $bE_{\mathbf{k}}$, whereas

$$LHS = \sum_n e^{i\mathbf{k}.\mathbf{R}_n} a \int \phi^*(\mathbf{r} - \boldsymbol{\delta}) H \phi(\mathbf{r} - \mathbf{R}_n) d^3r$$

The integral vanishes except for three values of $\mathbf{R}_n$, namely, $\mathbf{R}_1 = \mathbf{0}$, $\mathbf{R}_2 = a(\sqrt{3}/2, -1/2)$, and $\mathbf{R}_3 = a(\sqrt{3}/2, 1/2)$. For each of these values of $\mathbf{R}_n$, the integral is $-t$. These three $\mathbf{R}_n$ vectors are simply the negative of the three $\mathbf{R}_n$ vectors encountered earlier. We thus obtain,

$$-atg^*_{\mathbf{k}} = bE_{\mathbf{k}}$$

To sum up, the constants a and b satisfy the two homogeneous equations:

$$E_{\mathbf{k}}a + tg_{\mathbf{k}}b = 0$$
$$tg^*_{\mathbf{k}}a + E_{\mathbf{k}}b = 0$$

To have a nontrivial solution $(a,\ b \neq 0)$, the determinant of the coefficients must vanish,

$$\begin{vmatrix} E_{\mathbf{k}} & tg_{\mathbf{k}} \\ tg^*_{\mathbf{k}} & E_{\mathbf{k}} \end{vmatrix} = 0 \Rightarrow E^2_{\mathbf{k}} - t^2 \left|g_{\mathbf{k}}\right|^2 = 0$$
$$\Longrightarrow E_{\mathbf{k}} = \pm t \left|g_{\mathbf{k}}\right|$$

The dispersion of the valence π-band is given by $E_{\mathbf{k}} = -tg_{\mathbf{k}}$, while that for the conduction π-band is $E_{\mathbf{k}} = +tg_{\mathbf{k}}$. For pure, undoped graphene at zero temperature, all states in the valence band are occupied whereas all states in the conduction band are empty. For the valence band,

$$-t\left|g_{\mathbf{k}}\right| a + tg_{\mathbf{k}}b = 0 \Rightarrow a = \frac{g_{\mathbf{k}}}{\left|g_{\mathbf{k}}\right|}b$$

The wave function for the valence band states is thus given by

$$\psi^v_{\mathbf{k}} = \frac{1}{\sqrt{2}}\left(\frac{g_{\mathbf{k}}}{\left|g_{\mathbf{k}}\right|}\psi^A_{\mathbf{k}} + \psi^B_{\mathbf{k}}\right)$$

For the conduction band,

$$\psi^c_{\mathbf{k}} = \frac{1}{\sqrt{2}}\left(-\frac{g_{\mathbf{k}}}{\left|g_{\mathbf{k}}\right|}\psi^A_{\mathbf{k}} + \psi^B_{\mathbf{k}}\right)$$

(c)

$$\left|g_{\mathbf{k}}\right| = \sqrt{g^*_{\mathbf{k}}g_{\mathbf{k}}}$$

Let $\sqrt{3}k_x a/2 = \alpha,\ k_y a/2 = \beta$. Then

$$g_{\mathbf{k}} = 1 + e^{i(\beta-\alpha)} + e^{-i(\beta+\alpha)} = 1 + e^{-i\alpha}\left(e^{i\beta} + e^{-i\beta}\right)$$
$$= 1 + 2cos\beta e^{-i\alpha}$$

Therefore,

$$g^*_{\mathbf{k}}g_{\mathbf{k}} = \left(1 + 2cos\beta e^{i\alpha}\right)\left(1 + 2cos\beta e^{-i\alpha}\right) = 1 + 4cos^2\beta + 2cos\beta\left(e^{i\alpha} + e^{-i\alpha}\right)$$
$$= 1 + 4cos^2\beta + 4cos\alpha cos\beta$$

Using the trigonometric identity

$$cos2\beta = 2cos^2\beta - 1$$

we can write

$$4cos^2\beta = 2cos2\beta + 2$$

Hence,

$$g^*_{\mathbf{k}}g_{\mathbf{k}} = 3 + 4cos\alpha cos\beta + 2cos(2\beta)$$

(d) Let $k_x = 2\pi/\sqrt{3}a + k'_x$, $k_y = 2\pi/3a + k'_y$, where k'_x and k'_y are small: $k'_x, k'_y << \pi/a$. Setting $k'_x a = x$ and $k'_y a = y$,

$$E_{\mathbf{k}} = \pm t \left[3 + 4cos\left(\pi + \frac{\sqrt{3}}{2}x\right) cos\left(\frac{\pi}{3} + \frac{y}{2}\right) + 2cos\left(2\pi/3 + y\right) \right]^{1/2}$$
$$= \pm t \left\{ 3 - 4cos(\sqrt{3}x/2) \left[\frac{1}{2}cos(y/2) - \frac{\sqrt{3}}{2}sin(y/2) \right] - cosy - \sqrt{3}siny \right\}^{1/2}$$

where in the last step we used the formula $cos(a+b) = cosacosb - sinasinb$. Expanding:

$$cos\theta = 1 - \theta^2/2! + \cdots, \quad sin\theta = \theta - \theta^3/3! + \cdots,$$

we obtain

$$E_{\mathbf{k}} = \pm t \left\{ 3 - 4(1 - 3x^2/8)(1/2 - y^2/16 - \sqrt{3}y/4) - 1 + y^2/2 - \sqrt{3}y \right\}^{1/2}$$
$$= \pm t \left[3 - 2 + y^2/4 + \sqrt{3}y + 3x^2/4 - 1 + y^2/2 - \sqrt{3}y \right]^{1/2}$$
$$= \pm t \left[\frac{3}{4}\left(x^2 + y^2\right) \right]^{1/2} = \pm \frac{\sqrt{3}}{2} ta \left(k_x^{'2} + k_y^{'2} \right)^{1/2}$$
$$= \pm \frac{\sqrt{3}}{2} tak'$$

There are, of course, terms of higher order in k' which we have neglected since they are less important when k' is small. Measuring $\mathbf{k}$ from point K in the FBZ, we can write

$$E_{\mathbf{k}} = \pm \hbar v_F k$$

where $v_F = \sqrt{3}ta/2\hbar$ is the magnitude of the Fermi velocity, and the $-(+)$ sign refers to the valence (conduction) band.

We have expanded around point K; it is easily verified that the same linear dispersion is obtained near point K$'$.

(e) Consider a shell near point K, bounded by the constant energy surfaces $\epsilon = \hbar v_F k$ and $\epsilon + d\epsilon = \hbar v_F k + \hbar v_F dk$. The area of the shell is $2\pi k dk$. Each $\mathbf{k}$-point occupies an area in $\mathbf{k}$-space given by $(2\pi)^2/A$, where A is the area of the graphene crystal. Since there are two states for each $\mathbf{k}$-point ($|\mathbf{k}\uparrow\rangle$ and $|\mathbf{k}\downarrow\rangle$), the number of states in the shell is

$$N = 2(2\pi k dk)/(2\pi)^2/A = Akdk/\pi$$

The density of states is thus

$$D(\epsilon) = \frac{dN}{d\epsilon} = \frac{Ak}{\pi}\frac{dk}{d\epsilon} = \frac{Ak}{\pi\hbar v_F} = \frac{A|\epsilon|}{\pi(\hbar v_F)^2} = \frac{4A|\epsilon|}{3\pi a^2 t^2}$$
$$\Longrightarrow d(\epsilon) \equiv \frac{1}{A}D(\epsilon) = \frac{4|\epsilon|}{3\pi a^2 t^2}$$

Since there are two valleys, one near point K and another near point K$'$, the total density of states per unit area is

$$d_{total}(\epsilon) = \frac{8|\epsilon|}{3\pi a^2 t^2}$$

5. *More on graphene.*

The p_z orbital on each atom is represented by the wave function

$$\phi(\mathbf{r}) = Ar\,cos\theta e^{-Zr/2a_0}$$

Here, A is a normalization constant, a_0 is the Bohr radius, θ is the angle between $\mathbf{r}$ and the z-axis (the one perpendicular to the graphene plane), and Ze is the effective charge on the carbon nucleus, as seen by the electron in the p_z orbital ($Z \simeq 3$). We want to evaluate

$$I(\mathbf{q}) = \int \phi^*(\mathbf{r}) e^{-i\mathbf{q}.\mathbf{r}} \phi(\mathbf{r}) d^3r$$

where $\mathbf{q}$ is a two-dimensional vector in the FBZ of graphene.

First, note that since $\phi(\mathbf{r})$ is normalized,

$$2\pi A^2 \int_0^\infty r^4 e^{-Zr/a_0} dr \int_{-1}^{2} cos^2\theta dcos\theta = 1$$
$$\implies \frac{4\pi}{3} A^2 \int_0^\infty r^4 e^{-Zr/a_0} = 1$$

Expanding $e^{-i\mathbf{q}.\mathbf{r}}$, we can write

$$I(\mathbf{q}) = A^2 \sum_{n=0}^{\infty} \frac{1}{n!} \int_0^\infty r^4 e^{-Zr/a_0} dr \int_0^{2\pi} d\phi \int_{-1}^{1} d(cos\theta)\, cos^2\theta\, (-i\mathbf{q}.\mathbf{r})^n$$

If we choose the x-axis to be along the direction of $\mathbf{q}$, then $\mathbf{q}.\mathbf{r} = qr\,sin\theta cos\theta$. Therefore,

$$I(\mathbf{q}) = A^2 \sum_{n=0}^{\infty} \frac{(-iq)^n}{n!} \int_0^\infty r^{4+n} e^{-Zr/a_0} dr \int_0^\pi cos^2\theta\, sin^{n+1}\theta\, d\theta \int_0^{2\pi} cos^n\phi\, d\phi$$

Note that

$$\int_0^{2\pi} cos^n\phi d\phi = 0 \text{ if } n \text{ is odd;}$$

hence,

$$I(\mathbf{q}) = A^2 \sum_{n=0}^{\infty} (-1)^n \frac{q^{2n}}{(2n)!} \int_0^\infty r^{4+2n} e^{-Zr/a_0} dr \int_0^\pi (1 - sin^2\theta)\, sin^{2n+1}\theta\, d\theta \int_0^{2\pi} cos^{2n}\phi\, d\phi$$

Using

$$\int_0^{\pi} sin^{2n+1}\theta\, d\theta = \frac{2[(2n)!!]}{(2n+1)!!}, \quad \int_0^{\pi} sin^{2n+3}\theta\, d\theta = \frac{2[(2n+2)!!]}{(2n+3)!!}$$

$$\int_0^{2\pi} cos^{2n}\phi\, d\phi = 2\pi\frac{(2n-1)!!}{(2n)!!}, \quad \int_0^{\infty} r^{4+2n} e^{-Zr/a_0} dr = \frac{(2n+4)!}{4!}\left(\frac{a_0}{Z}\right)^{2n}\int_0^{\infty} r^4 e^{-Zr/a_0} dr,$$

and noting that

$$\frac{(2n)!!}{(2n+1)!!} - \frac{(2n+2)!!}{(2n+3)!!} = \frac{(2n)!!}{(2n+3)!!},$$

and using the normalization condition, we obtain

$$\begin{aligned} I(\mathbf{q}) &= \sum_{n=0}^{\infty}(-1)^n \frac{(n+1)(n+2)}{2}\left[\left(\frac{qa_0}{Z}\right)^2\right]^2 \\ &= \frac{1}{\left[1+(qa_0/Z)^2\right]^3} \end{aligned}$$

Since $Z \simeq 3$, then for small values of q : $qa_0 << 1$, $I(\mathbf{q}) \simeq 1$.

This result is not surprising: $\phi^*(\mathbf{r})\phi(\mathbf{r})$ is maximum at $r = 2a_0/Z \simeq 2a_0/3$ and decays exponentially for larger values of r. For $r > 3a_0$, $\phi^*(\mathbf{r})\phi(\mathbf{r})$ is almost vanishing. On the other hand, $e^{i\mathbf{q}.\mathbf{r}} \simeq 1$ for $r \precsim 3a_0$ since $qa_0 << 1$. So for values of r where $\phi^*(\mathbf{r})\phi(\mathbf{r})$ is appreciable, $e^{i\mathbf{q}.\mathbf{r}} = 1$. Since $\phi(\mathbf{r})$ is normalized, $I(\mathbf{q}) \simeq 1$.

6. *Matrix elements of graphene wave functions.*

$$\psi^A_{\mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{N}}\sum_n e^{i\mathbf{k}.\mathbf{R}_n}\phi(\mathbf{r}-\mathbf{R}_n), \quad \psi^B_{\mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{N}}\sum_n e^{i\mathbf{k}.\mathbf{R}_n}\phi(\mathbf{r}-\boldsymbol{\delta}-\mathbf{R}_n),$$

$$\psi^v_{\mathbf{k}} = \frac{1}{\sqrt{2}}\left[\frac{g_{\mathbf{k}}}{|g_{\mathbf{k}}|}\psi^A_{\mathbf{k}} + \psi^B_{\mathbf{k}}\right], \quad \psi^c_{\mathbf{k}} = \frac{1}{\sqrt{2}}\left[-\frac{g_{\mathbf{k}}}{|g_{\mathbf{k}}|}\psi^A_{\mathbf{k}} + \psi^B_{\mathbf{k}}\right]$$

(i)

$$I_1 = \left\langle \psi^A_{\mathbf{k}} \left| e^{-i\mathbf{q}.\mathbf{r}} \right| \psi^A_{\mathbf{k}+\mathbf{q}} \right\rangle = \frac{1}{N}\sum_{n,n'} e^{-i\mathbf{k}.\mathbf{R}_n} e^{i(\mathbf{k}+\mathbf{q}).\mathbf{R}_{n'}} \int e^{-i\mathbf{q}.\mathbf{r}}\phi^*(\mathbf{r}-\mathbf{R}_n)\phi(\mathbf{r}-\mathbf{R}_{n'})d^3r$$

Ignoring overlap between orbitals on different sites, the integral vanishes unless $n = n'$; hence

$$I_1 = \frac{1}{N}\sum_n e^{i\mathbf{q}.\mathbf{R}_n}\int e^{-i\mathbf{q}.\mathbf{r}}\left|\phi(\mathbf{r}-\mathbf{R}_n)\right|^2 d^3r = \frac{1}{N}\sum_n \int e^{-i\mathbf{q}.(\mathbf{r}-\mathbf{R}_n)}\left|\phi(\mathbf{r}-\mathbf{R}_n)\right|^2 d^3r$$

By a change of variable: $\mathbf{r} \to \mathbf{r} - \mathbf{R}_n$,

$$I_1(\mathbf{q}) = \frac{1}{N}\sum_n \int e^{-i\mathbf{q}.\mathbf{r})}\left|\phi(\mathbf{r})\right|^2 d^3r \simeq 1$$

In the last step, we made use of the result of problem 2.5.

(ii) Following the same steps as above, it is readily shown that

$$\left\langle \psi_{\mathbf{k}}^{B} \left| e^{-i\mathbf{q}.\mathbf{r}} \right| \psi_{\mathbf{k+q}}^{B} \right\rangle \simeq 1, \quad \left\langle \psi_{\mathbf{k}}^{A} \left| e^{-i\mathbf{q}.\mathbf{r}} \right| \psi_{\mathbf{k+q}}^{B} \right\rangle = \left\langle \psi_{\mathbf{k}}^{B} \left| e^{-i\mathbf{q}.\mathbf{r}} \right| \psi_{\mathbf{k+q}}^{A} \right\rangle = 0$$

The second equation results from neglecting overlap between atomic orbitals on different sites.

(iii)

$$\begin{aligned}\left\langle \psi_{\mathbf{k}}^{v} \left| e^{-i\mathbf{q}.\mathbf{r}} \right| \psi_{\mathbf{k+q}}^{v} \right\rangle = \frac{1}{2} \Bigg[& \frac{g_{\mathbf{k}}^{*} g_{\mathbf{k+q}}}{|g_{\mathbf{k}} g_{\mathbf{k+q}}|} \left\langle \psi_{\mathbf{k}}^{A} | e^{-i\mathbf{q}.\mathbf{r}} | \psi_{\mathbf{k+q}}^{A} \right\rangle + \left\langle \psi_{\mathbf{k}}^{B} | e^{-i\mathbf{q}.\mathbf{r}} | \psi_{\mathbf{k+q}}^{B} \right\rangle \\ & + \frac{g_{\mathbf{k}}^{*}}{|g_{\mathbf{k}}|} \left\langle \psi_{\mathbf{k}}^{A} | e^{-i\mathbf{q}.\mathbf{r}} | \psi_{\mathbf{k+q}}^{B} \right\rangle + \frac{g_{\mathbf{k}}}{|g_{\mathbf{k}}|} \left\langle \psi_{\mathbf{k}}^{B} | e^{-i\mathbf{q}.\mathbf{r}} | \psi_{\mathbf{k+q}}^{A} \right\rangle \Bigg]\end{aligned}$$

Using the results of (i) and (ii),

$$\left\langle \psi_{\mathbf{k}}^{v} \left| e^{-i\mathbf{q}.\mathbf{r}} \right| \psi_{\mathbf{k+q}}^{v} \right\rangle \simeq \frac{1}{2} \left[1 + \frac{g_{\mathbf{k}}^{*}\, g_{\mathbf{k+q}}}{|g_{\mathbf{k}}\, g_{\mathbf{k+q}}|} \right]$$

(iv) Similarly, it is readily shown that

$$\begin{aligned}\left\langle \psi_{\mathbf{k}}^{c} \left| e^{-i\mathbf{q}.\mathbf{r}} \right| \psi_{\mathbf{k+q}}^{c} \right\rangle &= \left\langle \psi_{\mathbf{k}}^{v} \left| e^{-i\mathbf{q}.\mathbf{r}} \right| \psi_{\mathbf{k+q}}^{v} \right\rangle \\ \left\langle \psi_{\mathbf{k}}^{c} \left| e^{-i\mathbf{q}.\mathbf{r}} \right| \psi_{\mathbf{k+q}}^{v} \right\rangle &= \left\langle \psi_{\mathbf{k}}^{v} \left| e^{-i\mathbf{q}.\mathbf{r}} \right| \psi_{\mathbf{k+q}}^{c} \right\rangle = \frac{1}{2} \left[1 - \frac{g_{\mathbf{k}}^{*}\, g_{\mathbf{k+q}}}{|g_{\mathbf{k}}\, g_{\mathbf{k+q}}|} \right]\end{aligned}$$

(v)

$$g_{\mathbf{k}} = 1 + e^{i\left(-\frac{\sqrt{3}}{2} k_x a + \frac{1}{2} k_y a\right)} + e^{-i\left(\frac{\sqrt{3}}{2} k_x a + \frac{1}{2} k_y a\right)}$$

We assume that $\mathbf{k}$ is near the point K or K' ($g_{\mathbf{k}}$ vanishes at these points). Expanding about point K,

$$\begin{aligned} g_{\mathbf{k}} &= \left.\frac{\partial g_{\mathbf{k}}}{\partial k_x}\right|_K \left(k_x - \frac{2\pi}{\sqrt{3}a} \right) + \left.\frac{\partial g_{\mathbf{k}}}{\partial k_y}\right|_K \left(k_y - \frac{2\pi}{3a} \right) \\ &= \frac{i\sqrt{3}a}{2} \left(k_x - \frac{2\pi}{\sqrt{3}a} \right) + \frac{\sqrt{3}a}{2} \left(k_y - \frac{2\pi}{3a} \right) \end{aligned}$$

Measuring $\mathbf{k}$ from point K,

$$g_{\mathbf{k}} = \frac{i\sqrt{3}a}{2} (k_x - ik_y) = i\frac{\sqrt{3}}{2} k a e^{-i\theta_{\mathbf{k}}}$$

where $\theta_{\mathbf{k}}$ is the angle between $\mathbf{k}$ and the x-axis. Therefore,

$$|g_{\mathbf{k}} g_{\mathbf{k+q}}| = \frac{3a^2}{4} k |\mathbf{k} + \mathbf{q}|$$

and

$$g_{\mathbf{k}}^{*} g_{\mathbf{k+q}} = \frac{3a^2}{4} k |\mathbf{k} + \mathbf{q}| e^{i\left(\theta_{\mathbf{k}} - \theta_{\mathbf{k+q}}\right)}$$

Hence,

$$\left\langle \psi^v_{\mathbf{k}} \left| e^{-i\mathbf{q}.\mathbf{r}} \right| \psi^v_{\mathbf{k}+\mathbf{q}} \right\rangle = \frac{1}{2}\left[1 + e^{i\left(\theta_{\mathbf{k}} - \theta_{\mathbf{k}+\mathbf{q}}\right)}\right]$$

and

$$\begin{aligned} \left|\left\langle \psi^v_{\mathbf{k}} \left| e^{-i\mathbf{q}.\mathbf{r}} \right| \psi^v_{\mathbf{k}+\mathbf{q}} \right\rangle\right|^2 &= \frac{1}{4}\left[1 + e^{i\left(\theta_{\mathbf{k}} - \theta_{\mathbf{k}+\mathbf{q}}\right)}\right]\left[1 + e^{-i\left(\theta_{\mathbf{k}} - \theta_{\mathbf{k}+\mathbf{q}}\right)}\right] \\ &= \frac{1}{2}\left(1 + cos\theta\right) \end{aligned}$$

where θ is the angle between $\mathbf{k}$ and $\mathbf{k}+\mathbf{q}$:

$$cos\theta = \frac{\mathbf{k}.(\mathbf{k}+\mathbf{q})}{k|\mathbf{k}+\mathbf{q}|} = \frac{k^2 + kq\,cos\phi}{k|\mathbf{k}+\mathbf{q}|} = \frac{k + q\,cos\phi}{|\mathbf{k}+\mathbf{q}|}$$

where ϕ is the angle between $\mathbf{k}$ and $\mathbf{q}$.
Following the same steps as above, we find

$$\left|\left\langle \psi^c_{\mathbf{k}} \left| e^{-i\mathbf{q}.\mathbf{r}} \right| \psi^v_{\mathbf{k}+\mathbf{q}} \right\rangle\right|^2 = \frac{1}{2}\left(1 - \frac{k + q\,cos\phi}{|\mathbf{k}+\mathbf{q}|}\right)$$

Since

$$\left\langle \psi^c_{\mathbf{k}} \left| e^{-i\mathbf{q}.\mathbf{r}} \right| \psi^c_{\mathbf{k}+\mathbf{q}} \right\rangle = \left\langle \psi^v_{\mathbf{k}} \left| e^{-i\mathbf{q}.\mathbf{r}} \right| \psi^v_{\mathbf{k}+\mathbf{q}} \right\rangle$$

and

$$\left\langle \psi^v_{\mathbf{k}} \left| e^{-i\mathbf{q}.\mathbf{r}} \right| \psi^c_{\mathbf{k}+\mathbf{q}} \right\rangle = \left\langle \psi^c_{\mathbf{k}} \left| e^{-i\mathbf{q}.\mathbf{r}} \right| \psi^v_{\mathbf{k}+\mathbf{q}} \right\rangle$$

we can write

$$F_{ss'}(\mathbf{k},\mathbf{q}) = \frac{1}{2}\left(1 + s\,s'\,\frac{k + q\,cos\phi}{|\mathbf{k}+\mathbf{q}|}\right)$$

where $s,\ s' = -1\ (+1)$ if $s,\ s' = v\ (c)$.

7. *Density of states.*

$$D(\epsilon)d\epsilon = 2\frac{(2\pi)^3}{V}\int dk_\perp dS_\epsilon$$

In the above, the function $dk_\perp$ is integrated over the surface in $\mathbf{k}$-space on which the energy is a constant equal to ϵ. $dk_\perp$ is the perpendicular distance in $\mathbf{k}$-space between the inner and outer surfaces of the shell.

The point to note here is that for the constant energy surface $\epsilon(\mathbf{k}) = \epsilon$, the gradient $\boldsymbol{\nabla}_{\mathbf{k}}\epsilon(\mathbf{k})$ is perpendicular to the constant energy surface. Therefore,

$$\left|\boldsymbol{\nabla}_{\mathbf{k}}\epsilon\right| dk_\perp = d\epsilon$$

Hence,

$$D(\epsilon)d\epsilon = 2\frac{(2\pi)^3}{V}\int \frac{dS_\epsilon}{\left|\boldsymbol{\nabla}_{\mathbf{k}}\epsilon\right|}d\epsilon$$

We note that $d\epsilon$ is simply a constant; the integration is not over ϵ, but rather over the constant energy surface. Cancelling $d\epsilon$, we obtain the desired result:

$$D(\epsilon) = 2\frac{(2\pi)^3}{V}\int \frac{dS_\epsilon}{|\boldsymbol{\nabla}_{\mathbf{k}}\epsilon|}$$

Chapter 3

Second Quantization

1. *Noninteracting electrons on a square lattice.*

The two lattice vectors are $\mathbf{a}_1 = a(1,0)$, $\mathbf{a}_2 = a(0,1)$. The Hamiltonian is

$$H = -t \sum_{<ij>\sigma} c^{\dagger}_{i\sigma} c_{j\sigma}$$

Expanding in terms of momentum operators,

$$c^{\dagger}_{i\sigma} = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}\in \mathrm{FBZ}} e^{-i\mathbf{k}.\mathbf{R}_i} c^{\dagger}_{\mathbf{k}\sigma}, \quad c_{j\sigma} = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}\in \mathrm{FBZ}} e^{i\mathbf{k}.\mathbf{R}_j} c_{\mathbf{k}\sigma},$$

the Hamiltonian is rewritten as

$$\begin{aligned} H &= -(t/N) \sum_{<ij>\sigma} \sum_{\mathbf{k}\mathbf{k}'} e^{-i\mathbf{k}'.\mathbf{R}_i} e^{i\mathbf{k}.\mathbf{R}_j} c^{\dagger}_{\mathbf{k}'\sigma} c_{\mathbf{k}\sigma} \\ &= -(t/N) \sum_{<ij>\sigma} \sum_{\mathbf{k}\mathbf{k}'} e^{-i(\mathbf{k}'-\mathbf{k}).\mathbf{R}_i} e^{i\mathbf{k}.(\mathbf{R}_j-\mathbf{R}_i)} c^{\dagger}_{\mathbf{k}'\sigma} c_{\mathbf{k}\sigma} \end{aligned}$$

The sum over $\mathbf{k}$ and $\mathbf{k}'$ is restricted to the values within the first Brillouin zone (FBZ).

For any given lattice site i, $\mathbf{R}_j - \mathbf{R}_i$ can only take four values, namely, $\pm a(1,0)$ and $\pm a(0,1)$. Hence,

$$\begin{aligned} \sum_{<ij>} e^{-i(\mathbf{k}'-\mathbf{k}).\mathbf{R}_i} e^{i\mathbf{k}.(\mathbf{R}_j-\mathbf{R}_i)} &= \left(e^{ik_x a} + e^{-ik_x a} + e^{ik_y a} + e^{-ik_y a}\right) \sum_i e^{\mathbf{k}'-\mathbf{k}).\mathbf{R}_i} \\ &= (2cos(k_x a) + 2cos(k_y a) N \delta_{\mathbf{k}\mathbf{k}'} \end{aligned}$$

In the last step we used the result of problem 2.1.

We thus find

$$H = \sum_{\mathbf{k}\sigma} 2t\left[cos(k_x a) + cos(k_y a)\right] c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}$$

where

$$\epsilon_{\mathbf{k}} = 2t\left[cos(k_x a) + cos(k_y a)\right]$$

This is the dispersion of the energy band.

2. *Graphene revisited.*

(a) The Hamiltonian is

$$H = -t \sum_{i\sigma} \sum_{\delta=1}^{3} a_{i\sigma}^\dagger b_{i+\delta,\sigma} + H.C.$$

The creation and annihilation operators are expanded as follows:

$$a_{i\sigma}^\dagger = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}\in\mathrm{FBZ}} e^{-i\mathbf{k}.\mathbf{R}_i} a_{\mathbf{k}\sigma}^\dagger, \quad b_{i\sigma} = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}\in\mathrm{FBZ}} e^{i\mathbf{k}.\mathbf{R}_i} b_{\mathbf{k}\sigma}$$

Putting these into the expression for the Hamiltonian, we find

$$H = -\frac{t}{N} \sum_{\mathbf{k}\mathbf{k}'} \sum_{i\sigma} \sum_{\boldsymbol{\delta}} e^{-i\mathbf{k}'.\mathbf{R}_i} e^{i\mathbf{k}.(\mathbf{R}_i+\boldsymbol{\delta})} a_{\mathbf{k}'\sigma}^\dagger b_{\mathbf{k}\sigma} + H.C.$$

Note that

$$\sum_{\boldsymbol{\delta}} e^{i\mathbf{k}.\boldsymbol{\delta}} = g_{\mathbf{k}}$$

where $g_{\mathbf{k}}$ was defined earlier in problem 2.4. Thus

$$\begin{aligned} H &= -\frac{t}{N} \sum_{\mathbf{k}\mathbf{k}'\sigma} g_{\mathbf{k}} a_{\mathbf{k}'\sigma}^\dagger b_{\mathbf{k}\sigma} \sum_i e^{i(\mathbf{k}-\mathbf{k}').\mathbf{R}_i} + H.C. \\ &= -t \sum_{\mathbf{k}\sigma} g_{\mathbf{k}} a_{\mathbf{k}\sigma}^\dagger b_{\mathbf{k}\sigma} - t \sum_{\mathbf{k}\sigma} g_{\mathbf{k}}^* b_{\mathbf{k}\sigma}^\dagger a_{\mathbf{k}\sigma} \\ &= -t \sum_{\mathbf{k}\sigma} \begin{pmatrix} a_{\mathbf{k}\sigma}^\dagger & b_{\mathbf{k}\sigma}^\dagger \end{pmatrix} \begin{pmatrix} 0 & g_{\mathbf{k}} \\ g_{\mathbf{k}}^* & 0 \end{pmatrix} \begin{pmatrix} a_{\mathbf{k}\sigma} \\ b_{\mathbf{k}\sigma} \end{pmatrix} \end{aligned}$$

(b) The matrix

$$G = \begin{pmatrix} 0 & g_{\mathbf{k}} \\ g_{\mathbf{k}}^* & 0 \end{pmatrix}$$

has eigenvalues $\pm|g_{\mathbf{k}}|$. The eigenvector corresponsing to the eigenvalue $-|g_{\mathbf{k}}|$ is

$$\frac{1}{\sqrt{2}} \begin{pmatrix} -g_{\mathbf{k}}/|g_{\mathbf{k}}| \\ 1 \end{pmatrix}$$

and that corresponsing to the eigenvalue $+|g_{\mathbf{k}}|$ is

$$\frac{1}{\sqrt{2}} \begin{pmatrix} g_{\mathbf{k}}/|g_{\mathbf{k}}| \\ 1 \end{pmatrix}$$

We form the matrix A whose columns are the above two eigenvectors, and its inverse A^{-1},

$$A = \frac{1}{\sqrt{2}} \begin{bmatrix} -\frac{g_{\mathbf{k}}}{|g_{\mathbf{k}}|} & \frac{g_{\mathbf{k}}}{|g_{\mathbf{k}}|} \\ 1 & 1 \end{bmatrix}, \quad A^{-1} = \frac{1}{\sqrt{2}} \begin{bmatrix} -\frac{g_{\mathbf{k}}^*}{|g_{\mathbf{k}}|} & 1 \\ \frac{g_{\mathbf{k}}^*}{|g_{\mathbf{k}}|} & 1 \end{bmatrix}$$

It is easily verified that

$$A^{-1}GA = \begin{bmatrix} -|g_{\mathbf{k}}| & 0 \\ 0 & |g_{\mathbf{k}}| \end{bmatrix}$$

The Hamiltonian is now written as

$$\begin{aligned} H &= -t \sum_{\mathbf{k}\sigma} \begin{pmatrix} a^\dagger_{\mathbf{k}\sigma} & b^\dagger_{\mathbf{k}\sigma} \end{pmatrix} AA^{-1} \begin{pmatrix} 0 & g_{\mathbf{k}} \\ g^*_{\mathbf{k}} & 0 \end{pmatrix} AA^{-1} \begin{pmatrix} a_{\mathbf{k}\sigma} \\ b_{\mathbf{k}\sigma} \end{pmatrix} \\ &= -t \sum_{\mathbf{k}\sigma} \begin{pmatrix} c^\dagger_{1\mathbf{k}\sigma} & c^\dagger_{2\mathbf{k}\sigma} \end{pmatrix} \begin{pmatrix} -|g_{\mathbf{k}}| & 0 \\ 0 & |g_{\mathbf{k}}| \end{pmatrix} \begin{pmatrix} c_{1\mathbf{k}\sigma} \\ c_{2\mathbf{k}\sigma} \end{pmatrix} \\ &= -t \sum_{\mathbf{k}\sigma} \sum_{n=1}^{2} E_{n\mathbf{k}} c^\dagger_{n\mathbf{k}\sigma} c_{n\mathbf{k}\sigma} \end{aligned}$$

where

$$\begin{pmatrix} c_{1\mathbf{k}\sigma} \\ c_{2\mathbf{k}\sigma} \end{pmatrix} = A^{-1} \begin{pmatrix} a_{\mathbf{k}\sigma} \\ b_{\mathbf{k}\sigma} \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} -\frac{g^*_{\mathbf{k}}}{|g_{\mathbf{k}}|} a_{\mathbf{k}\sigma} + b_{\mathbf{k}\sigma} \\ \frac{g^*_{\mathbf{k}}}{|g_{\mathbf{k}}|} a_{\mathbf{k}\sigma} + b_{\mathbf{k}\sigma} \end{pmatrix}$$

3. *Commutators.*

(a)

$$\left[c_{\mathbf{k}\sigma}, \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} \right] = \left[c_{\mathbf{k}\sigma}, \sum_{\mathbf{k}'\sigma'} \epsilon_{\mathbf{k}'} c^\dagger_{\mathbf{k}'\sigma'} c_{\mathbf{k}'\sigma'} \right] = \sum_{\mathbf{k}'\sigma'} \epsilon_{\mathbf{k}'} \left[c_{\mathbf{k}\sigma}, c^\dagger_{\mathbf{k}'\sigma'} c_{\mathbf{k}'\sigma'} \right]$$

If c and $c^\dagger$ are boson operators, then

$$[A, BC] = B[A, C] + [A, B]C$$

gives

$$\begin{aligned} \left[c_{\mathbf{k}\sigma}, c^\dagger_{\mathbf{k}'\sigma'} c_{\mathbf{k}'\sigma'} \right] &= c^\dagger_{\mathbf{k}'\sigma'} \left[c_{\mathbf{k}\sigma}, c_{\mathbf{k}'\sigma'} \right] + \left[c_{\mathbf{k}\sigma}, c^\dagger_{\mathbf{k}'\sigma'} \right] c_{\mathbf{k}'\sigma'} \\ &= 0 + \delta_{\mathbf{k}\mathbf{k}'} \delta_{\sigma\sigma'} c_{\mathbf{k}'\sigma'} \end{aligned}$$

If, on the other hand, c and $c^\dagger$ are fermion operators, then the formula

$$[A, BC] = \{A, B\}C - B\{A, C\}$$

gives

$$\begin{aligned} \left[c_{\mathbf{k}\sigma}, c^\dagger_{\mathbf{k}'\sigma'} c_{\mathbf{k}'\sigma'} \right] &= \left\{ c_{\mathbf{k}\sigma}, c^\dagger_{\mathbf{k}'\sigma'} \right\} c_{\mathbf{k}'\sigma'} - c^\dagger_{\mathbf{k}'\sigma'} \left\{ c_{\mathbf{k}\sigma}, c_{\mathbf{k}'\sigma'} \right\} \\ &= \delta_{\mathbf{k}\mathbf{k}'} \delta_{\sigma\sigma'} c_{\mathbf{k}'\sigma'} \end{aligned}$$

Therefore, whether c and $c^\dagger$ are boson or fermion operators, we have

$$\left[c_{\mathbf{k}\sigma}, \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} \right] = \sum_{\mathbf{k}'\sigma'} \epsilon_{\mathbf{k}'} \delta_{\mathbf{k}\mathbf{k}'} \delta_{\sigma\sigma'} c_{\mathbf{k}'\sigma'} = \epsilon_{\mathbf{k}} c_{\mathbf{k}\sigma}$$

(b) For boson operators,

$$\left[c^\dagger_{\mathbf{k}\sigma}, \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}\right] = \sum_{\mathbf{k}'\sigma'} \epsilon_{\mathbf{k}'} \left[c^\dagger_{\mathbf{k}\sigma}, c^\dagger_{\mathbf{k}'\sigma'} c_{\mathbf{k}'\sigma'}\right] = \sum_{\mathbf{k}'\sigma'} \epsilon_{\mathbf{k}'} c^\dagger_{\mathbf{k}'\sigma'} \left[c^\dagger_{\mathbf{k}\sigma}, c_{\mathbf{k}'\sigma'}\right]$$
$$= -\sum_{\mathbf{k}'\sigma'} \epsilon_{\mathbf{k}'} c^\dagger_{\mathbf{k}'\sigma'} \delta_{\mathbf{k}\mathbf{k}'} \delta_{\sigma\sigma'} = -\epsilon_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma}$$

For fermion operators,

$$\left[c^\dagger_{\mathbf{k}\sigma}, \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}\right] = \sum_{\mathbf{k}'\sigma'} \epsilon_{\mathbf{k}'} \left[c^\dagger_{\mathbf{k}\sigma}, c^\dagger_{\mathbf{k}'\sigma'} c_{\mathbf{k}'\sigma'}\right] = -\sum_{\mathbf{k}'\sigma'} \epsilon_{\mathbf{k}'} c^\dagger_{\mathbf{k}'\sigma'} \left\{c^\dagger_{\mathbf{k}\sigma}, c_{\mathbf{k}'\sigma'}\right\}$$
$$= -\sum_{\mathbf{k}'\sigma'} \epsilon_{\mathbf{k}'} c^\dagger_{\mathbf{k}'\sigma'} \delta_{\mathbf{k}\mathbf{k}'} \delta_{\sigma\sigma'} = -\epsilon_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma}$$

The same answer is obtained whether c and $c^\dagger$ are boson or fermion operators.

4. *Field and number operators.*

The total number of particles operator is given by

$$N = \sum_\sigma \int d^3r \Psi^\dagger_\sigma(\mathbf{r}) \Psi_\sigma(\mathbf{r})$$

For bosons,

$$[N, \Psi_\sigma(\mathbf{r})] = \sum_{\sigma'} \int d^3r' \left[\Psi^\dagger_{\sigma'}(\mathbf{r}')\Psi_{\sigma'}(\mathbf{r}'), \Psi_\sigma(\mathbf{r})\right]$$

Using $[AB, C] = A[B, C] + [A, C]B$, we find

$$\left[\Psi^\dagger_{\sigma'}(\mathbf{r}')\Psi_{\sigma'}(\mathbf{r}'), \Psi_\sigma(\mathbf{r})\right] = \Psi^\dagger_{\sigma'}(\mathbf{r}') \left[\Psi_{\sigma'}(\mathbf{r}'), \Psi_\sigma(\mathbf{r})\right] + \left[\Psi^\dagger_{\sigma'}(\mathbf{r}'), \Psi_\sigma(\mathbf{r})\right] \Psi_{\sigma'}(\mathbf{r}')$$

For boson field operators,

$$[\Psi_{\sigma'}(\mathbf{r}'), \Psi_\sigma(\mathbf{r})] = 0, \quad \left[\Psi^\dagger_{\sigma'}(\mathbf{r}'), \Psi_\sigma(\mathbf{r})\right] = -\delta_{\sigma\sigma'}\delta(\mathbf{r} - \mathbf{r}')$$

For fermion operators,

$$\left[\Psi^\dagger_{\sigma'}(\mathbf{r}')\Psi_{\sigma'}(\mathbf{r}'), \Psi_\sigma(\mathbf{r})\right] = \Psi^\dagger_{\sigma'}(\mathbf{r}') \left\{\Psi_{\sigma'}(\mathbf{r}'), \Psi_\sigma(\mathbf{r})\right\} - \left\{\Psi^\dagger_{\sigma'}(\mathbf{r}'), \Psi_\sigma(\mathbf{r})\right\} \Psi_{\sigma'}(\mathbf{r}')$$
$$= 0 - \delta_{\sigma\sigma'}\delta(\mathbf{r} - \mathbf{r}')\Psi_\sigma(\mathbf{r})$$

Hence, for both bosons and fermions,

$$[N, \Psi_\sigma(\mathbf{r})] = -\sum_{\sigma'} \int d^3r' \delta_{\sigma\sigma'}\delta(\mathbf{r} - \mathbf{r}')\Psi_{\sigma'}(\mathbf{r}') = -\Psi_\sigma(\mathbf{r})$$

Now consider $[N, \Psi_\sigma^\dagger(\mathbf{r})]$. For boson operators,

$$\left[\Psi_{\sigma'}^\dagger(\mathbf{r}')\Psi_{\sigma'}(\mathbf{r}'), \Psi_\sigma(\mathbf{r})\right] = \Psi_{\sigma'}^\dagger(\mathbf{r}')\left[\Psi_{\sigma'}(\mathbf{r}'), \Psi_\sigma^\dagger(\mathbf{r})\right] = \delta_{\sigma\sigma'}\delta(\mathbf{r}-\mathbf{r}')\Psi_{\sigma'}^\dagger(\mathbf{r}')$$

For fermion operators,

$$\left[\Psi_{\sigma'}^\dagger(\mathbf{r}')\Psi_{\sigma'}(\mathbf{r}'), \Psi_\sigma(\mathbf{r})\right] = \Psi_{\sigma'}^\dagger(\mathbf{r}')\left\{\Psi_{\sigma'}(\mathbf{r}'), \Psi_\sigma^\dagger(\mathbf{r})\right\} = \delta_{\sigma\sigma'}\delta(\mathbf{r}-\mathbf{r}')\Psi_{\sigma'}^\dagger(\mathbf{r}')$$

Hence, for both bosons and fermions,

$$\left[N, \Psi_\sigma^\dagger(\mathbf{r})\right] = \Psi_\sigma^\dagger(\mathbf{r})$$

Define $\Psi_\sigma(\mathbf{r}, \theta)$ by

$$\Psi_\sigma(\mathbf{r}, \theta) = e^{iN\theta}\Psi_\sigma(\mathbf{r})e^{-iN\theta}$$

Taking derivatives with respect to θ,

$$\frac{d}{d\theta}\Psi_\sigma(\mathbf{r}, \theta) = iN\Psi_\sigma(\mathbf{r}, \theta) - i\Psi_\sigma(\mathbf{r}, \theta)N = i\left[N, \Psi_\sigma(\mathbf{r}, \theta)\right]$$

Since N commutes with $e^{\pm iN\theta}$, we can write

$$\begin{aligned}
[N, \Psi_\sigma(\mathbf{r}, \theta)] &= Ne^{iN\theta}\Psi_\sigma(\mathbf{r})e^{-iN\theta} - e^{iN\theta}\Psi_\sigma(\mathbf{r})e^{-iN\theta}N \\
&= e^{iN\theta}N\Psi_\sigma(\mathbf{r})e^{-iN\theta} - e^{iN\theta}\Psi_\sigma(\mathbf{r})Ne^{-iN\theta} = e^{iN\theta}\left[N, \Psi_\sigma(\mathbf{r})\right]e^{-iN\theta} \\
&= -\Psi_\sigma(\mathbf{r}, \theta)
\end{aligned}$$

where in the last step we used $[N, \Psi_\sigma(\mathbf{r})] = -\Psi_\sigma(\mathbf{r})$. Thus,

$$\frac{d}{d\theta}\Psi_\sigma(\mathbf{r}, \theta) = -i\Psi_\sigma(\mathbf{r}, \theta) \Rightarrow \Psi_\sigma(\mathbf{r}, \theta) = e^{-i\theta}\Psi_\sigma(\mathbf{r}, \theta = 0) = e^{-i\theta}\Psi_\sigma(\mathbf{r})$$

Taking the adjoint on both sides,

$$\Psi_\sigma^\dagger(\mathbf{r}, \theta) = e^{i\theta}\Psi_\sigma^\dagger(\mathbf{r})$$

5. *Spin operators.*

The spin operator for the N electrons is

$$\mathbf{S} = \sum_{i=1}^{N}\mathbf{s}_i$$

The second quantized form of S_x is

$$S_x = \sum_{\mathbf{k}\sigma\mathbf{k}'\sigma'}\langle\mathbf{k}'\sigma'|s_x|\mathbf{k}\sigma\rangle c_{\mathbf{k}'\sigma'}^\dagger c_{\mathbf{k}\sigma} = \sum_{\mathbf{k}\sigma\sigma'}\langle\sigma'|\sigma\rangle c_{\mathbf{k}\sigma'}^\dagger c_{\mathbf{k}\sigma}$$

In writing the above, we have used $s_x|\mathbf{k}\sigma\rangle = |\mathbf{k}\rangle s_x|\sigma\rangle$ and $\langle\mathbf{k}|\mathbf{k}'\rangle = \delta_{\mathbf{k}\mathbf{k}'}$. The state $|\sigma\rangle$ is either $|\uparrow\rangle$ or $|\downarrow\rangle$. Using the results of problem 1.5: $\langle\uparrow|s_x|\uparrow\rangle = \langle\downarrow|s_x|\downarrow\rangle 0$, $\langle\uparrow|s_x|\downarrow\rangle = \hbar/2 = \langle\downarrow|s_x|\uparrow\rangle$, we find

$$S_x = \frac{\hbar}{2}\sum_{\mathbf{k}}\left(c^\dagger_{\mathbf{k}\uparrow}c_{\mathbf{k}\downarrow} + c^\dagger_{\mathbf{k}\downarrow}c_{\mathbf{k}\uparrow}\right)$$

For s_y we have

$$\langle\uparrow|s_y|\uparrow\rangle = \langle\downarrow|s_y|\downarrow\rangle = 0, \quad \langle\uparrow|s_y|\downarrow\rangle = -i\hbar/2 = -\langle\downarrow|s_y|\uparrow\rangle$$

Hence,

$$S_y = i\frac{\hbar}{2}\sum_{\mathbf{k}}\left(c^\dagger_{\mathbf{k}\downarrow}c_{\mathbf{k}\uparrow} - c^\dagger_{\mathbf{k}\uparrow}c_{\mathbf{k}\downarrow}\right)$$

For s_z we have

$$\langle\uparrow|s_z|\uparrow\rangle = \hbar/2 \quad \langle\downarrow|s_z|\downarrow\rangle = -\hbar/2, \quad \langle\uparrow|s_z|\downarrow\rangle = \langle\downarrow|s_z|\uparrow\rangle = 0$$

It follows that

$$S_z = \frac{\hbar}{2}\sum_{\mathbf{k}}\left(c^\dagger_{\mathbf{k}\uparrow}c_{\mathbf{k}\uparrow} - c^\dagger_{\mathbf{k}\downarrow}c_{\mathbf{k}\downarrow}\right)$$

6. *Number-density operator.*

$$n(\mathbf{r}) = \sum_\sigma \Psi^\dagger_\sigma(\mathbf{r})\Psi_\sigma(\mathbf{r}) = \sum_\sigma\sum_{n\mathbf{k}}\sum_{n'\mathbf{k}'}\phi^*_{n\mathbf{k}}(\mathbf{r})\phi_{n'\mathbf{k}'}(\mathbf{r})c^\dagger_{n\mathbf{k}\sigma}c_{n'\mathbf{k}'\sigma}$$

In writing the above, we used the formula for the expansion of the field operators in terms of the creation and annihilation operators. The function $\phi_{n\mathbf{k}}(\mathbf{r})$ is a Bloch function, and it can be written as

$$\phi_{n\mathbf{k}}(\mathbf{r}) = u_{n\mathbf{k}}(\mathbf{r})e^{i\mathbf{k}.\mathbf{r}}, \quad u_{n\mathbf{k}}(\mathbf{r}) = u_{n\mathbf{k}}(\mathbf{r}+\mathbf{R})$$

where $\mathbf{R}$ is any lattice vector. The Fourier transform of $n(\mathbf{r})$ is

$$n_{\mathbf{q}} = \int n(\mathbf{r})e^{-i\mathbf{q}.\mathbf{r}}d^3r = \sum_\sigma\sum_{n\mathbf{k}}\sum_{n'\mathbf{k}'}c^\dagger_{n\mathbf{k}\sigma}c_{n'\mathbf{k}'\sigma}\int u^*_{n\mathbf{k}}(\mathbf{r})u_{n'\mathbf{k}'}(\mathbf{r})e^{i(\mathbf{k}'-\mathbf{k}-\mathbf{q}).\mathbf{r}}d^3r$$

Shifting the integration variable from $\mathbf{r}$ to $\mathbf{r}+\mathbf{R}$, the integral does not change; however, the integrand gets multiplied by $e^{i(\mathbf{k}'-\mathbf{k}-\mathbf{q}).\mathbf{R})}$. This quantity must be equal to 1 for all lattice vectors $\mathbf{R}$; this implies that $\mathbf{k}'-\mathbf{k}-\mathbf{q} = \mathbf{G}$, where $\mathbf{G}$ is a reciprocal lattice vector.

****

Another way to arrive at the above conclusion is to note that $f(\mathbf{r}) = u^*_{n\mathbf{k}}(\mathbf{r})u_{n'\mathbf{k}'}(\mathbf{r})$ is a periodic function: $f(\mathbf{r}) = f(\mathbf{r}+\mathbf{R})$. Expanding $f(\mathbf{r})$ in a Fourier series

$$f(\mathbf{r}) = \frac{1}{V}\sum_{\mathbf{q}'}f_{\mathbf{q}'}e^{i\mathbf{q}'.\mathbf{r}},$$

and using

$$f(\mathbf{r}) = f(\mathbf{r}+\mathbf{R}) = \frac{1}{V}\sum_{\mathbf{q}'} f_{\mathbf{q}'} e^{i\mathbf{q}'.(\mathbf{r}+\mathbf{R})},$$

we find that $e^{i\mathbf{q}'.\mathbf{R}} = 1$, which means that $\mathbf{q}'$ is a reciprocal lattice vector. Thus

$$f(\mathbf{r}) = \frac{1}{V}\sum_{\mathbf{G}} f_{\mathbf{G}} e^{i\mathbf{G}.\mathbf{r}},$$

and

$$\begin{aligned}\int f(\mathbf{r}) e^{i(\mathbf{k}'-\mathbf{k}-\mathbf{q}).\mathbf{r}} d^3r &= \frac{1}{V}\sum_{\mathbf{G}} f_{\mathbf{G}} \int e^{i(\mathbf{k}'-\mathbf{k}-\mathbf{q}+\mathbf{G}).\mathbf{r}} d^3r \\ &= \sum_{\mathbf{G}} f_{\mathbf{G}} \delta_{\mathbf{k}'-\mathbf{k}-\mathbf{q},-\mathbf{G}}\end{aligned}$$

In other words, the integral vanishes unless $\mathbf{k}' = \mathbf{k}+\mathbf{q}+\mathbf{G}$ for some lattice vector $\mathbf{G}$.

Note:

To see that $\int e^{i\mathbf{k}.\mathbf{r}} d^3r = V\delta_{\mathbf{k},\mathbf{0}}$, suppose that the crystal is a cube of side L and that the lattice vectors are along the x, y, and z directions. Then

$$\int e^{i\mathbf{k}.\mathbf{r}} d^3r = \int_0^L e^{ik_x x} dx \int_0^L e^{ik_y y} dy \int_0^L e^{ik_z z} dz$$

Now consider

$$\int_0^L e^{ik_x x} dx = \frac{e^{ik_x L} - 1}{ik_x}$$

Since $k_x = 0, \pm 2\pi/L, \pm 4\pi/L, \ldots$, the numerator vanishes, and the integral thus vanishes unless $k_x = 0$, in which case the integral equals L.

****

To summarize, in the expression for $n_{\mathbf{q}}$, the integral vanishes unless $\mathbf{k}' = \mathbf{k}+\mathbf{q}+\mathbf{G}$, where $\mathbf{G}$ is a reciprocal lattice vector. Since $\mathbf{k}$, $\mathbf{k}'$ $\in$FBZ, then for any given $\mathbf{q}$, $\mathbf{G}$ is the particular reciprocal lattice vector that carries $\mathbf{k}+\mathbf{q}$, should it lie outside the FBZ, back into the FBZ. If $\mathbf{k}+\mathbf{q}$ $\in$FBZ, then $\mathbf{G}=0$. We thus write $\mathbf{k}' = \mathbf{k}+\mathbf{q}$ with the understanding that $\mathbf{k}+\mathbf{q}$ lies in the FBZ. Therefore,

$$\begin{aligned}n_{\mathbf{q}} &= \sum_{\sigma}\sum_{nn'\mathbf{k}} c^\dagger_{n\mathbf{k}\sigma} c_{n'\mathbf{k}+\mathbf{q}\sigma} \int \phi^*_{n\mathbf{k}}(\mathbf{r}) e^{-i\mathbf{q}.\mathbf{r}} \phi_{n'\mathbf{k}+\mathbf{q}}(\mathbf{r}) d^3r \\ &= \sum_{\mathbf{k}\sigma}\sum_{nn'} \langle n\mathbf{k}\sigma| e^{-i\mathbf{q}.\mathbf{r}} |n'\mathbf{k}+\mathbf{q}\sigma\rangle c^\dagger_{n\mathbf{k}\sigma} c_{n'\mathbf{k}+\mathbf{q}\sigma}\end{aligned}$$

7. *Current density.*

$$\begin{aligned}\mathbf{j}(\mathbf{r}) &= -\frac{e}{2m}\sum_i \left[\left(\mathbf{p}_i + \frac{e}{c}\mathbf{A}(\mathbf{r}_i)\right)\delta(\mathbf{r}-\mathbf{r}_i) + \delta(\mathbf{r}-\mathbf{r}_i)\left(\mathbf{p}_i + \frac{e}{c}\mathbf{A}(\mathbf{r}_i)\right)\right] \\ &= -\frac{e}{2m}\sum_i [\mathbf{p}_i\delta(\mathbf{r}-\mathbf{r}_i) + \delta(\mathbf{r}-\mathbf{r}_i)\mathbf{p}_i] - \frac{e^2}{2mc}\sum_i [\mathbf{A}(\mathbf{r}_i)\delta(\mathbf{r}-\mathbf{r}_i) + \delta(\mathbf{r}-\mathbf{r}_i)\mathbf{A}(\mathbf{r}_i)]\end{aligned}$$

Since $\mathbf{A}(\mathbf{r}_i)$ commutes with $\mathbf{r}_i$, the second term becomes

$$\mathbf{j}^D(\mathbf{r}) = -\frac{e^2}{mc}\sum_i \mathbf{A}(\mathbf{r}_i)\delta(\mathbf{r}-\mathbf{r}_i)$$

Its second quantized form is

$$\begin{aligned}\mathbf{j}^D(\mathbf{r}) &= -\frac{e^2}{mc}\sum_\sigma \int \Psi^\dagger_\sigma(\mathbf{r}_1)\mathbf{A}(\mathbf{r}_1)\delta(\mathbf{r}-\mathbf{r}_1)\Psi_\sigma(\mathbf{r}_1)d^3r_1 = -\frac{e^2}{mc}\mathbf{A}(\mathbf{r})\sum_\sigma \Psi^\dagger_\sigma(\mathbf{r})\Psi_\sigma(\mathbf{r}) \\ &= -\frac{e^2}{mc}\mathbf{A}(\mathbf{r})n(\mathbf{r})\end{aligned}$$

The paramagnetic current is given by

$$\mathbf{j}^P(\mathbf{r}) = -\frac{e}{2m}\sum_i [\mathbf{p}_i\delta(\mathbf{r}-\mathbf{r}_i) + \delta(\mathbf{r}-\mathbf{r}_i)\mathbf{p}_i]$$

Its second quantized form is

$$\begin{aligned}\mathbf{j}^P(\mathbf{r}) &= \frac{ie\hbar}{2m}\sum_\sigma \left[\int \Psi^\dagger_\sigma(\mathbf{r}_1)\boldsymbol{\nabla}_{\mathbf{r}_1}\delta(\mathbf{r}-\mathbf{r}_1)\Psi_\sigma(\mathbf{r}_1)d^3r_1 + \int \Psi^\dagger_\sigma(\mathbf{r}_1)\delta(\mathbf{r}-\mathbf{r}_1)\boldsymbol{\nabla}_{\mathbf{r}_1}\Psi_\sigma(\mathbf{r}_1)d^3r_1\right] \\ &\equiv \frac{ie\hbar}{2m}(\mathbf{A}+\mathbf{B})\end{aligned}$$

To evaluate this, consider a complete set of states $\{\phi_n(\mathbf{r})|\sigma\rangle\}$. Using

$$\Psi_\sigma(\mathbf{r}) = \sum_n \phi + n(\mathbf{r})c_{n\sigma}, \quad \Psi^\dagger_\sigma(\mathbf{r}) = \sum_n \phi^*_n(\mathbf{r})c^\dagger_{n\sigma},$$

the second term becomes

$$\begin{aligned}\mathbf{B} &= \sum_\sigma\sum_{nn'} c^\dagger_{n'\sigma}c_{n\sigma}\int \phi^*_{n'}(\mathbf{r}_1)\delta(\mathbf{r}-\mathbf{r}_1)\boldsymbol{\nabla}_{\mathbf{r}_1}\phi_n(\mathbf{r}_1)d^3r_1 \\ &= \sum_\sigma\sum_{nn'} c^\dagger_{n'\sigma}c_{n\sigma}\phi^*_{n'}(\mathbf{r})\boldsymbol{\nabla}_{\mathbf{r}}\phi_n(\mathbf{r}) \\ &= \sum_\sigma \Psi^\dagger_\sigma(\mathbf{r})\boldsymbol{\nabla}\Psi_\sigma(\mathbf{r})\end{aligned}$$

The first term is given by

$$\mathbf{A} = \sum_\sigma\sum_{nn'} c^\dagger_{n'\sigma}c_{n\sigma}\int \phi^*_{n'}(\mathbf{r}_1)\boldsymbol{\nabla}_{\mathbf{r}_1}\delta(\mathbf{r}-\mathbf{r}_1)\phi_n(\mathbf{r}_1)d^3r_1$$

Recall how the adjoint of an operator X is defined:

$$\int f^* X g d^3r = \int (X^\dagger f)^* g d^3r$$

Thus

$$\mathbf{A} = \sum_{\sigma} \sum_{nn'} c^{\dagger}_{n'\sigma} c_{n\sigma} \int \left(\boldsymbol{\nabla}^{\dagger}_{\mathbf{r}_1} \phi_{n'}(\mathbf{r}_1) \right)^* \delta(\mathbf{r} - \mathbf{r}_1) \phi_n(\mathbf{r}_1) d^3 r_1$$

Noting that $\boldsymbol{\nabla}^{\dagger} = -\boldsymbol{\nabla}$ (recall that $\mathbf{p}^{\dagger} = \mathbf{p} \Rightarrow (-i\hbar\boldsymbol{\nabla})^{\dagger} = -i\hbar\boldsymbol{\nabla}$), we find

$$\begin{aligned}
\mathbf{A} &= -\sum_{\sigma} \sum_{nn'} c^{\dagger}_{n'\sigma} c_{n\sigma} \int \left(\boldsymbol{\nabla}_{\mathbf{r}_1} \phi^*_{n'}(\mathbf{r}_1) \right) \delta(\mathbf{r} - \mathbf{r}_1) \phi_n(\mathbf{r}_1) d^3 r_1 \\
&= -\sum_{\sigma} \sum_{nn'} c^{\dagger}_{n'\sigma} c_{n\sigma} \left(\boldsymbol{\nabla} \phi^*_{n'}(\mathbf{r}) \right) \phi_n(\mathbf{r}) \\
&= -\sum_{\sigma} \left(\boldsymbol{\nabla} \Psi^{\dagger}_{\sigma}(\mathbf{r}) \right) \Psi_{\sigma}(\mathbf{r})
\end{aligned}$$

The required expression for $\mathbf{j}^P(\mathbf{r})$ is thus obtained.
****

An alternative method to determine $\mathbf{A}$ is as follows.

$$\begin{aligned}
\mathbf{A} &= \sum_{\sigma} \sum_{nn'} c^{\dagger}_{n'\sigma} c_{n\sigma} I \\
I &= \int \phi^*_{n'}(\mathbf{r}_1) \boldsymbol{\nabla}_{\mathbf{r}_1} \delta(\mathbf{r} - \mathbf{r}_1) \phi_n(\mathbf{r}_1) d^3 r_1
\end{aligned}$$

The operator $\delta(\mathbf{r} - \mathbf{r}_1)$ first acts on the function $\phi_n(\mathbf{r}_1)$ to yield the function $\delta(\mathbf{r} - \mathbf{r}_1)\phi_n(\mathbf{r}_1)$ which is equal to the function $\delta(\mathbf{r} - \mathbf{r}_1)\phi_n(\mathbf{r})$. Thus

$$I = \phi_n(\mathbf{r}) \int \phi^*_{n'}(\mathbf{r}_1) \boldsymbol{\nabla}_{\mathbf{r}_1} \delta(\mathbf{r} - \mathbf{r}_1) d^3 r_1$$

In the above , $\delta(\mathbf{r} - \mathbf{r}_1)$ is the Dirac-delta function (not an operator). The operator $\boldsymbol{\nabla}_{\mathbf{r}_1}$ now acts on the function $\delta(\mathbf{r} - \mathbf{r}_1)$,

$$\boldsymbol{\nabla}_{\mathbf{r}_1} \delta(\mathbf{r} - \mathbf{r}_1) = -\boldsymbol{\nabla}_{\mathbf{r}} \delta(\mathbf{r} - \mathbf{r}_1)$$

Therefore,

$$I = -\phi_n(\mathbf{r}) \int \phi^*_{n'}(\mathbf{r}_1) \boldsymbol{\nabla}_{\mathbf{r}} \delta(\mathbf{r} - \mathbf{r}_1) d^3 r_1$$

Since the integration is over $\mathbf{r}_1$, we can move $\boldsymbol{\nabla}_{\mathbf{r}}$ to outside the integral,

$$I = -\phi_n(\mathbf{r}) \boldsymbol{\nabla}_{\mathbf{r}} \int \phi^*_{n'}(\mathbf{r}_1) \delta(\mathbf{r} - \mathbf{r}_1) d^3 r_1 = -\phi_n(\mathbf{r}) \boldsymbol{\nabla} \phi^*_{n'}(\mathbf{r})$$

Hence,

$$\mathbf{A} = -\sum_{\sigma} \sum_{nn'} c^{\dagger}_{n'\sigma} c_{n\sigma} \phi_n(\mathbf{r}) \boldsymbol{\nabla} \phi^*_{n'}(\mathbf{r}) = -\sum_{\sigma} \left(\boldsymbol{\nabla} \Psi^{\dagger}_{\sigma}(\mathbf{r}) \right) \Psi_{\sigma}(\mathbf{r})$$

****

The Fourier transform of $\mathbf{j}^P(\mathbf{r})$ is given by

$$\begin{aligned}\mathbf{j}^P_{\mathbf{q}} &= \int \mathbf{j}^P(\mathbf{r})e^{-i\mathbf{q}.\mathbf{r}}d^3r \\ &= \frac{ie\hbar}{2m}\sum_\sigma \int \left[\Psi^\dagger_\sigma(\mathbf{r})\boldsymbol{\nabla}\Psi_\sigma(\mathbf{r}) - \left(\boldsymbol{\nabla}\Psi^\dagger_\sigma(\mathbf{r})\right)\Psi_\sigma(\mathbf{r})\right] e^{-i\mathbf{q}.\mathbf{r}}d^3r\end{aligned}$$

Expanding the field operators, using plane waves as basis:

$$\Psi_\sigma(\mathbf{r}) = \frac{1}{\sqrt{V}}\sum_{\mathbf{k}} e^{i\mathbf{k}.\mathbf{r}}c_{\mathbf{k}\sigma}, \quad \Psi^\dagger_\sigma(\mathbf{r}) = \frac{1}{\sqrt{V}}\sum_{\mathbf{k}} e^{-i\mathbf{k}.\mathbf{r}}c^\dagger_{\mathbf{k}\sigma},$$

we obtain

$$\begin{aligned}\mathbf{j}^P_{\mathbf{q}} &= \frac{ie\hbar}{2mV}\sum_\sigma\sum_{\mathbf{k}\mathbf{k}'}\left[\int\left(e^{-i\mathbf{k}.\mathbf{r}}(i\mathbf{k}')e^{i\mathbf{k}'.\mathbf{r}}e^{-i\mathbf{q}.\mathbf{r}} + i\mathbf{k}e^{-i\mathbf{k}.\mathbf{r}}e^{i\mathbf{k}'.\mathbf{r}}e^{-i\mathbf{q}.\mathbf{r}}\right)d^3r\right]c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}'\sigma} \\ &= -\frac{e\hbar}{2mV}\sum_\sigma\sum_{\mathbf{k}\mathbf{k}'}(\mathbf{k}'+\mathbf{k})\int e^{i(\mathbf{k}'-\mathbf{k}-\mathbf{q}).\mathbf{r}}d^3r\, c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}'\sigma}\end{aligned}$$

Since

$$\int e^{i(\mathbf{k}'-\mathbf{k}-\mathbf{q}).\mathbf{r}}d^3r = V\delta\mathbf{k}', \mathbf{k}+\mathbf{q}$$

we find

$$\mathbf{j}^P_{\mathbf{q}} = -\frac{e\hbar}{2m}\sum_{\mathbf{k}\sigma}(2\mathbf{k}+\mathbf{q})c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}+\mathbf{q}\sigma}$$

8. *Contact potential.*

$$H' = (g/2)\sum_{i\neq j}\delta(\mathbf{r}_i - \mathbf{r}_j)$$

In terms of field operators, V is written as

$$\begin{aligned}H' &= (g/2)\sum_{\sigma_1\sigma_2}\int\int \Psi^\dagger_{\sigma_1}(\mathbf{r}_1)\Psi^\dagger_{\sigma_2}(\mathbf{r}_2)\delta(\mathbf{r}_1-\mathbf{r}_2)\Psi_{\sigma_2}(\mathbf{r}_2)\Psi_{\sigma_1}(\mathbf{r}_1)d^3r_1d^3r_2 \\ &= (g/2)\sum_{\sigma_1\sigma_2}\int \Psi^\dagger_{\sigma_1}(\mathbf{r})\Psi^\dagger_{\sigma_2}(\mathbf{r})\Psi_{\sigma_2}(\mathbf{r})\Psi_{\sigma_1}(\mathbf{r})d^3r\end{aligned}$$

If we use a set of plane waves as a basis,

$$H' = \frac{g}{2}\sum_{\mathbf{k}_1\sigma_1}\sum_{\mathbf{k}_2\sigma_2}\sum_{\mathbf{k}_3\sigma_3}\sum_{\mathbf{k}_4\sigma_4}\langle\mathbf{k}_1\sigma_1\mathbf{k}_2\sigma_2|\delta(\mathbf{r}_1-\mathbf{r}_2)|\mathbf{k}_3\sigma_3\mathbf{k}_4\sigma_4\rangle c^\dagger_{\mathbf{k}_1\sigma_1}c^\dagger_{\mathbf{k}_2\sigma_2}c_{\mathbf{k}_4\sigma_4}c_{\mathbf{k}_3\sigma_3}$$

The matrix element is given by

$$\begin{aligned}
M &\equiv \langle \mathbf{k}_1\sigma_1\mathbf{k}_2\sigma_2|\delta(\mathbf{r}_1-\mathbf{r}_2)|\mathbf{k}_3\sigma_3\mathbf{k}_4\sigma_4\rangle \\
&= \frac{1}{V^2}\delta_{\sigma_1\sigma_3}\delta_{\sigma_2\sigma_4}\int\int e^{-i\mathbf{k}_1.\mathbf{r}_1}e^{-i\mathbf{k}_2.\mathbf{r}_2}\delta(\mathbf{r}_1-\mathbf{r}_2)e^{i\mathbf{k}_3.\mathbf{r}_1}e^{i\mathbf{k}_4.\mathbf{r}_2} \\
&= \frac{1}{V^2}\delta_{\sigma_1\sigma_3}\delta_{\sigma_2\sigma_4}\int e^{i(\mathbf{k}_3+\mathbf{k}_4-\mathbf{k}_1-\mathbf{k}_2).\mathbf{r}}d^3r \\
&= \frac{1}{V}\delta_{\sigma_1\sigma_3}\delta_{\sigma_2\sigma_4}\delta_{\mathbf{k}_1-\mathbf{k}_3,\mathbf{k}_4-\mathbf{k}_2}
\end{aligned}$$

Let $\mathbf{k}_1-\mathbf{k}_3=\mathbf{q}$. Then, for M not to vanish, we should have $\mathbf{k}_2-\mathbf{k}_4=-\mathbf{q}$; hence

$$\begin{aligned}
H' &= \frac{g}{2V}\sum_{\mathbf{q}}\sum_{\mathbf{k}_3\sigma_3}\sum_{\mathbf{k}_4\sigma_4} c^\dagger_{\mathbf{k}_3+\mathbf{q}\sigma_3}c^\dagger_{\mathbf{k}_4-\mathbf{q}\sigma_4}c_{\mathbf{k}_4\sigma_4}c_{\mathbf{k}_3\sigma_3} \\
&= \frac{g}{2V}\sum_{\mathbf{q}}\sum_{\mathbf{k}\sigma}\sum_{\mathbf{k}'\sigma'} c^\dagger_{\mathbf{k}+\mathbf{q}\sigma}c^\dagger_{\mathbf{k}'-\mathbf{q}\sigma'}c_{\mathbf{k}'\sigma'}c_{\mathbf{k}\sigma}
\end{aligned}$$

We could have arrived at this result more quickly. The interaction is of the form

$$H' = \frac{1}{2}\sum_{i\neq j} v(i,j), \quad v(i,j) = g\delta(\mathbf{r}_i-\mathbf{r}_j)$$

The system is translationally invariant; hence

$$H' = \frac{1}{2V}\sum_{\mathbf{k}\sigma}\sum_{\mathbf{k}'\sigma'}\sum_{\mathbf{q}} v_{\mathbf{q}}c^\dagger_{\mathbf{k}+\mathbf{q}\sigma}c^\dagger_{\mathbf{k}'-\mathbf{q}\sigma'}c_{\mathbf{k}'\sigma'}c_{\mathbf{k}\sigma}$$

where $v_{\mathbf{q}}$, the Fourier transform of $v(\mathbf{r}_i-\mathbf{r}_j)$ is

$$v_{\mathbf{q}} = \int v(\mathbf{r})e^{-i\mathbf{q}.\mathbf{r}}d^3r = \int g\delta(\mathbf{r})e^{-i\mathbf{q}.\mathbf{r}}d^3r = g$$

9. *Spin waves.*

$$H = -\frac{J}{2}\sum_{<ij>}\mathbf{S}_i.\mathbf{S}_j = -\frac{J}{2}\sum_{i,m}\mathbf{S}_i.\mathbf{S}_{i+m}$$

The sum over i runs over all the lattice vectors $\mathbf{R}_i$ $(i=1,2,\ldots,N)$, while the sum over m runs over the Z lattice vectors connecting i to its nearest neighbors $(m=1,2,\ldots,Z)$. Z is called the coordination number. The raising and lowering spin operators are

$$S_i^+ = S_i^x + iS_i^y, \quad S_i^- = S_i^x - iS_i^y$$

We transform to boson operators a_i and $a_i^\dagger$,

$$S_i^+ = [2s - a_i^\dagger a_i]^{1/2}a_i, \quad S_i^- = a_i^\dagger[2s-a_i^\dagger a_i]^{1/2}$$

The operators a_i and $a_i^\dagger$ satisfy the usual boson commutation relations:

$$[a_i,a_j] = [a_i^\dagger,a_j^\dagger] = 0, \quad [a_i,a_j^\dagger] = \delta_{ij}$$

(a)

$$\begin{aligned}
S_i^- S_i^+ &= (S_i^x - iS_i^y)(S_i^x + iS_i^y) = (S_i^x)^2 + (S_i^y)^2 + i(S_i^x S_i^y - S_i^y S_i^x) \\
&= (S_i^x)^2 + (S_i^y)^2 - S_i^z \\
&\Rightarrow (S_i^x)^2 + (S_i^y)^2 = S_i^- S_i^+ + S_i^z
\end{aligned}$$

In order to simplify notation, in what follows we drop the subscript i and write x, y, and z as subscripts instead of superscripts. We thus write the above relation as

$$S_x^2 + S_y^2 = S^- S^+ + S_z$$

Using $S_z^2 = s(s+1) - S_x^2 - S_y^2 = s(s+1) - S^- S^+ - S_z$, we find

$$\begin{aligned}
S_z^2 + S_z &= s(s+1) - S^- S^+ = s(s+1) - 2sa^\dagger(1 - a^\dagger a/2s)a \\
&= s(s+1) - 2sa^\dagger a + a^\dagger a^\dagger aa
\end{aligned}$$

Using the commutation relation $[a, a^\dagger] = 1$, we obtain

$$\begin{aligned}
S_z^2 + S_z &= s(s+1) - 2sa^\dagger a + a^\dagger(aa^\dagger - 1)a = s(s+1) - (2s+1)a^\dagger a + (a^\dagger a)^2 \\
&\Rightarrow S_z(S_z + 1) = (s - a^\dagger a)(s - a^\dagger a + 1)
\end{aligned}$$

This equation has two solutions

$$S_z = s - a^\dagger a \text{ or } S_z = a^\dagger a - s - 1$$

However, the second solution is not acceptable because S^+, S^-, and S_z satisfy the follwing commutation relation

$$[S^+, S^-] = 2S_z$$

As we now check, it is the first solution that satisfies this commutation relation.

$$\begin{aligned}
[S^+, S^-] &= S^+ S^- - S^- S^+ = \sqrt{2s - a^\dagger a}\; aa^\dagger \sqrt{2s - a^\dagger a} - a^\dagger \sqrt{2s - a^\dagger a}\sqrt{2s - a^\dagger a}\; a \\
&= \sqrt{2s - a^\dagger a}\; (a^\dagger a + 1)\sqrt{2s - a^\dagger a} - a^\dagger(2s - a^\dagger)a
\end{aligned}$$

Next we use the fact that $a^\dagger a$ commutes with any function of $a^\dagger a$ that can be expanded in a power series in $a^\dagger a$. Thus

$$\begin{aligned}
[S^+, S^-] &= a^\dagger a(2s - a^\dagger a) + 2s - a^\dagger a - a^\dagger(2s - aa^\dagger + 1)a \\
&= 2(s - a^\dagger a)
\end{aligned}$$

We can also form S_x and S_y in terms of a and $a^\dagger$ and verify easily that the usual commutation relations are satisfied.

(b) First we note that

$$\mathbf{S}_i.\mathbf{S}_{i+m} = S_i^z S_{i+m}^z + \frac{1}{2}[S_i^+ S_{i+m}^- + S_i^- S_{i+m}^+]$$

We are interested in expanding the Hamiltonian up to quadratic terms in a and $a^\dagger$. Hence we write

$$
\begin{aligned}
S_i^+ &= \sqrt{2s - a_i^\dagger a_i}\; a_i \simeq \sqrt{2s}\; a_i \\
S_i^- &= a_i^\dagger \sqrt{2s - a^\dagger a} = \sqrt{2s}\; a_i^\dagger \\
S_i^z &= s - a_i^\dagger a_i
\end{aligned}
$$

Including other terms in S_i^+ and/or S_i^- will lead to terms in H of order higher than quadratic. Physically, the above approximation for S_i^+ and S_i^- can be justified at low temperatures where there are only few excitations above the ground state, for then the thermal average $\langle a_i^\dagger a_i \rangle$ will be of order $1/N$, which is negligible compared to $2s$.

The Hamiltonian is now written as

$$
H = -\frac{J}{2} \sum_{i,m} [(s - a_i^\dagger a_i)(s - a_{i+m}^\dagger a_{i+m}) + s a_i a_{i+m}^\dagger + s a_i^\dagger a_{i+m}]
$$

Ignoring terms containing four operators, we can write

$$
H = -\frac{J}{2} \sum_{i,m} s^2 + \frac{Js}{2} \sum_{i,m} (a_i^\dagger a_i + a_{i+m}^\dagger a_{i+m}) - \frac{Js}{2} \sum_{i,m} (a_i^\dagger a_{i+m} + a_i a_{i+m}^\dagger)
$$

Noting that

$$
\begin{aligned}
&\sum_{i,m} s^2 = NZs^2, \quad \sum_{i,m} a_i^\dagger a_i = \sum_{i,m} a_{i+m}^\dagger a_{i+m} = Z \sum_i a_i^\dagger a_i \\
&a_i a_{i+m}^\dagger = a_{i+m}^\dagger a_i, \quad \sum_{i,m} a_{i+m}^\dagger a_i = \sum_{i,m} a_i^\dagger a_{i+m}
\end{aligned}
$$

The Hamiltonian reduces to

$$
H = E_0 + ZJs \sum_i a_i^\dagger a_i - Js \sum_{i,m} a_i^\dagger a_{i+m}
$$

where

$$
E_0 = -\frac{1}{2} JNZs^2
$$

is the ground state energy.

We now consider the transformation

$$
a_{\mathbf{k}} = \frac{1}{\sqrt{N}} \sum_i e^{i\mathbf{k}.\mathbf{R}_i} a_i, \quad a_{\mathbf{k}}^\dagger = \frac{1}{\sqrt{N}} \sum_i e^{-i\mathbf{k}.\mathbf{R}_i} a_i^\dagger
$$

Inverting the transformation, we obtain

$$
a_i = \frac{1}{\sqrt{N}} \sum_{\mathbf{k} \in \mathrm{FBZ}} e^{-i\mathbf{k}.\mathbf{R}_i} a_{\mathbf{k}}, \quad a_i^\dagger = \frac{1}{\sqrt{N}} \sum_{\mathbf{k} \in \mathrm{FBZ}} e^{i\mathbf{k}.\mathbf{R}_i} a_{\mathbf{k}}^\dagger
$$

The operators $a_{\mathbf{k}}$ and $a_{\mathbf{k}}^\dagger$ satisfy the usual commutation relations. For example,

$$[a_{\mathbf{k}}, a_{\mathbf{k}'}^\dagger] = \frac{1}{N}\sum_{i,j} e^{i\mathbf{k}.\mathbf{R}_i} e^{-i\mathbf{k}'.\mathbf{R}_j}[a_i, a_j^\dagger] = \frac{1}{N}\sum_{i,j} e^{i\mathbf{k}.\mathbf{R}_i} e^{-i\mathbf{k}'.\mathbf{R}_j}\delta_{ij} = \frac{1}{N}\sum_{i} e^{i(\mathbf{k}-\mathbf{k}').\mathbf{R}_i}$$
$$= \delta_{\mathbf{k}\mathbf{k}'}$$

In the last step we used the result from problem 2.1. We now have

$$\sum_i a_i^\dagger a_i = \frac{1}{N}\sum_i \sum_{\mathbf{k}\mathbf{k}'} e^{i(\mathbf{k}-\mathbf{k}').\mathbf{R}_i} a_{\mathbf{k}}^\dagger a_{\mathbf{k}'}$$

On the RHS, summing over i first, we find

$$\sum_i a_i^\dagger a_i = \frac{1}{N}\sum_{\mathbf{k}\mathbf{k}'} N\delta_{\mathbf{k}\mathbf{k}'} a_{\mathbf{k}}^\dagger a_{\mathbf{k}'} = \sum_{\mathbf{k}} a_{\mathbf{k}}^\dagger a_{\mathbf{k}}$$

Next, we evalute

$$\sum_{i,m} a_i^\dagger a_{i+m} = \frac{1}{N}\sum_{i,m}\sum_{\mathbf{k}\mathbf{k}'} e^{i\mathbf{k}.\mathbf{R}_i} e^{-i\mathbf{k}'.(\mathbf{R}_i+\boldsymbol{\delta}_m)} a_{\mathbf{k}}^\dagger a_{\mathbf{k}'}$$

where $\boldsymbol{\delta}_m$ is the lattice vector connecting the lattice site i to the site $i+m$, which is one of the nearest neighbors of i. We define the quantity $\beta(\mathbf{k}')$ by

$$\beta(\mathbf{k}') = \frac{1}{Z}\sum_m e^{-i\mathbf{k}'.\boldsymbol{\delta}_m}$$

Thus

$$\begin{aligned}
\sum_{i,m} a_i^\dagger a_{i+m} &= \frac{1}{N}\sum_{\mathbf{k}\mathbf{k}'} Z\beta(\mathbf{k}')\sum_i e^{i(\mathbf{k}-\mathbf{k}').\mathbf{R}_i} a_{\mathbf{k}}^\dagger a_{\mathbf{k}'} \\
&= \frac{1}{N}\sum_{\mathbf{k}\mathbf{k}'} Z\beta(\mathbf{k}') N\delta_{\mathbf{k}\mathbf{k}'} a_{\mathbf{k}}^\dagger a_{\mathbf{k}'} \\
&= Z\sum_{\mathbf{k}} \beta(\mathbf{k}) a_{\mathbf{k}}^\dagger a_{\mathbf{k}}
\end{aligned}$$

Assembling all the pieces together,

$$H = E_0 + ZJs\sum_{\mathbf{k}}[1-\beta(\mathbf{k})]a_{\mathbf{k}}^\dagger a_{\mathbf{k}} = E_0 + \sum_{kv}\hbar\omega_{\mathbf{k}} a_{\mathbf{k}}^\dagger a_{\mathbf{k}}$$

where $\hbar\omega_{\mathbf{k}} = ZJs[1-\beta(\mathbf{k})]$. Note that as $\mathbf{k}\to 0$, $\beta(\mathbf{k})\to 1$ and $\omega_{\mathbf{k}}\to 0$.

Chapter 4

Electron Gas

1. *Constrained ground state.*

   For the unpolarized state,

$$F_F = \hbar^2 k_F^2/2m = \frac{\hbar^2}{2m}(3\pi N/V)^{2/3}$$

   For the polarized state,

$$\begin{aligned}
N_\uparrow &= \frac{4\pi k_{F\uparrow}^3/3}{(2\pi)^3/V} \\
\Longrightarrow k_{F\uparrow} &= (6\pi^2 N_\uparrow/V)^{1/3} = \left[\frac{6\pi^2 N(1+p)}{2V}\right]^{1/3} = k_F(1+p)^{1/3}
\end{aligned}$$

   Similarly,

$$k_{F\downarrow} = k_F(1-p)^{1/3}$$

   The total energy is

$$E = \sum_{\mathbf{k},k<k_{F\uparrow}} \frac{\hbar^2 k^2}{2m} + \sum_{\mathbf{k},k<k_{F\downarrow}} \frac{\hbar^2 k^2}{2m}$$

   Replacing the sum by an integral,

$$\begin{aligned}
E &= \frac{\hbar^2}{2m}\frac{V}{(2\pi)^3}\left[\int_0^{k_{F\uparrow}} k^2 d^3k + \int_0^{k_{F\downarrow}} k^2 d^3k\right] \\
&= \frac{\hbar^2}{2m}\frac{V}{(2\pi)^3}4\pi\left[\int_0^{k_{F\uparrow}} k^4 dk + \int_0^{k_{F\downarrow}} k^4 dk\right] = \frac{\hbar^2}{2m}\frac{V}{10\pi^2}[k_{F\uparrow}^5 + k_{F\downarrow}^5] \\
&= \frac{\hbar^2}{2m}\frac{V}{10\pi^2}k_F^5[(1+p)^{5/3} + (1-p)^{5/3}]
\end{aligned}$$

   Noting that

$$\frac{\hbar^2}{2m}k_F^5 = \frac{\hbar^2 k_F^2}{2m}k_F^3 = E_F(3\pi^2 N/V),$$

we obtain

$$E_N = \frac{3E_F}{5}\left[\frac{(1+p)^{5/3}+(1-p)^{5/3}}{2}\right] = \frac{E_0}{N}\left[\frac{(1+p)^{5/3}+(1-p)^{5/3}}{2}\right]$$

2. *Correlation function.*

$$G_\sigma(\mathbf{r},\mathbf{r}') = \langle\Phi_0|\Psi_\sigma^\dagger(\mathbf{r})\Psi_\sigma(\mathbf{r}')|\Phi_0\rangle = \frac{1}{V}\sum_{\mathbf{kk}'} e^{i\mathbf{k}.\mathbf{r}}e^{-i\mathbf{k}'.\mathbf{r}'}\langle\Phi_0|c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}'\sigma}|\Phi_0\rangle$$

In the ground state $|\Phi_0\rangle$, all single-particle states within the Fermi sphere are occupied, whereas all states outside the Fermi sphere are empty. Thus $c_{\mathbf{k}'\sigma}|\Phi_0\rangle$ vanishes unless $k' < k_F$. If $k' < k_F$, then $c_{\mathbf{k}'\sigma}$ annihilates an electron in state $|\mathbf{k}'\sigma\rangle$. The operator $c^\dagger_{\mathbf{k}\sigma}$ then creates an electron in state $|\mathbf{k}\sigma\rangle$. Thus, for the matrix element $\langle\Phi_0|c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}'\sigma}|\Phi_0\rangle$ to be nonzero, $\mathbf{k}$ and $\mathbf{k}'$ must be equal, in which case $\langle\Phi_0|c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}'\sigma}|\Phi_0\rangle = 1$.

$$G_\sigma(\mathbf{r},\mathbf{r}') = \sum_{\mathbf{k}}^{k<k_F} e^{i\mathbf{k}.(\mathbf{r}-\mathbf{r}')} = \frac{1}{V}\frac{V}{(2\pi)^3}\int_{FS} e^{i\mathbf{k}.(\mathbf{r}-\mathbf{r}')}d^3k$$

The integration is over the Fermi sphere. Let $\mathbf{r}-\mathbf{r}' = \mathbf{x}$, and choose the z-direction to be along $\mathbf{k}$. Then

$$G_\sigma(\mathbf{r},\mathbf{r}') = G_\sigma(\mathbf{x}) = \frac{1}{(2\pi)^3}\int_0^{k_F} k^2dk\int_{-1}^{1} d(cos\theta)\int_0^{2\pi} d\phi e^{ikx\,cos\theta}$$

Integration over ϕ gives 2π. The integral over θ is straightforward,

$$G_\sigma(\mathbf{x}) = \frac{1}{4\pi^2}\int_0^{k_F} k^2\,\frac{e^{ikx}-e^{-ikx}}{ikx}dk = \frac{1}{2\pi^2 x}\int_0^{k_F} k\,sin(kx)dk$$

The integration over k is carried out by parts: $u = k,\ dv = sin(kx)dk \Rightarrow v = -cos(kx)/x$. Thus,

$$\begin{aligned}
G_\sigma(\mathbf{x}) &= \frac{1}{2\pi^2 x}\left[-\left.\frac{k cos(kx)}{x}\right|_0^{k_F} + \frac{1}{x}\int_0^{k_F} cos(kx)dk\right] \\
&= \frac{1}{2\pi^2x^3}[sin(k_Fx)-(k_Fx)cos(k_Fx)] = \frac{k_F^3}{2\pi^2}\left[\frac{sin(k_Fx)-(k_Fx)cos(k_Fx)}{(k_Fx)^3}\right] \\
&= \frac{3n}{2}\left[\frac{sin(k_Fx)-(k_Fx)cos(k_Fx)}{(k_Fx)^3}\right]
\end{aligned}$$

In the last step, we used the formula $k_F^3 = 3\pi^2 n$, where $n = N/V$ is the density of electrons. In the limit as $x\to\infty$, $G_\sigma(\mathbf{x})\to 0$. On the other hand,

$$\begin{aligned}
\lim_{x\to 0} G_\sigma(\mathbf{x}) &= \frac{1}{2\pi^2x^3}\left[k_Fx - \frac{(k_Fx)^3}{3!} - k_Fx + \frac{(k_Fx)^3}{2!}\right] = k_F^3/6\pi^2 = \frac{3\pi^2 N/V}{6\pi^2} \\
&= n/2
\end{aligned}$$

We remark that $G_\sigma(\mathbf{r},\mathbf{r}')$ is the overlap of states $\Psi_\sigma(\mathbf{r}')|\Phi_0\rangle$ and $\Psi_\sigma(\mathbf{r})|\Phi_0\rangle$. These states are not normalized. In fact,

$$\langle\Phi_0|\Psi^\dagger_\sigma(\mathbf{r})\Psi_\sigma(\mathbf{r})|\Phi_0\rangle = \frac{1}{2}\langle\Phi_0|\sum_\sigma \Psi^\dagger_\sigma(\mathbf{r})\Psi_\sigma(\mathbf{r})|\Phi_0\rangle = \frac{1}{2}\langle\Phi_0|n(\mathbf{r})|\Phi_0\rangle = n/2$$

Thus, the state $\sqrt{\frac{2}{n}}\Psi_\sigma(\mathbf{r})|\Phi_0\rangle$ is normalized. Therefore, the probability amplitude for the ground state with one particle at $\mathbf{r}$ removed to be found in the ground state with one particle at $\mathbf{r}'$ removed is $g_\sigma(\mathbf{r},\mathbf{r}') = \frac{2}{n}G_\sigma(\mathbf{r},\mathbf{r}')$.

As $\mathbf{r}\to\mathbf{r}'$, $g_\sigma(\mathbf{r},\mathbf{r}')\to 1$. For larger values of $k_F x$, the function $g_\sigma(x)$ displays damped oscillations.

3. *Pair correlation function.*

$$D_{\sigma\sigma'}(\mathbf{r},\mathbf{r}') = \langle\Phi_0|\Psi^\dagger_\sigma(\mathbf{r})\Psi^\dagger_{\sigma'}(\mathbf{r}')\Psi_{\sigma'}(\mathbf{r}')\Psi_\sigma(\mathbf{r})|\Phi_0\rangle$$

Expanding

$$\Psi_\sigma(\mathbf{r}) = \frac{1}{\sqrt{V}}\sum_{\mathbf{k}} e^{i\mathbf{k}.\mathbf{r}}c_{\mathbf{k}\sigma}, \quad \Psi^\dagger_\sigma(\mathbf{r}) = \frac{1}{\sqrt{V}}\sum_{\mathbf{k}} e^{-i\mathbf{k}.\mathbf{r}}c^\dagger_{\mathbf{k}\sigma},$$

we obtain

$$\begin{aligned} D_{\sigma\sigma'}(\mathbf{r},\mathbf{r}') &= \frac{1}{V^2}\sum_{\mathbf{k}_1\mathbf{k}_2}\sum_{\mathbf{k}_3\mathbf{k}_4} e^{i\mathbf{k}_1.\mathbf{r}}e^{i\mathbf{k}_2.\mathbf{r}'}e^{-i\mathbf{k}_3.\mathbf{r}'}e^{-i\mathbf{k}_4.\mathbf{r}}\langle\Phi_0|c^\dagger_{\mathbf{k}_4\sigma}c^\dagger_{\mathbf{k}_3\sigma'}c_{\mathbf{k}_2\sigma'}c_{\mathbf{k}_1\sigma}|\Phi_0\rangle \\ &= \frac{1}{V^2}\sum_{\mathbf{k}_1\mathbf{k}_2}\sum_{\mathbf{k}_3\mathbf{k}_4} e^{i(\mathbf{k}_1-\mathbf{k}_4).\mathbf{r}}e^{i(\mathbf{k}_2-\mathbf{k}_3).\mathbf{r}'}\langle\Phi_0|c^\dagger_{\mathbf{k}_4\sigma}c^\dagger_{\mathbf{k}_3\sigma'}c_{\mathbf{k}_2\sigma'}c_{\mathbf{k}_1\sigma}|\Phi_0\rangle \end{aligned}$$

(i) Consider first the case $\sigma\neq\sigma'$. For the matrix element to be nonzero, we must have $\mathbf{k}_4=\mathbf{k}_1$ and $\mathbf{k}_3=\mathbf{k}_2$. Thus

$$D_{\sigma\sigma'}(\mathbf{r},\mathbf{r}') = \frac{1}{V^2}\sum_{\mathbf{k}\mathbf{k}'}\langle\Phi_0|c^\dagger_{\mathbf{k}\sigma}c^\dagger_{\mathbf{k}'\sigma'}c_{\mathbf{k}'\sigma'}c_{\mathbf{k}\sigma}|\Phi_0\rangle$$

Since $\sigma\neq\sigma'$, we have $c_{\mathbf{k}'\sigma'}c_{\mathbf{k}\sigma} = -c_{\mathbf{k}\sigma}c_{\mathbf{k}'\sigma'}$ and $c^\dagger_{\mathbf{k}'\sigma'}c_{\mathbf{k}\sigma} = -c_{\mathbf{k}\sigma}c^\dagger_{\mathbf{k}'\sigma'}$. Therefore

$$\begin{aligned} D_{\sigma\sigma'}(\mathbf{r},\mathbf{r}') &= \frac{1}{V^2}\sum_{\mathbf{k}\mathbf{k}'}\langle\Phi_0|n_{\mathbf{k}\sigma}n_{\mathbf{k}'\sigma'}|\Phi_0\rangle = \frac{1}{V^2}N_\sigma N_{\sigma'} = \frac{1}{V^2}\frac{N}{2}\frac{N}{2} \\ &= (n/2)^2 \end{aligned}$$

(ii) Next, consider the case $\sigma=\sigma'$. For $D_{\sigma\sigma'}(\mathbf{r},\mathbf{r}')$ to be nonzero, either ($\mathbf{k}_4=\mathbf{k}_1$ and $\mathbf{k}_3=\mathbf{k}_2$) or ($\mathbf{k}_3=\mathbf{k}_1$ and $\mathbf{k}_4=\mathbf{k}_2$). Thus

$$D_{\sigma\sigma'}(\mathbf{r},\mathbf{r}') = \frac{1}{V^2}\sum_{\mathbf{k}\mathbf{k}'}\langle\Phi_0|c^\dagger_{\mathbf{k}\sigma}c^\dagger_{\mathbf{k}'\sigma}c_{\mathbf{k}'\sigma}c_{\mathbf{k}\sigma}|\Phi_0\rangle + \frac{1}{V^2}\sum_{\mathbf{k}\mathbf{k}'}e^{i(\mathbf{k}-\mathbf{k}').(\mathbf{r}-\mathbf{r}')}\langle\Phi_0|c^\dagger_{\mathbf{k}'\sigma}c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}'\sigma}c_{\mathbf{k}\sigma}|\Phi_0\rangle$$

Consider the first term,

$$\begin{aligned}\langle\Phi_0|c^\dagger_{\mathbf{k}\sigma}c^\dagger_{\mathbf{k}'\sigma}c_{\mathbf{k}'\sigma}c_{\mathbf{k}\sigma}|\Phi_0\rangle &= -\langle\Phi_0|c^\dagger_{\mathbf{k}\sigma}c^\dagger_{\mathbf{k}'\sigma}c_{\mathbf{k}\sigma}c_{\mathbf{k}'\sigma}|\Phi_0\rangle \\ &= -\delta_{\mathbf{k}\mathbf{k}'}\langle\Phi_0|c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}'\sigma}|\Phi_0\rangle + \langle\Phi_0|c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}c^\dagger_{\mathbf{k}'\sigma}c_{\mathbf{k}'\sigma}|\Phi_0\rangle \\ &= -\delta_{\mathbf{k}\mathbf{k}'}\langle\Phi_0|n_{\mathbf{k}\sigma}|\Phi_0\rangle + \langle\Phi_0|n_{\mathbf{k}\sigma}n_{\mathbf{k}'\sigma}|\Phi_0\rangle\end{aligned}$$

Now consider the second term

$$\begin{aligned}\langle\Phi_0|c^\dagger_{\mathbf{k}'\sigma}c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}'\sigma}c_{\mathbf{k}\sigma}|\Phi_0\rangle &= \delta_{\mathbf{k}\mathbf{k}'}\langle\Phi_0|c^\dagger_{\mathbf{k}'\sigma}c_{\mathbf{k}\sigma}|\Phi_0\rangle - \langle\Phi_0|c^\dagger_{\mathbf{k}'\sigma}c_{\mathbf{k}'\sigma}c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}|\Phi_0\rangle \\ &= \delta_{\mathbf{k}\mathbf{k}'}\langle\Phi_0|n_{\mathbf{k}\sigma}|\Phi_0\rangle - \langle\Phi_0|n_{\mathbf{k}'\sigma}n_{\mathbf{k}\sigma}|\Phi_0\rangle\end{aligned}$$

Hence,

$$\begin{aligned}D_{\sigma\sigma}(\mathbf{r},\mathbf{r}') &= \frac{1}{V^2}\sum_{\mathbf{k}\mathbf{k}'}[1-e^{i(\mathbf{k}-\mathbf{k}').\mathbf{x}}]\langle\Phi_0|n_{\mathbf{k}'\sigma}n_{\mathbf{k}\sigma}|\Phi_0\rangle \\ &= \frac{1}{V^2}\sum_{\mathbf{k}\mathbf{k}'}[1-e^{i(\mathbf{k}-\mathbf{k}').\mathbf{x}}]n_{\mathbf{k}'\sigma}n_{\mathbf{k}\sigma} \\ &= \frac{1}{V^2}\frac{N}{2}\frac{N}{2} - \frac{1}{V}\sum_{\mathbf{k}}e^{i\mathbf{k}.\mathbf{x}}n_{\mathbf{k}\sigma}\frac{1}{V}\sum_{\mathbf{k}'}e^{-i\mathbf{k}'.\mathbf{x}}n_{\mathbf{k}'\sigma} \\ &= (n/2)^2 - [G_\sigma(\mathbf{x})]^2\end{aligned}$$

where

$$\begin{aligned}G_\sigma(\mathbf{x}) &= \frac{1}{2\pi^2x^3}[sin(k_Fx)-(k_Fx)cos(k_Fx)] \\ &= \frac{3n}{2}\left[\frac{sin(k_Fx)-(k_Fx)cos(k_Fx)}{(k_Fx)^3}\right]\end{aligned}$$

This was evaluated in the previous problem. Thus

$$\begin{aligned}D_{\sigma\sigma}(\mathbf{x}) &= (n/2)^2\left\{1-9\left[\frac{sin(k_Fx)-(k_Fx)cos(k_Fx)}{(k_Fx)^3}\right]^2\right\} \\ &\equiv (n/2)^2 g(k_Fx)\end{aligned}$$

The function $g(k_Fx)$ is zero at $k_Fx=0$, rises to 1 for a value of k_Fx between π and 2π, and then undergoes damped oscillations.

To interpret this result, consider the system of N electrons in the ground state $|\Phi_0\rangle$. Suppose an electron with spin σ is removed from position $\mathbf{r}$ to yield the $(N-1)$-particle state $\sqrt{2/n}\Psi_\sigma(\mathbf{r})|\Phi_0\rangle$. In this state the density distribution of electrons with spin σ' is

$$\frac{2}{n}\langle\Phi_0|\Psi^\dagger_\sigma(\mathbf{r})n_{\sigma'}(\mathbf{r}')\Psi_\sigma(\mathbf{r})|\Phi_0\rangle = (2/n)D_{\sigma\sigma'}(\mathbf{r},\mathbf{r}')$$

What we found was that

$$(2/n)D_{\sigma\sigma'}(\mathbf{r},\mathbf{r}') = \begin{cases} n/2 & \sigma \neq \sigma' \\ (n/2)g_{\sigma\sigma}(k_F x) & \sigma = \sigma' \end{cases}$$

For electrons with spin $\sigma' \neq \sigma$, the removal of an electron at $\mathbf{r}$ with spin σ has no effect; the density is still $n/2$. However, for electrons with spin σ, the density is greatly reduced for $|\mathbf{r}-\mathbf{r}'| \lesssim k_F^{-1}$. In other words, it is unlikely to find two electrons with the same spin at a separation $\lesssim k_F^{-1}$. This is known as an exchange hole, or correlation hole, associated with an electron of a given spin. Thus, electrons with the same spin tend to stay away from each other, which is purely a consequence of the antisymmetry of the wave function, not the result of any genuine repulsion between the electrons.

To elaborate this point further, consider

$$\begin{aligned} D_{\sigma\sigma'}(\mathbf{r}-\mathbf{r}') &= \langle\Phi_0|\Psi^\dagger_\sigma(\mathbf{r})\Psi^\dagger_{\sigma'}(\mathbf{r}')\Psi_{\sigma'}(\mathbf{r}')\Psi_\sigma(\mathbf{r})|\Phi_0\rangle \\ &= -\langle\Phi_0|\Psi^\dagger_\sigma(\mathbf{r})\Psi^\dagger_{\sigma'}(\mathbf{r}')\Psi_\sigma(\mathbf{r})\Psi_{\sigma'}(\mathbf{r}')|\Phi_0\rangle \end{aligned}$$

Replacing $\Psi^\dagger_{\sigma'}(\mathbf{r}')\Psi_\sigma(\mathbf{r})$ with $\delta_{\sigma\sigma'}\delta(\mathbf{r}-\mathbf{r}') - \Psi_\sigma(\mathbf{r})\Psi^\dagger_{\sigma'}(\mathbf{r}')$, we obtain

$$\begin{aligned} D_{\sigma\sigma'}(\mathbf{r}-\mathbf{r}') &= \langle\Phi_0|\Psi^\dagger_\sigma(\mathbf{r})\Psi_\sigma(\mathbf{r})\Psi^\dagger_{\sigma'}(\mathbf{r}')\Psi_{\sigma'}(\mathbf{r}')|\Phi_0\rangle - \delta_{\sigma\sigma'}\delta(\mathbf{r}-\mathbf{r}')\langle\Phi_0|\Psi^\dagger_\sigma(\mathbf{r})\Psi_\sigma(\mathbf{r})|\Phi_0\rangle \\ &= \langle\Phi_0|n_\sigma(\mathbf{r})n_{\sigma'}(\mathbf{r}')|\Phi_0\rangle - \delta_{\sigma\sigma'}\delta(\mathbf{r}-\mathbf{r}')\langle\Phi_0|n_\sigma(\mathbf{r})|\Phi_0\rangle \\ &= \sum_{i,j}\langle\Phi_0|\delta(\mathbf{r}-\mathbf{r}_{i,\sigma})\delta(\mathbf{r}'-\mathbf{r}_{j,\sigma'})|\Phi_0\rangle - \delta_{\sigma\sigma'}\delta(\mathbf{r}-\mathbf{r}')n/2 \\ &= \sum_{i,j}\langle\Phi_0|\delta(\mathbf{r}-\mathbf{r}'+\mathbf{r}'-\mathbf{r}_{i,\sigma})\delta(\mathbf{r}'-\mathbf{r}_{j,\sigma'})|\Phi_0\rangle - \delta_{\sigma\sigma'}\delta(\mathbf{r}-\mathbf{r}')n/2 \end{aligned}$$

Let $\mathbf{x} = \mathbf{r}-\mathbf{r}'$. Then

$$D_{\sigma\sigma'}(\mathbf{x}) = \sum_{i,j}\langle\Phi_0|\delta(\mathbf{x}-\mathbf{r}_{i\sigma}+\mathbf{r}_{j,\sigma'})\delta(\mathbf{r}'-\mathbf{r}_{j,\sigma'})|\Phi_0\rangle - \delta_{\sigma\sigma'}\delta(\mathbf{x})n/2$$

We have already seen earlier that $D_{\sigma\sigma'}$ depends only on $\mathbf{x}$ and not on $\mathbf{r}$ and $\mathbf{r}'$ separately. Since $D_{\sigma\sigma'}$ does not depend on $\mathbf{r}'$, we integrate over $\mathbf{r}'$ ($\frac{1}{V}\int d^3r' = 1$),

$$D_{\sigma\sigma'}(\mathbf{x}) = \frac{1}{V}\sum_{i,j}\langle\Phi_0|\delta[\mathbf{x}-(\mathbf{r}_{i\sigma}-\mathbf{r}_{j,\sigma'})]|\Phi_0\rangle - \delta_{\sigma\sigma'}\delta(\mathbf{x})n/2$$

Let us consider now the two cases: $\sigma \neq \sigma'$ and $\sigma = \sigma'$.

(i) $\sigma \neq \sigma'$,

$$D_{\sigma\sigma'}(\mathbf{x}) = \frac{1}{V}\sum_{i,j}\langle\Phi_0|\delta[\mathbf{x}-(\mathbf{r}_{i\sigma}-\mathbf{r}_{j,\sigma'})]|\Phi_0\rangle$$

We have seen that in this case $D_{\sigma\sigma'} = (n/2)^2$. The above expression for $D_{\sigma\sigma'}(\mathbf{x})$ can be interpreted as being proportional to the probability density that two electrons with opposite spins are separated in space by $\mathbf{x}$. Since $D_{\sigma\sigma'} = (n/2)^2$, this probability density is independent of $\mathbf{x}$.

(ii) $\sigma = \sigma'$,

$$D_{\sigma\sigma}(\mathbf{x}) = \frac{1}{V}\sum_{i,j}\langle\Phi_0|\delta[\mathbf{x} - (\mathbf{r}_{i\sigma} - \mathbf{r}_{j,\sigma})]|\Phi_0\rangle - \frac{n}{2}\delta(\mathbf{x})$$

The last term may be rewritten as

$$\begin{aligned}\frac{n}{2}\delta(\mathbf{x}) = \frac{N}{2V}\delta(\mathbf{x}) &= \frac{1}{V}\sum_i \delta(\mathbf{x} - \mathbf{r}_{i\sigma} + \mathbf{r}_{i\sigma}) \\ &= \frac{1}{V}\sum_i\langle\Phi_0|\delta(\mathbf{x} - \mathbf{r}_{i\sigma} + \mathbf{r}_{i\sigma})|\Phi_0\rangle\end{aligned}$$

Hence

$$D_{\sigma\sigma}(\mathbf{x}) = \frac{1}{V}\sum_{i\neq j}\langle\Phi_0|\delta[\mathbf{x} - (\mathbf{r}_{i\sigma} - \mathbf{r}_{j,\sigma})]|\Phi_0\rangle$$

This shows that $D_{\sigma\sigma}(\mathbf{x})$ is proportional to the probability density that two electrons with the same spin orientation are separated by $\mathbf{x}$. We have seen that in this case $D_{\sigma\sigma}(\mathbf{x})$ is very small for $x \lesssim k_F^{-1}$. Thus, two electrons with the same spin orientation are unlikely to be very close to each other.

4. *Coulomb interaction in 2D.*

$$\begin{aligned}v_{\mathbf{q}} &= e^2\int \frac{1}{r}e^{-i\mathbf{q}.\mathbf{r}}d^3r = e^2\int_0^\infty dr\int_0^{2\pi} d\theta e^{-iqr cos\theta} \\ &= 2\pi e^2\int_0^\infty J_0(qr)dr = \frac{2\pi e^2}{q}\int_0^\infty J_0(x)dx \\ &= 2\pi e^2/q\end{aligned}$$

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Notes on Bessel's function:

Consider the generating function

$$f(x,t) = exp\left[\frac{x}{2}\left(t - \frac{1}{t}\right)\right]$$

Bessel's functions of the first jind, $J_n(x)$, are defined using this generating function as follows:

$$f(x,t) = \sum_{n=-\infty}^{\infty} J_n(x)t^n$$

It is clear that $J_n(x)$ is a real function of x. It can be shown that

$$J_{-n}(x) = (-1)^n J_n(x)$$

To obtain an integral representation of $J_0(x)$, let $t = e^{-i\theta}$. Then

$$\frac{x}{2}\left(t - \frac{1}{t}\right) = \frac{x}{2}(e^{-i\theta} - e^{i\theta}) = -ix\, sin\theta$$

Thus,

$$\begin{aligned}
e^{-ix\,sin\theta} &= J_0(x) + J_1(x)e^{-i\theta} + J_{-1}(x)e^{i\theta} + J_2(x)e^{-2i\theta} + J_{-2}(x)e^{2i\theta} + \cdots \\
&= J_0(x) + J_1(x)[e^{-i\theta} - e^{i\theta}] + J_2(x)[e^{-2i\theta} + e^{2i\theta}] + J_3(x)[e^{-3i\theta} - e^{3i\theta}] + \cdots \\
&= J_0(x) - 2i[J_1(x)sin\theta + J_3(x)sin3\theta + \cdots] + 2[J_2(x)cos2\theta + J_4(x)cos4\theta + \cdots]
\end{aligned}$$

Integrating over θ from 0 to 2π, we obtain

$$2\pi J_0(x) = \int_0^{2\pi} e^{-ix\,sin\theta} d\theta$$

Hence,

$$J_0(x) = \frac{1}{2\pi}\int_0^{2\pi} e^{-ix\,sin\theta} d\theta$$

Since

$$e^{-ix\,sin\theta} = \sum_n \frac{(-ix)^2}{n!} sin^n\theta$$

and

$$\int_0^{2\pi} sin^n\theta\, d\theta = \int_0^{2\pi} cos^n\theta\, d\theta$$

it follows that

$$J_0(x) = \frac{1}{2\pi}\int_0^{2\pi} e^{-ix\,cos\theta} d\theta$$

We used this result to obtain $v_{\mathbf{q}}$. Since $J_0(x)$ is real, we also have

$$J_0(x) = \frac{1}{2\pi}\int_0^{2\pi} e^{ix\,cos\theta} d\theta$$

The other result we used was that $\int_0^\infty J_0(x)dx = 1$. To prove this, consider

$$\int_0^\infty J_0(x)dx = \frac{1}{2\pi}\int_0^{2\pi} d\theta \int_0^\infty dx\, e^{ix\,cos\theta}$$

The integrand is oscillatory at ∞. To do the integral, we introduce a damping factor η,

$$\int_0^\infty dx\, e^{ix\,cos\theta} = \lim_{\eta\to 0^+}\int_0^\infty dx\, e^{ix\,(cos\theta + i\eta)} = \lim_{\eta\to 0^+}\frac{i}{cos\theta + i\eta}$$

Thus

$$I \equiv \int_0^\infty J_0(x)dx = \frac{i}{2\pi}\lim_{\eta\to 0^+}\int_0^{2\pi}\frac{d\theta}{cos\theta + i\eta}$$

Let $z = e^{i\theta}$, then $dz = iz\,d\theta \Rightarrow d\theta = dz/(iz)$. We also have $cos\theta = (z + 1/z)/2$. Therefore,

$$I = \frac{1}{\pi}\int_C \frac{dz}{z^2 + 2i\eta z + 1}$$

where the integration is over the unit circle. The poles are at

$$z_1 = -i(\eta + \sqrt{\eta^2+1}), \quad z_2 = -i\eta + i\sqrt{\eta^2+1}$$

The pole at z_2 lies within the unit circle. By the residue theorem,

$$I = \lim_{\eta\to 0^+} \frac{1}{\pi} 2\pi i \lim_{z\to z_2} \frac{1}{z - z_1} = \lim_{\eta\to 0^+} 2i \frac{1}{2i\sqrt{\eta^2+1}} = \lim_{\eta\to 0^+} \frac{1}{\sqrt{\eta^2+1}}$$
$$= 1$$

5. *Exchange energy in 2D.*

As seen in the previous problem, in 2D we have $v_{\mathbf{q}} = 2\pi e^2/q$. The first-order energy shift is

$$\Delta E = \frac{1}{2A} \sum_{\mathbf{q}}{}' \sum_{\mathbf{k}\sigma} \sum_{\mathbf{k}'\sigma'} v_{\mathbf{q}} \langle F | c^\dagger_{\mathbf{k}+\mathbf{q}\sigma} c^\dagger_{\mathbf{k}'-\mathbf{q}\sigma'} c_{\mathbf{k}'\sigma'} c_{\mathbf{k}\sigma} | F \rangle$$

The prime on the summation indicates that the term $\mathbf{q} = \mathbf{0}$ is excluded. Since $\mathbf{q} \neq \mathbf{0}$, it follows that $c^\dagger_{\mathbf{k}'-\mathbf{q}\sigma'} c_{\mathbf{k}'\sigma'} = -c_{\mathbf{k}'\sigma'} c^\dagger_{\mathbf{k}'-\mathbf{q}\sigma'}$. Hence,

$$\Delta E = -\frac{1}{2A} \sum_{\mathbf{q}}{}' \sum_{\mathbf{k}\sigma} \sum_{\mathbf{k}'\sigma'} \frac{2\pi e^2}{q} \langle F | c^\dagger_{\mathbf{k}+\mathbf{q}\sigma} c_{\mathbf{k}'\sigma'} c^\dagger_{\mathbf{k}'-\mathbf{q}\sigma'} c_{\mathbf{k}\sigma} | F \rangle$$

The exchange term is obtained for the case $\mathbf{k}' = \mathbf{k} + \mathbf{q}$, $\sigma = \sigma'$. The exchange contribution is thus given by

$$\Delta E_x = -\frac{\pi e^2}{A} \sum_{\mathbf{q}}{}' \sum_{\mathbf{k}\sigma} \frac{1}{q} \langle F | c^\dagger_{\mathbf{k}+\mathbf{q}\sigma} c_{\mathbf{k}+\mathbf{q}\sigma} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} | F \rangle$$
$$= -\frac{2\pi e^2}{A} \sum_{\mathbf{kq}}{}' \frac{1}{q} \theta(k_F - k)\theta(k_F - |\mathbf{k}+\mathbf{q}|)$$

Replacing $\sum_{\mathbf{k}}$ by $(A/(2\pi)^2) \int d^2k$, we obtain

$$\Delta E_x = -\frac{e^2}{2\pi} \sum_{\mathbf{q}}{}' \frac{1}{q} \int d^2k \theta(k_F - k)\theta(k_F - |\mathbf{k}+\mathbf{q}|)$$

The integral over d^2k is the area $A'(\mathbf{q})$ of the region of intersection of two Fermi circles, one centered at $\mathbf{k} = \mathbf{0}$ and another centered at $\mathbf{k} = -\mathbf{q}$; thus,

$$\Delta E_x = -\frac{e^2}{2\pi} \sum_{\mathbf{q}} \frac{1}{q} A'(\mathbf{q})$$

where

$$A'(\mathbf{q}) = 2\left[K_F^2 cos^{-1}(q/2k_F) - (q/2)\sqrt{k_F^2 - d^2/4}\right]$$

Replacing the summation over **q** by integration, we obtain

$$\Delta E_x = \frac{e^2 A}{4\pi^2} \int_0^{2k_F} A'(q)dq$$

Define $x = q/2k_F$. Then

$$\Delta E_x = -\frac{e^2 A k_F^3}{\pi^2} \int_0^1 [cos^{-1}x - x\sqrt{1-x^2}]dx = -\frac{e^2 A k_F^3}{\pi^2}(I_1 - I_2)$$

where

$$I_1 = \int_0^1 cos^{-1}x dx\,, \quad I_2 = \int_0^1 x\sqrt{1-x^2}dx$$

I_1 is evaluated by parts $(u = cos^{-1}x,\ dv = dx)$ and I_2 is elementary. We find that $I_1 = 1,\ I_2 = 1/3$. Hence,

$$\Delta E_x = -\frac{2e^2 A k_F^3}{3\pi^2} = -\frac{2e^2 A k_F^2}{3\pi^2} k_F = -\frac{2e^2 A 2\pi (N/A)}{3\pi^2} k_F = -\frac{4Ne^2}{3\pi} k_F$$

$$\Longrightarrow \frac{\Delta E_x}{N} = -\frac{4e^2}{3\pi} k_F$$

Chapter 5

A Brief review of statistical mechanics

1. *Stirling's formula.*

$$N! = \int_0^\infty e^{-t} t^N dt$$

Let $t = N + \sqrt{N}\,x = N(1 + x/\sqrt{N})$, then

$$t^N = N^N \left(1 + \frac{x}{\sqrt{N}}\right)^N, \quad e^{-t} = e^{-N} e^{-\sqrt{N}\,x}, \quad dt = \sqrt{N}\,dx$$

Thus,

$$N! = \sqrt{N}\,N^N e^{-N} \int_{-\sqrt{N}}^\infty e^{-\sqrt{N}\,x} \left(1 + \frac{x}{\sqrt{N}}\right)^N dx$$

The integrand $f(x)$ is maximum at $x = 0$ ($f(0) = 1$) and falls off to zero on both sides of the maximum (it is easy to check that the derivative of $f(x)$ vanishes at $x = 0$).

Let us expand $ln\,f(x) = ln \left[e^{-\sqrt{N}\,x}\left(1 + \frac{x}{\sqrt{N}}\right)^N\right] = -\sqrt{N}\,x + N\,ln(1 + x/\sqrt{N})$ about $x = 0$,

$$ln\,f(x) = ln\,f(0) + \frac{\partial}{\partial x} ln\,f(x)\Big|_0 x + \frac{1}{2!}\frac{\partial^2}{\partial x^2} ln\,f(x)\Big|_0 x^2 + \frac{1}{3!}\frac{\partial^3}{\partial x^3} ln\,f(x)\Big|_0 x^3 + \cdots$$

Noting that

$$\frac{\partial}{\partial x} ln\,f(x) = -\sqrt{N} + \frac{\sqrt{N}}{1 + x/\sqrt{N}} = \sqrt{N}\left[\frac{-x/\sqrt{N}}{1 + x/\sqrt{N}}\right] = \frac{-x/}{1 + x/\sqrt{N}}$$

$$\frac{\partial^2}{\partial x^2} ln\,f(x) = \frac{\partial}{\partial x}\left[\frac{-x}{1 + x/\sqrt{N}}\right] = -\left(1 + \frac{x}{\sqrt{N}}\right)^{-2}$$

$$\frac{\partial^3}{\partial x^3} ln\,f(x) = \frac{2}{\sqrt{N}}\left(1 + \frac{x}{\sqrt{N}}\right)^{-3}$$

We find

$$ln f(x) = -\frac{x^2}{2} + \frac{x^3}{3\sqrt{N}} + \cdots$$
$$exp[ln f(x)] = exp\left[-\frac{x^2}{2} + \frac{x^3}{3\sqrt{N}} + \cdots\right]$$

Hence,

$$N! \simeq \sqrt{N} N^N e^{-N} \int_{-\sqrt{N}}^{\infty} e^{-x^2/2} dx$$

For $x = -\sqrt{N}$, $e^{-x^2/2} = e^{-N/2}$ is exceedingly small and the limit may be safely pushed to $-\infty$,

$$N! \simeq \sqrt{N} N^N e^{-N} \int_{-\infty}^{\infty} e^{-x^2/2} dx = \sqrt{2\pi N}\, N^N e^{-N}$$

Therefore,

$$ln N! \simeq N ln N - N + \frac{1}{2} ln(2\pi N)$$

For $N >> 1$, the last term is negligible compared to the first two; hence

$$ln N! \simeq N ln N - N$$

2. *Vacancies and interstitials in graphene.*

(a) Since there are M vacancies and a total of N lattice sites, the number of ways of choosing the vacancies is the number of ways of choosing M objects from among N objects; this is given by

$$\Omega_v = \frac{N!}{M!(N-M)!}$$

The removed atoms are placed at the centers of hexagons. A hexagon has 6 atoms, bet each atom is shared by 3 hexagons; hence there are two atoms per hexagon. Since there is a total of N atoms, the total number of interstitial sites (hexagon centers) is $N/2$. Thus, we have M atoms that are to be distributed among $N/2$ sites; the number of ways to do that is

$$\Omega_i = \frac{(N/2)!}{M!(N/2-M)!}$$

The number of distinct configurations, where each configuration is a graphene crystal with N carbon atoms, M vacancies, and M interstitials, is thus equal to $\Omega = \Omega_v \Omega_i$. The entropy is given by

$$S = k ln \Omega = k ln \Omega_v + k ln \Omega_i$$

Using Stirling's approximation (see problem 5.1): $N >> 1 \Rightarrow ln N! = N ln N - N$, we obtain for the entropy

$$S = k[N ln N - M ln M - (N-M) ln(N-M) + (N/2) ln(N/2) - M ln M - (N/2 - M) ln(N/2 - M)]$$

(b) The temperature T is related to the entropy S through the formula $1/T = \partial S/\partial E$. Since $E = M\varepsilon$, it follows that

$$\frac{1}{T} = \frac{1}{\varepsilon}\frac{\partial S}{\partial M} = \frac{k}{\varepsilon}[ln(N-M) + ln(N/2 - M) - 2ln M]$$
$$\Longrightarrow e^{\varepsilon/kT} = (N-M)(N/2-M)/M^2$$

Defining $x = M/N = E/(N\varepsilon)$, the above equation reduces to

$$2(e^{\varepsilon/kT} - 1)x^2 + 3x - 1 = 0,$$

which is a quadratic equation in x, whose solution (x is positive) is

$$x = \frac{-3 + \sqrt{8e^{\varepsilon/kT} + 1}}{4(e^{\varepsilon/kT} - 1)}$$

In the low-temperature and high-temperature limits, the above expression reduces to

$$E = N\varepsilon \begin{cases} (1/2)^{1/2} e^{-\varepsilon/2kT} & kT << \varepsilon \\ 1/3 & kT >> \varepsilon \end{cases}$$

3. *Magnetic susceptibility*

(a) One atom is the small system and the rest of the crystal is the heat reservoir. There are two states with energies $-\mu B$ and $+\mu B$. The partition function of the system is

$$Z = e^{-\mu B/kT} + e^{\mu B/kT}$$

The probability that the magnetic moment points in the direction of $\mathbf{B}$ is $P_1 = e^{\mu B/kT}/Z$, while the probability that in points in the direction opposite to $\mathbf{B}$ is $P_2 = e^{-\mu B/kT}/Z$. The average value of μ is thus given by

$$\bar{\mu} = P_1\mu + P_2(-\mu) = \mu(P_1 - P_2) = \mu\left(\frac{e^{\mu B/kT} - e^{-\mu B/kT}}{e^{\mu B/kT} + e^{-\mu B/kT}}\right)$$
$$= \mu\, tanh(\mu B/kT)$$

Thus, the magnetization is

$$M = n\mu\, tanh(\mu B/kT)$$

(b) For $x = \mu B/kT << 1$,

$$M \simeq n\mu\left[\frac{1 + x - 1 + x}{1 + x + 1 - x}\right] = n\mu x = \frac{n\mu^2 B}{kT}$$
$$\Longrightarrow \chi = \frac{\partial M}{\partial B} = \frac{n\mu^2}{kT}$$

4. *Entropy.*

   The free energy $F = E - TS$ is given by $-kT\,lnZ$. Hence $TS = kT\,lnZ + E$. We thus find (with $\beta = 1/(kT)$)

$$S = k[lnZ + \beta E] = k[lnZ + \beta \sum_n p_n E_n]$$

   The probability for a state with energy E_n to be occupied is p_n,

$$p_n = \frac{e^{-\beta E_n}}{Z} \Rightarrow e^{-\beta E_n} = Zp_n \Rightarrow -\beta E_n = ln(Zp_n) \Rightarrow \beta E_n = -ln(Zp_n)$$

   Therefore,

$$\begin{aligned} S &= k\left[lnZ - \sum_n p_n ln(Zp_n)\right] = k\left[lnZ - \sum_n p_n lnZ - \sum_n p_n ln p_n\right] \\ &= -k\sum_n p_n ln p_n \end{aligned}$$

   In the last step we used $\sum_n p_n = 1$.

5. *Statistical operator.*

   From the definition of the statistical operator.

$$\begin{aligned} &\rho = \sum_i p_i|\psi_i\rangle\langle\psi_i| \\ &\Rightarrow \rho^2 = \sum_{i,j} p_i p_j |\psi_i\rangle\langle\psi_i|\psi_j\rangle\langle\psi_j| = \sum_{i,j} p_i p_j |\psi_i\rangle\delta_{ij}\langle\psi_j| = \sum p_i^2|\psi_i\rangle\langle\psi_i| \end{aligned}$$

   Hence

$$\begin{aligned} Tr[\rho^2] &= \sum_m\sum_i p_i^2\langle\psi_m|\psi_i\rangle\langle\psi_i|\psi_m\rangle = \sum_i p_i^2\sum_m\langle\psi_i|\psi_m\rangle\langle\psi_m|\psi_i\rangle \\ &= \sum_i p_i^2\langle\psi_i|\psi_i\rangle = \sum_i p_i^2 \le 1 \end{aligned}$$

6. *Ising model in one dimension.*

   (a) A state of the system is represented as an N-row $\{s_1\ s_2\ \cdots s_N\}$ where each entry is either $+1$ or -1. The total number of states is 2^N. Summing over the states means summing over $s_1, s_2, \cdots, s_N$ independently. Thus, the partition function is given by

$$\begin{aligned} Z &= \sum_{s_1=-1,+1}\ \sum_{s_2=-1,+1}\cdots\sum_{s_N=-1,+1} e^{-\beta E_{\{s_1\ s_2\cdots s_N\}}} \\ &= \sum_{s_1=-1,+1}\ \sum_{s_2=-1,+1}\cdots\sum_{s_N=-1,+1} e^{\beta J\sum_{i=1}^N s_i s_{i+1} + (1/2)\beta h\sum_{i=1}^N s_i + s_{i+1}} \end{aligned}$$

We note that the mean value of the total magnetization, $\langle M \rangle = \langle \sum_i s_i \rangle$, can be obtained from the partition function. Taking the derivative of the Helmholtz free energy $F = -kT lnZ$ with respect to the applied field, we obtain

$$\begin{aligned}\frac{\partial F}{\partial h} &= -\frac{kT}{Z}\frac{\partial Z}{\partial h} = -\frac{kT}{Z}\frac{\partial}{\partial h}\sum_{s_1}\cdots\sum_{s_N} e^{\beta J\sum_{i=1}^N s_i s_{i+1} + \beta h \sum_{i=1}^N s_i} \\ &= -\frac{1}{Z}\sum_{\{s_1 s_2 \cdots s_N\}} (s_1 + \cdots + s_N) e^{-\beta E_{\{s_1 s_2 \cdots s_N\}}} = -\langle \sum_i s_i \rangle \\ &= -\langle M \rangle\end{aligned}$$

We define a 2x2 matrix T whose matrix elements are

$$\langle s|T|s'\rangle = e^{\beta J s s' + \beta h (s+s')/2}, \quad s, s' = 1, -1$$

T is called a transfer matrix. The equation for the partition function may now be written as

$$\begin{aligned}Z &= \sum_{s_1=-1,+1}\ \sum_{s_2=-1,+1}\cdots\sum_{s_N=-1,+1}\prod_{i=1}^N e^{\beta J s_i s_{i+1} + (1/2)\beta h (s_i + s_{i+1})} \\ &= \sum_{s_1=-1,+1}\ \sum_{s_2=-1,+1}\cdots\sum_{s_N=-1,+1}\prod_{i=1}^N \langle s_i|T|s_{i+1}\rangle \\ &\sum_{s_1=-1,+1}\ \sum_{s_2=-1,+1}\cdots\sum_{s_N=-1,+1} \langle s_1|T|s_2\rangle\langle s_2|T|s_3\rangle\cdots\langle s_N|T|s_{N+1} = s_1\rangle \\ &= \sum_{s_1=-1,+1} \langle s_1|T^N|s_1\rangle = Tr[T^N]\end{aligned}$$

The completeness property of spin states $(|1\rangle\langle 1| + |-1\rangle\langle -1|)$ was used above in the step before the last.

(b) Since T is a real symmetric matrix, it can be diagonalized by an orthogonal transformation: $T = O^T D O$, where the 2x2 matrix O is orthogonal ($O^T = O^{-1}$), O^T is the transpose of O and D is a 2x2 diagonal matrix whose diagonal elements are the eigenvalues of O. It follows that

$$\begin{aligned}Tr[T^N] &= Tr[O^T D O O^T D O \cdots O^T D O] = Tr[O^T D^N O] = Tr[O O^T D^N] \\ &= Tr[D^N]\end{aligned}$$

We have used (i) $OO^T = 1$ (by virtue of O being orthogonal), and (ii) the invariance of the trace under cyclic permutations. The eigenvalues of D are readily found; they are given by

$$\lambda_\pm = e^{\beta J}\left[cosh(\beta h) \pm \sqrt{sinh^2(\beta h) + e^{-4\beta J}}\right]$$

The diagonal elements of D are λ_+ and λ_-. Hence, the diagonal elements of D^N are λ_+^N and λ_-^N, and

$$Tr[T^N] = Tr[D^N] = \lambda_+^N + \lambda_-^N = \lambda_+^N[1 + (\lambda_-/\lambda_+)^N] \xrightarrow{N\to\infty} \lambda_+^N$$

The last step follows because $0 < \lambda_-/\lambda_+ < 1$. The Helmholtz free energy is given by

$$\begin{aligned} F &= -kT\,lnZ = -NkT\,ln\lambda_+ \\ &= -NJ - NkT\,ln\left[cosh(\beta h) + \sqrt{sinh^2(\beta h) + e^{-4\beta J}}\right] \end{aligned}$$

(c) The mean magnetization per one magnetic moment (or spin) is

$$m = -\frac{1}{N}\frac{\partial F}{\partial h} = \frac{sinh(\beta h)}{\sqrt{sinh^2(\beta h) + e^{-4\beta J}}} \xrightarrow{h \to 0} 0$$

Chapter 6

Correlation and Green's functions

1. *Time dependence.*

$$A(t) = e^{i\bar{H}t/\hbar} A e^{-i\bar{H}t/\hbar}$$

$$\langle T\, A(t)\, B(t')\rangle = \theta(t-t')\langle\, A(t)\, B(t')\rangle \pm \theta(t'-t)\langle B(t')\, A(t)\rangle$$

The lower sign $(-)$ refers to the case when A and B are fermion operators, while the upper sign $(+)$ refers to the case when A and B are boson operators.

$$\begin{aligned}\langle\, A(t)\, B(t')\rangle &= \langle e^{i\bar{H}t/\hbar} A e^{-i\bar{H}(t-t')/\hbar} B e^{-i\bar{H}t'/\hbar}\rangle \\ &= Z_G^{-1} Tr\left[e^{-\beta\bar{H}} e^{i\bar{H}t/\hbar} A e^{-i\bar{H}(t-t')/\hbar} B e^{-i\bar{H}t'/\hbar}\right]\end{aligned}$$

Using the invariance of the trace under cyclic permutations, we move $e^{-i\bar{H}t'/\hbar}$ to the far left and then commute it through $e^{-\beta\bar{H}}$,

$$\begin{aligned}\langle\, A(t)\, B(t')\rangle &= Z_G^{-1} Tr\left[e^{-\beta\bar{H}} e^{i\bar{H}(t-t')/\hbar} A e^{-i\bar{H}(t-t')/\hbar} B\right] \\ &= \langle A(t-t')B(0)\rangle\end{aligned}$$

Similarly,

$$\langle B(t')A(t)\rangle = Z_G^{-1} Tr\left[e^{-\beta\bar{H}} e^{i\bar{H}t'/\hbar} B e^{i\bar{H}(t-t')/\hbar} A e^{-i\bar{H}t/\hbar}\right]$$

Commuting $e^{-i\bar{H}t'/\hbar}$ through $e^{-\beta\bar{H}}$, then moving it to the far right, we obtain

$$\begin{aligned}\langle B(t')A(t)\rangle &= Z_G^{-1} Tr\left[e^{-\beta\bar{H}} B e^{i\bar{H}(t-t')/\hbar} A e^{-i\bar{H}(t-t')/\hbar}\right] \\ &= \langle B(0)A(t-t')\rangle\end{aligned}$$

Hence

$$\begin{aligned}\langle T\, A(t)\, B(t')\rangle &= \theta(t-t')\langle A(t-t')B(0)\rangle \pm \theta(t'-t)\langle B(0)A(t-t')\rangle \\ &= \langle T A(t-t')B(0)\rangle\end{aligned}$$

This proves that the correlation function $-i\langle T\, A(t)\, B(t')\rangle$ depends on $t-t'$, not on t and t' separately.

2. *Translational invariance.*

(a)

$$[\Psi_\sigma(\mathbf{r}), \mathbf{P}] = \sum_{\sigma'} \left[\Psi_\sigma(\mathbf{r}), \int \Psi^\dagger_{\sigma'}(\mathbf{r}')(-i\hbar\boldsymbol{\nabla}_{\mathbf{r}'})\Psi_{\sigma'}(\mathbf{r}')d^3r'\right]$$

Note that it is the commutator of $\Psi_\sigma(\mathbf{r})$ (not $\Psi^\dagger_\sigma(\mathbf{r})$ as the problem incorrectly states) with $\mathbf{P}$.

For bosons, using

$$[A, BC] = [A, B]C + B[A, C],$$

we find

$$[\Psi_\sigma(\mathbf{r}), \mathbf{P}] = \sum_{\sigma'} \left[\int [\Psi_\sigma(\mathbf{r}), \Psi^\dagger_{\sigma'}(\mathbf{r}')](-i\hbar\boldsymbol{\nabla}_{\mathbf{r}'})\Psi_{\sigma'}(\mathbf{r}')d^3r' \right.$$
$$\left. + \int \Psi^\dagger_{\sigma'}(\mathbf{r}')[\Psi_\sigma(\mathbf{r}), (-i\hbar\boldsymbol{\nabla}_{\mathbf{r}'})\Psi_{\sigma'}(\mathbf{r}')]d^3r'\right]$$

Noting that

$$[\Psi_\sigma(\mathbf{r}), (-i\hbar\boldsymbol{\nabla}_{\mathbf{r}'})\Psi_{\sigma'}(\mathbf{r}')] = -i\hbar\boldsymbol{\nabla}_{\mathbf{r}'}[\Psi_\sigma(\mathbf{r}), \Psi_{\sigma'}(\mathbf{r}')] = 0$$

and that

$$[\Psi_\sigma(\mathbf{r}), \Psi^\dagger_{\sigma'}(\mathbf{r}')] = \delta_{\sigma\sigma'}\delta(\mathbf{r} - \mathbf{r}')$$

we find

$$\begin{aligned}[\Psi_\sigma(\mathbf{r}), \mathbf{P}] &= \sum_{\sigma'} \delta_{\sigma\sigma'} \int \delta(\mathbf{r} - \mathbf{r}')(-i\hbar\boldsymbol{\nabla}_{\mathbf{r}'})\Psi_{\sigma'}(\mathbf{r}')]d^3r' \\ &= -i\hbar\boldsymbol{\nabla}\Psi_\sigma(\mathbf{r})\end{aligned}$$

This is a differential equation for $\Psi_\sigma(\mathbf{r})$ that is to be solved subject to the condition that at $\mathbf{r} = \mathbf{0}$, $\Psi_\sigma(\mathbf{r}) = \Psi_\sigma(0)$. It is straightforward to check that the solution is

$$\Psi_\sigma(\mathbf{r}) = e^{-i\mathbf{P}.\mathbf{r}/\hbar}\Psi_\sigma(0)e^{i\mathbf{P}.\mathbf{r}/\hbar}$$

Indeed,

$$-i\hbar\boldsymbol{\nabla}\Psi_\sigma(\mathbf{r}) = -\mathbf{P}e^{-i\mathbf{P}.\mathbf{r}/\hbar}\Psi_\sigma(0)e^{i\mathbf{P}.\mathbf{r}/\hbar} + e^{-i\mathbf{P}.\mathbf{r}/\hbar}\Psi_\sigma(0)\mathbf{P}e^{i\mathbf{P}.\mathbf{r}/\hbar}$$

Since $\mathbf{P}$ commutes with $e^{i\mathbf{P}.\mathbf{r}/\hbar}$, the above equation can be written as

$$-i\hbar\boldsymbol{\nabla}\Psi_\sigma(\mathbf{r}) = -\mathbf{P}\Psi_\sigma(\mathbf{r}) + \Psi_\sigma(\mathbf{r})\mathbf{P} = [\Psi_\sigma(\mathbf{r}), \mathbf{P}]$$

(b)

$$\begin{aligned}C &= \langle\Psi(\mathbf{r}\sigma t)\Psi^\dagger(\mathbf{r}'\sigma' t')\rangle \\ &= Z_G^{-1}Tr\left[e^{-\beta\bar{H}}T(\mathbf{r})\Psi(\mathbf{0}\sigma t)T(-\mathbf{r})T(\mathbf{r}')\Psi^\dagger(\mathbf{0}\sigma' t')T(-\mathbf{r}')\right]\end{aligned}$$

where $T(\mathbf{r}) = e^{-i\mathbf{P}.\mathbf{r}/\hbar}$. Moving $T(-\mathbf{r}')$ to the far left and commuting it through $e^{-\beta\bar{H}}$, we obtain

$$\begin{aligned} C &= Z_G^{-1} Tr\left[e^{-\beta\bar{H}} T(\mathbf{r}-\mathbf{r}')\Psi(\mathbf{0}\sigma t)T(-\mathbf{r}+\mathbf{r}')\Psi^\dagger(\mathbf{0}\sigma' t')\right] \\ &= \langle\Psi(\mathbf{r}-\mathbf{r}'\sigma t)\Psi^\dagger(\mathbf{0}\sigma' t')\rangle = C(\mathbf{r}-\mathbf{r}'; \sigma t; \sigma' t') \end{aligned}$$

Since all single-particle Green's functions are linear combinations of $C(\mathbf{r}\sigma t; \mathbf{r}'\sigma' t')$ and $C(\mathbf{r}'\sigma' t'; \mathbf{r}\sigma t)$ with coefficients consisting of $\theta(t-t')$ and $\theta(t'-t)$, it follows that, in a translationally invariant system, all single-particle Green's functions are functions of $\mathbf{r}-\mathbf{r}'$.

3. *Spectral function.*

From Eq. (6.35),

$$A(\mathbf{k}\sigma,\omega) = 2\pi Z_G^{-1}\sum_{nm} e^{-\beta\bar{E}_n}\left|\langle m|c^\dagger_{\mathbf{k}\sigma}|n\rangle\right|^2\left(1\mp e^{-\beta\hbar\omega}\right)\delta\left[\omega-\left(\bar{E}_m-\bar{E}_n\right)/\hbar\right]$$

Thus

$$\begin{aligned} I &= \int_{-\infty}^{\infty} A(\mathbf{k}\sigma,\omega)d\omega \\ &= 2\pi Z_G^{-1}\sum_{nm} e^{-\beta\bar{E}_n}\left|\langle m|c^\dagger_{\mathbf{k}\sigma}|n\rangle\right|^2\left[1\mp e^{-\beta(\bar{E}_m-\bar{E}_n)}\right] \\ &= 2\pi Z_G^{-1}\sum_{nm}\left(e^{-\beta\bar{E}_n}\mp e^{-\beta\bar{E}_m)}\right)\langle m|c^\dagger_{\mathbf{k}\sigma}|n\rangle\langle n|c_{\mathbf{k}\sigma}|m\rangle \\ &= 2\pi Z_G^{-1}\left[\sum_{nm} e^{-\beta\bar{E}_n}\langle n|c_{\mathbf{k}\sigma}|m\rangle\langle m|c^\dagger_{\mathbf{k}\sigma}|n\rangle \mp \sum_{nm} e^{-\beta\bar{E}_m}\langle m|c^\dagger_{\mathbf{k}\sigma}|n\rangle\langle n|c_{\mathbf{k}\sigma}|m\rangle\right] \end{aligned}$$

Using the resulution of identity ($1=\sum_m |m\rangle\langle m|$ or $1=\sum_n |n\rangle\langle n|$), we find

$$I = 2\pi Z_G^{-1}\left[\sum_n e^{-\beta\bar{E}_n}\langle n|c_{\mathbf{k}\sigma}c^\dagger_{\mathbf{k}\sigma}|n\rangle \mp \sum_m e^{-\beta\bar{E}_m}\langle m|c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}|m\rangle\right]$$

Relabeling m in the second sum as n,

$$\begin{aligned} I &= 2\pi Z_G^{-1}\sum_n e^{-\beta\bar{E}_n}\langle n|c_{\mathbf{k}\sigma}c^\dagger_{\mathbf{k}\sigma}\mp c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}|n\rangle = 2\pi Z_G^{-1}\sum_n e^{-\beta\bar{E}_n}\langle n|1|n\rangle \\ &= 2\pi Z_G^{-1}\sum_n e^{-\beta\bar{E}_n} = 2\pi \end{aligned}$$

4. *Advanced Green's function.*

$$\begin{aligned} G^A(\mathbf{k}\sigma,t) &= i\theta(-t)\langle[c_{\mathbf{k}\sigma}(t), c^\dagger_{\mathbf{k}\sigma}(0)]_\mp\rangle \\ &= i\theta(-t)\left[\langle c_{\mathbf{k}\sigma}(t)c^\dagger_{\mathbf{k}\sigma}(0)\rangle \mp \langle c^\dagger_{\mathbf{k}\sigma}(0)c_{\mathbf{k}\sigma}(t)\rangle\right] \end{aligned}$$

Using Eqs. (6.30) and (6.32),

$$\begin{aligned}
\langle c_{\mathbf{k}\sigma}(t)c^{\dagger}_{\mathbf{k}\sigma}(0)\rangle &= -\int_{-\infty}^{\infty} P(\mathbf{k}\sigma,\epsilon)e^{-i\epsilon t}\frac{d\epsilon}{2\pi} \\
\langle c^{\dagger}_{\mathbf{k}\sigma}(0)c_{\mathbf{k}\sigma}(t)\rangle &= -\int_{-\infty}^{\infty} e^{-\beta\hbar\epsilon}P(\mathbf{k}\sigma,\epsilon)e^{-i\epsilon t}\frac{d\epsilon}{2\pi}
\end{aligned}$$

where $P(\mathbf{k}\sigma,\epsilon)$ is given in Eq. (6.31). Therefore,

$$G^A(\mathbf{k}\sigma,t) = -i\theta(-t)\int_{-\infty}^{\infty}(1\mp e^{-\beta\hbar\epsilon})P(\mathbf{k}\sigma,\epsilon)e^{-i\epsilon t}\frac{d\epsilon}{2\pi}$$

The Fourier transform is

$$G^A(\mathbf{k}\sigma,\omega) = \int_{-\infty}^{\infty} e^{i\omega t}G^A(\mathbf{k}\sigma,t)dt$$

Since $G^A(\mathbf{k}\sigma,t)$ vanishes for $t>0$,

$$G^A(\mathbf{k}\sigma,\omega) = -i\int_{-\infty}^{\infty}(1\mp e^{-\beta\hbar\epsilon})P(\mathbf{k}\sigma,\epsilon)\frac{d\epsilon}{2\pi}\int_{-\infty}^{0} e^{i(\omega-\epsilon)t}dt$$

The integral over t is oscillatory at $-\infty$, so we introduce a damping factor,

$$\begin{aligned}
\int_{-\infty}^{0} e^{i(\omega-\epsilon)t}dt = \int_{-\infty}^{0} e^{i(\omega-\epsilon-i0^+)t}dt &= \left.\frac{e^{i(\omega-\epsilon-i0^+)t}}{i(\omega-\epsilon-i0^+)}\right|_{-\infty}^{0} \\
&= \frac{1}{i(\omega-\epsilon-i0^+)}
\end{aligned}$$

Hence

$$G^A(\mathbf{k}\sigma,\omega) = -\int_{-\infty}^{\infty}\frac{(1\mp e^{-\beta\hbar\epsilon})P(\mathbf{k}\sigma,\epsilon)}{\omega-\epsilon-i0^+}\frac{d\epsilon}{2\pi}$$

The spectral density function $A(\mathbf{k}\sigma,\epsilon) = -(1\mp e^{-\beta\hbar\epsilon})P(\mathbf{k}\sigma,\epsilon)$ [see Eq. (6.35)]. Thus

$$G^A(\mathbf{k}\sigma,\omega) = -\int_{-\infty}^{\infty}\frac{A(\mathbf{k}\sigma,\epsilon)}{\omega-\epsilon-i0^+}\frac{d\epsilon}{2\pi}$$

5. *Advanced correlation function.*

The advanced correlation function is defined as

$$C^A_{AB}(t) = i\theta(-t)\langle[A(t),B(0)]_{\mp}\rangle$$

The ensemble average of the commutator was evaluated in Sec. 6.4.3,

$$C^A_{AB}(t) = i\theta(-t)Z_G^{-1}\sum_{nm} e^{i(\bar{E}_n-\bar{E}_m)t/\hbar}\langle n|A|m\rangle\langle m|B|n\rangle\left(e^{-\beta\bar{E}_n}\mp e^{-\beta\bar{E}_m}\right)$$

The Fourier transform is

$$C_{AB}^A(\omega) = \int_{-\infty}^{\infty} e^{i\omega t)} C_{AB}^A(t)dt$$
$$= iZ_G^{-1} \sum_{nm} \langle n|A|m\rangle\langle m|B|n\rangle \left(e^{-\beta \bar{E}_n} \mp e^{-\beta \bar{E}_m}\right) \int_{-\infty}^{0} e^{i[\omega - (\bar{E}_m - \bar{E}_n)/\hbar]t} dt$$

The integral is evaluated as follows:

$$\int_{-\infty}^{0} e^{i[\omega-(\bar{E}_m-\bar{E}_n)/\hbar]t} dt = \lim_{\eta\to 0^+} \int_{-\infty}^{0} e^{i\,[\omega-(\bar{E}_m-\bar{E}_n)/\hbar - i\eta]\,t} dt$$
$$= \lim_{\eta\to 0^+} \frac{1}{i[\omega - (\bar{E}_m - \bar{E}_n)/\hbar - i\eta]}$$

Thus,

$$C_{AB}^A = Z_G^{-1} \sum_{nm} \frac{\langle n|A|m\rangle\langle m|B|n\rangle \left(e^{-\beta \bar{E}_n} \mp e^{-\beta \bar{E}_m}\right)}{\omega - (\bar{E}_m - \bar{E}_n)/\hbar - i0^+}$$

The poles are at $\omega = (\bar{E}_m - \bar{E}_n)/\hbar + i0^+$; they are all above the real axis.

6. *Greater and lesser functions.*

For fermions,

$$iG^>(\mathbf{k}\sigma, t) = \langle c_{\mathbf{k}\sigma}(t) c_{\mathbf{k}\sigma}^\dagger(0)\rangle = C(\mathbf{k}\sigma, t)$$

We have already shown in the text [see Eq. (6.43)] that

$$C(\mathbf{k}\sigma, \omega) = A(\mathbf{k}\sigma, \omega)(1 - f_\omega)$$

As for the lesser function,

$$iG^<(\mathbf{k}\sigma, t) = -\langle c_{\mathbf{k}\sigma}^\dagger(0) c_{\mathbf{k}\sigma}(t)\rangle = \int_{-\infty}^{\infty} e^{-\beta\hbar\epsilon} P(\mathbf{k}\sigma, \epsilon) e^{-i\epsilon t} \frac{d\epsilon}{2\pi}$$

[see Eq. (6.32)]. Therefore,

$$iG^<(\mathbf{k}\sigma, \omega) = \int_{-\infty}^{\infty} e^{i\omega t} iG^<(\mathbf{k}\sigma, t) dt$$
$$= \int_{-\infty}^{\infty} e^{-\beta\hbar\epsilon} P(\mathbf{k}\sigma, \epsilon) \frac{d\epsilon}{2\pi} \int_{-\infty}^{\infty} e^{i(\omega-\epsilon)t} dt$$

Using

$$\int_{-\infty}^{\infty} e^{i(\omega-\epsilon)t} dt = 2\pi\delta(\omega - \epsilon),$$

we find

$$iG^<(\mathbf{k}\sigma, \omega) = \int_{-\infty}^{\infty} e^{-\beta\hbar\epsilon} P(\mathbf{k}\sigma, \epsilon)\delta(\omega - \epsilon) d\epsilon = e^{-\beta\hbar\omega} P(\mathbf{k}\sigma, \omega)$$
$$= \frac{-e^{-\beta\hbar\omega} A(\mathbf{k}\sigma, \omega)}{1 + e^{-\beta\hbar\omega}}$$

In the last step we used the relation between $P(\mathbf{k}\sigma,\omega)$ and $A(\mathbf{k}\sigma,\omega)$ given in Eq. (6.35). Hence

$$iG^{<}(\mathbf{k}\sigma,\omega)=\frac{-A(\mathbf{k}\sigma,\omega)}{e^{\beta\hbar\omega}+1}=-A(\mathbf{k}\sigma,\omega)f_\omega$$

For bosons,

$$iG^{>}(\mathbf{k}\sigma,t)=\langle c_{\mathbf{k}\sigma}(t)c^\dagger_{\mathbf{k}\sigma}(0)\rangle=C(\mathbf{k}\sigma,t)$$

Hence,

$$iG^{>}(\mathbf{k}\sigma,\omega)=A(\mathbf{k}\sigma,\omega)\,(1+n_\omega)$$

[see Eq. (6.43)].

The lesser function, $iG^{<}(\mathbf{k}\sigma,t)=\langle c^\dagger_{\mathbf{k}\sigma}(0)c_{\mathbf{k}\sigma}(t)\rangle$, has the same expression as in the fermions case, except for a minus sign. Thus,

$$iG^{<}(\mathbf{k}\sigma,\omega)=-e^{-\beta\hbar\omega}P(\mathbf{k}\sigma,\omega)$$

Using Eq. (6.35), we find

$$iG^{<}(\mathbf{k}\sigma,\omega)=\frac{e^{-\beta\hbar\omega}A(\mathbf{k}\sigma,\omega)}{1-e^{-\beta\hbar\omega}}=\frac{A(\mathbf{k}\sigma,\omega)}{e^{\beta\hbar\omega}-1}=A(\mathbf{k}\sigma,\omega)n_\omega$$

7. *Causal Green's function.*

The causal, or time-ordered, Green's function is defined as

$$G(\mathbf{k}\sigma,t)=-i\langle T\,c_{\mathbf{k}\sigma}(t)c^\dagger_{\mathbf{k}\sigma}(0)\rangle\,,$$

where T is the time-ordering operator. The above can be written as

$$G(\mathbf{k}\sigma,t)=-i\theta(t)\langle c_{\mathbf{k}\sigma}(t)c^\dagger_{\mathbf{k}\sigma}(0)\rangle\mp\theta(-t)\langle c^\dagger_{\mathbf{k}\sigma}(0)c_{\mathbf{k}\sigma}(t)\rangle$$

Equations (6.30) and (6.33) give

$$\langle c_{\mathbf{k}\sigma}(t)c^\dagger_{\mathbf{k}\sigma}(0)\rangle=-\int_{-\infty}^{\infty}P(\mathbf{k}\sigma,\epsilon)e^{-i\epsilon t}\frac{d\epsilon}{2\pi}\equiv I(t)$$
$$\langle c^\dagger_{\mathbf{k}\sigma}(0)c_{\mathbf{k}\sigma}(t)\rangle=-\int_{-\infty}^{\infty}e^{-\beta\hbar\epsilon}P(\mathbf{k}\sigma,\epsilon)e^{-i\epsilon t}\frac{d\epsilon}{2\pi}\equiv J(t)$$

The Fourier transform of the causal Green's function is thus given by

$$G(\mathbf{k}\sigma,\omega)=\int_{-\infty}^{\infty}e^{i\omega t}G(\mathbf{k}\sigma,t)dt=-i\int_0^\infty I(t)e^{i\omega t}dt\mp i\int_{-\infty}^{0}J(t)e^{i\omega t}dt$$

$$\begin{aligned}\int_0^\infty I(t)e^{i\omega t}dt&=-\int_{-\infty}^{\infty}P(\mathbf{k}\sigma,\epsilon)\frac{d\epsilon}{2\pi}\int_0^\infty e^{i(\omega-\epsilon)t}dt\\&=-i\int_{-\infty}^{\infty}\frac{P(\mathbf{k}\sigma,\epsilon)}{\omega-\epsilon+i0^+}\frac{d\epsilon}{2\pi}\end{aligned}$$

$$\int_{-\infty}^{0} J(t)e^{i\omega t}dt = -\int_{-\infty}^{\infty} e^{-\beta\hbar\epsilon} P(\mathbf{k}\sigma,\epsilon)\frac{d\epsilon}{2\pi}\int_{-\infty}^{0} e^{i(\omega-\epsilon)t}dt$$
$$= i\int_{-\infty}^{\infty} \frac{e^{-\beta\hbar\epsilon}P(\mathbf{k}\sigma,\epsilon)}{\omega-\epsilon-i0^{+}}\,\frac{d\epsilon}{2\pi}$$

Thus,

$$G(\mathbf{k}\sigma,\omega) = -\int_{-\infty}^{\infty} \frac{P(\mathbf{k}\sigma,\epsilon)}{\omega-\epsilon+i0^{+}}\,\frac{d\epsilon}{2\pi} \pm \int_{-\infty}^{\infty} \frac{e^{-\beta\hbar\epsilon}P(\mathbf{k}\sigma,\epsilon)}{\omega-\epsilon-i0^{+}}\,\frac{d\epsilon}{2\pi}$$

We could now replace $P(\mathbf{k}\sigma,\epsilon)$ by its expression in Eq. (6.31)

$$P(\mathbf{k}\sigma,\epsilon) = -2\pi Z_G^{-1}\sum_{nm} e^{-\beta\bar{E}_n}|\langle m|c^{\dagger}_{\mathbf{k}\sigma}|n\rangle|^2\delta\left[\epsilon-\left(\bar{E}_m-\bar{E}_n\right)/\hbar\right]$$

and integrate over ϵ. The delta function makes the integral easy to perform,

$$G(\mathbf{k}\sigma,\omega) = Z_G^{-1}\sum_{nm}\frac{e^{-\beta\bar{E}_n}|\langle m|c^{\dagger}_{\mathbf{k}\sigma}|n\rangle|^2}{\omega-(\bar{E}_m-\bar{E}_n)/\hbar+i0^{+}} \mp Z_G^{-1}\sum_{nm}\frac{e^{-\beta\bar{E}_m}|\langle m|c^{\dagger}_{\mathbf{k}\sigma}|n\rangle|^2}{\omega-(\bar{E}_m-\bar{E}_n)/\hbar-i0^{+}}$$
$$= Z_G^{-1}\sum_{nm}|\langle m|c^{\dagger}_{\mathbf{k}\sigma}|n\rangle|^2\left[\frac{e^{-\beta\bar{E}_n}}{\omega-(\bar{E}_m-\bar{E}_n)/\hbar+i0^{+}} \mp \frac{e^{-\beta\bar{E}_m}}{\omega-(\bar{E}_m-\bar{E}_n)/\hbar-i0^{+}}\right]$$

8. *Relations among Green's functions.*

(a) The retarded correlation function is given in Eq, (6.67), and the advanced correlation function was calculated in problem 5. We can chhose $A = c_{\mathbf{k}\sigma}$ and $B = c^{\dagger}_{\mathbf{k}\sigma}$; then C^R_{AB} and C^A_{AB} become the retarded and advanced single-particle Green's functions. Thus,

$$G^R(\mathbf{k}\sigma,\omega) = Z_G^{-1}\sum_{nm}\frac{|\langle m|c^{\dagger}_{\mathbf{k}\sigma}|n\rangle|^2(e^{-\beta\bar{E}_n}\mp e^{-\beta\bar{E}_m})}{\omega-(\bar{E}_m-\bar{E}_n)/\hbar+i0^{+}}$$

and

$$G^A(\mathbf{k}\sigma,\omega) = Z_G^{-1}\sum_{nm}\frac{|\langle m|c^{\dagger}_{\mathbf{k}\sigma}|n\rangle|^2(e^{-\beta\bar{E}_n}\mp e^{-\beta\bar{E}_m})}{\omega-(\bar{E}_m-\bar{E}_n)/\hbar-i0^{+}}$$

The causal Green's function was evaluated in the previous problem. Using

$$\frac{1}{x\pm i0^{+}} = P(1/x)\mp i\delta(x),$$

we readily obtain

$$Re\,G(\mathbf{k}\sigma,\omega) = Re\,G^R(\mathbf{k}\sigma,\omega) = Re\,G^A(\mathbf{k}\sigma,\omega)$$

and

$$Im\,G^R(\mathbf{k}\sigma,\omega) = -Im\,G^A(\mathbf{k}\sigma,\omega)$$

(b) For fermions,

$$\begin{aligned}
Im\,G^R(\mathbf{k}\sigma,\omega) &= -\pi Z_G^{-1}\sum_{nm}|\langle m|c^\dagger_{\mathbf{k}\sigma}|n\rangle|^2(e^{-\beta\bar{E}_n}+e^{-\beta\bar{E}_m})\delta\left[\omega-(\bar{E}_m-\bar{E}_n)/\hbar\right] \\
&= -\pi Z_G^{-1}\sum_{nm}e^{-\beta\bar{E}_n}|\langle m|c^\dagger_{\mathbf{k}\sigma}|n\rangle|^2(1+e^{-\beta(\bar{E}_m-\bar{E}_n)})\delta\left[\omega-(\bar{E}_m-\bar{E}_n)/\hbar\right] \\
&= -\pi Z_G^{-1}\left(1+e^{-\beta\hbar\omega}\right)\sum_{nm}e^{-\beta\bar{E}_n}|\langle m|c^\dagger_{\mathbf{k}\sigma}|n\rangle|^2\delta\left[\omega-(\bar{E}_m-\bar{E}_n)/\hbar\right]
\end{aligned}$$

In the above, we have used the relation $\delta(x-a)f(x)=\delta(x-a)f(a)$.

$$\begin{aligned}
Im\,G(\mathbf{k}\sigma,\omega) &= -\pi Z_G^{-1}\sum_{nm}e^{-\beta\bar{E}_n}|\langle m|c^\dagger_{\mathbf{k}\sigma}|n\rangle|^2(1-e^{-\beta(\bar{E}_m-\bar{E}_n)})\delta\left[\omega-(\bar{E}_m-\bar{E}_n)/\hbar\right] \\
&= -\pi Z_G^{-1}\left(1-e^{-\beta\hbar\omega}\right)\sum_{nm}e^{-\beta\bar{E}_n}|\langle m|c^\dagger_{\mathbf{k}\sigma}|n\rangle|^2\delta\left[\omega-(\bar{E}_m-\bar{E}_n)/\hbar\right]
\end{aligned}$$

Hence,

$$\begin{aligned}
\frac{Im\,G^R(\mathbf{k}\sigma,\omega)}{Im\,G(\mathbf{k}\sigma,\omega)} &= \frac{1+e^{-\beta\hbar\omega}}{1-e^{-\beta\hbar\omega}} = \frac{e^{\beta\hbar\omega/2}+e^{-\beta\hbar\omega/2}}{e^{\beta\hbar\omega/2}-e^{-\beta\hbar\omega/2}} \\
&= \frac{1}{tanh(\beta\hbar\omega/2)}
\end{aligned}$$

For bosons, the $+$ and $-$ signs in teh above expression are interchanged,

$$\frac{Im\,G^R(\mathbf{k}\sigma,\omega)}{Im\,G(\mathbf{k}\sigma,\omega)} = \frac{1-e^{-\beta\hbar\omega}}{1+e^{-\beta\hbar\omega}} = tanh(\beta\hbar\omega/2)$$

9. *Greater and lesser correlation functions.*

$$iC^<_{AB}(t) = \langle B(0)A(t)\rangle = Z_G^{-1}Tr\left[e^{-\beta\bar{H}}B(0)e^{i\bar{H}t/\hbar}A(0)e^{-i\bar{H}t/\hbar}\right]$$

We first move $e^{-i\bar{H}t/\hbar}$ to the far left, then move $A(0)$ to the far left, then move $e^{i\bar{H}t/\hbar}$ to the far left; we end up with

$$\begin{aligned}
iC^<_{AB}(t) &= Z_G^{-1}Tr\left[e^{i\bar{H}t/\hbar}A(0)e^{-i\bar{H}t/\hbar}e^{-\beta\bar{H}}B(0)\right] \\
&= Z_G^{-1}Tr\left[e^{-\beta\bar{H}}e^{\beta\bar{H}}e^{i\bar{H}t/\hbar}A(0)e^{-i\bar{H}(t-i\beta\hbar)/\hbar}B(0)\right] \\
&= Z_G^{-1}Tr\left[e^{-\beta\bar{H}}e^{i\bar{H}(t-i\beta\hbar)/\hbar}A(0)e^{-i\bar{H}(t-i\beta\hbar)/\hbar}B(0)\right] \\
&= Z_G^{-1}Tr\left[e^{-\beta\bar{H}}A(t-i\beta\hbar)B(0)\right] = \langle A(t-i\beta\hbar)B(0)\rangle \\
&= iC^>_{AB}(t-i\beta\hbar)
\end{aligned}$$

This proves the first part of the question.

Taking the Fourier transform,

$$C^<_{AB}(\omega) = \int_{-\infty}^{\infty} e^{i\omega t} C^<_{AB}(t)dt = \int_{-\infty}^{\infty} e^{i\omega t} C^>_{AB}(t - i\beta\hbar)dt$$

Changing variables: $t \to t' = t - i\beta\hbar$,

$$C^<_{AB}(\omega) = \int_{-\infty}^{\infty} e^{i\omega t'} e^{-\beta\hbar\omega} C^>_{AB}(t')dt' = e^{-\beta\hbar\omega} C^>_{AB}(\omega)$$

We could arrive at the same results by writing the spectral representations of $C^<_{AB}(\omega)$ and $C^>_{AB}(\omega)$.

10. *Susceptibility.*

(a)

$$\hbar\chi_{AB}(t) = -i\theta(t)\langle[A(t), B(0)]\rangle$$

A and B are hermitian operators $\Rightarrow A^\dagger = A,\ B^\dagger = B$. We can write

$$\hbar\chi_{AB}(t) = -i\theta(t)\langle A(t)B(0)\rangle + i\theta(t)\langle B(0)A(t)\rangle$$

Its complex conjugate is

$$\hbar\chi^*_{AB}(t) = i\theta(t)\langle A(t)B(0)\rangle^* - i\theta(t)\langle B(0)A(t)\rangle^*$$

Note that for any operator A,

$$\begin{aligned}\langle A\rangle &= Z_G^{-1} Tr[e^{-\beta\bar{H}}A] = Z_G^{-1}\sum_m \langle m|e^{-\beta\bar{H}}A|m\rangle \\ &= Z_G^{-1}\sum_m e^{-\beta\bar{E}_m}\langle m|A|m\rangle \\ &\Longrightarrow \langle A\rangle^* = Z_G^{-1}\sum_m e^{-\beta\bar{E}_m}\langle m|A|m\rangle^* = Z_G^{-1}\sum_m e^{-\beta\bar{E}_m}\langle m|A^\dagger|m\rangle = \langle A^\dagger\rangle\end{aligned}$$

Hence,

$$\begin{aligned}\hbar\chi^*_{AB}(t) &= i\theta(t)\langle (A(t)B(0))^\dagger\rangle - i\theta(t)\langle (B(0)A(t))^\dagger\rangle \\ &= i\theta(t)\langle B^\dagger(0)A^\dagger(t)\rangle - i\theta(t)\langle A^\dagger(t)B^\dagger(0)\rangle\end{aligned}$$

Since A and B are hermitian,

$$\begin{aligned}\hbar\chi^*_{AB}(t) &= i\theta(t)\langle B(0)A(t)\rangle - i\theta(t)\langle A(t)B(0)\rangle \\ &= -i\theta(t)\langle[A(t), B(0)]\rangle = \hbar\chi_{AB}\end{aligned}$$

Thus, $\chi_{AB}(t)$ is real.

(b)

$$\chi_{AB}(\omega) = \int_{-\infty}^{\infty} e^{i\omega t}\chi_{AB}(t)dt$$

$$\Longrightarrow [\chi_{AB}(\omega)]^* = \int_{-\infty}^{\infty} e^{-i\omega t}[\chi_{AB}(t)]^* dt = \int_{-\infty}^{\infty} e^{-i\omega t}\chi_{AB}(t)dt = \chi_{AB}(-\omega)$$

11. *Kramers-Kronig relations.*

Since there are no poles inside the contour C,

$$I = \int_C \frac{\chi(\omega')d\omega'}{\omega' - \omega} = 0$$

Also

$$I = \int_{-\infty}^{\epsilon} \frac{\chi(\omega')d\omega'}{\omega' - \omega} + \int_{\epsilon}^{\infty} \frac{\chi(\omega')d\omega'}{\omega' - \omega} + \int_{C_1} \frac{\chi(\omega')d\omega'}{\omega' - \omega} + \int_{C_2} \frac{\chi(\omega')d\omega'}{\omega' - \omega}$$

C_2 is the large semicircle at infinity, and the integral over it vanishes by assumption (b). C_1 is the semicircle of radius ϵ, centered on ω. Writing $\omega' - \omega = \epsilon e^{i\theta}$, $d\omega' = i\epsilon e^{i\theta}d\theta = i(\omega' - \omega)d\theta$, we find

$$\int_{C_1} \frac{\chi(\omega')d\omega'}{\omega' - \omega} = i\int_{\pi}^{0} \chi(\omega + \epsilon e^{i\theta})d\theta$$

Taking the limit $\epsilon \to 0$,

$$\int_{C_1} \frac{\chi(\omega')d\omega'}{\omega' - \omega} = i\int_{\pi}^{0} \chi(\omega)d\theta = -i\pi\chi(\omega)$$

We note that

$$\lim_{\epsilon\to 0}\left[\int_{-\infty}^{\epsilon} \frac{\chi(\omega')d\omega'}{\omega' - \omega} + \int_{\epsilon}^{\infty} \frac{\chi(\omega')d\omega'}{\omega' - \omega}\right] = P\int_{-\infty}^{\infty} \frac{\chi(\omega')d\omega'}{\omega' - \omega}$$

Thus, $I = 0$ implies that

$$\chi(\omega) = \frac{1}{i\pi}P\int_{-\infty}^{\infty} \frac{\chi(\omega')d\omega'}{\omega' - \omega}$$

Taking the real part on both sides,

$$Re\,\chi(\omega) = \frac{1}{\pi}P\int_{-\infty}^{\infty} \frac{Im\,\chi(\omega')d\omega'}{\omega' - \omega} = \frac{1}{\pi}P\left[\int_{-\infty}^{0} \frac{Im\,\chi(\omega')d\omega'}{\omega' - \omega} + \int_{0}^{\infty} \frac{Im\,\chi(\omega')d\omega'}{\omega' - \omega}\right]$$

In the integral from $-\infty$ to 0, let $\omega'' = -\omega'$,

$$P\int_{-\infty}^{0} \frac{Im\,\chi(\omega')d\omega'}{\omega' - \omega} = P\int_{\infty}^{0} \frac{Im\,\chi(-\omega'')d\omega''}{\omega'' + \omega} = P\int_{0}^{\infty} \frac{Im\,\chi(\omega')d\omega'}{\omega' + \omega}$$

where we used the fact that $Im\,\chi(\omega)$ is an odd function of ω. Hence,

$$Re\,\chi(\omega) = \frac{1}{\pi}P\int_{0}^{\infty} Im\,\chi(\omega)\left[\frac{1}{\omega' + \omega} + \frac{1}{\omega' - \omega}\right]d\omega' = \frac{2}{\pi}P\int_{)}^{\infty} \frac{\omega' Im\,\chi(\omega')}{\omega'^2 - \omega^2}d\omega'$$

The expression for $Im\,\chi(\omega)$ follows in a similar way.

12. *Polarizability.*

$$C^R_{AB}(t-t') = -i\theta(t-t')\langle[A(t), B(t')]_\mp\rangle$$
$$\chi^0(\mathbf{q},\omega) = \frac{1}{\hbar}D^{R,0}(\mathbf{q},\omega)$$
$$D^{R,0}(\mathbf{q},t-t') = -i\theta(t-t')\frac{1}{V}\langle[n_H(\mathbf{q},t), n_H(-\mathbf{q},t')]\rangle$$

In the first expression, the $+(-)$ sign refers to fermions (bosons). The operator n_H is bosonic, and the subscript indicates that the operator is in the Heisenberg picture. We see that

$$\chi^0(\mathbf{q},\omega) = \frac{1}{\hbar V}C^R_{AB}(\mathbf{q},\omega)$$

if we set $A(t) = n_H(\mathbf{q},t)$ and $B(t') = n_H(-\mathbf{q},t')$. Thus

$$\chi^0(\mathbf{q},\omega) = \frac{1}{\hbar V}C^R_{n_\mathbf{q}n_{-\mathbf{q}}}(\mathbf{q},\omega)$$

where

$$n_\mathbf{q} = \sum_{\mathbf{k}\sigma} c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}+\mathbf{q}}\sigma$$

Equation (6.47) in the text now becomes

$$C^R_{n_\mathbf{q}n_{-\mathbf{q}}}(\mathbf{q},\omega) = Z_G^{-1}\sum_{nm}\frac{\langle n|n_\mathbf{q}|m\rangle\langle m|n_{-\mathbf{q}}|n\rangle(e^{-\beta\bar{E}_n} - e^{-\beta\bar{E}_m})}{\omega - (\bar{E}_m - \bar{E}_n)/\hbar + i0^+}$$

Note that

$$n_{-\mathbf{q}} = \sum_{\mathbf{k}\sigma} c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}-\mathbf{q}\sigma} = \sum_{\mathbf{k}\sigma} c^\dagger_{\mathbf{k}+\mathbf{q}\sigma}c_{\mathbf{k}\sigma} = n^\dagger_\mathbf{q}$$

Therefore,

$$C^R_{n_\mathbf{q}n_{-\mathbf{q}}}(\mathbf{q},\omega) = Z_G^{-1}\sum_{nm}\frac{|\langle n|n_\mathbf{q}|m\rangle|^2(e^{-\beta\bar{E}_n} - e^{-\beta\bar{E}_m})}{\omega - (\bar{E}_m - \bar{E}_n)/\hbar + i0^+}$$

The matrix element

$$\langle n|n_\mathbf{q}|m\rangle = \sum_{\mathbf{k}\sigma}\langle n|c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}+\mathbf{q}\sigma}|m\rangle$$

is nonvanishing if $|n\rangle$ differs from $|m\rangle$ by the replacement of a particle of coordinates $(\mathbf{k}+\mathbf{q}\sigma)$ with one of coordinates $(\mathbf{k}\sigma)$. Hence

$$\bar{E}_m - \bar{E}_n = \bar{\epsilon}_{\mathbf{k}+\mathbf{q}\sigma} - \bar{\epsilon}_{\mathbf{k}\sigma}$$

Furthermore,

$$\langle n|n_\mathbf{q}|m\rangle\langle m|n^\dagger_\mathbf{q}|n\rangle = \sum_{\mathbf{k}\sigma}\sum_{\mathbf{k}'\sigma'}\langle n|c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}+\mathbf{q}\sigma}|m\rangle\langle m|c^\dagger_{\mathbf{k}+\mathbf{q}\sigma}c_{\mathbf{k}\sigma}|n\rangle$$

The retarded correlation function now becomes

$$\begin{aligned}
C^R_{n_{\mathbf{q}}n_{-\mathbf{q}}}(\mathbf{q},\omega) = Z_G^{-1}\sum_{\mathbf{k}\sigma}&\frac{1}{\omega + (\bar{\epsilon}_{\mathbf{k}\sigma} - \bar{\epsilon}_{\mathbf{k}+\mathbf{q}\sigma})/\hbar + i0^+} \\
&\sum_{nm}\langle n|c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}+\mathbf{q}\sigma}|m\rangle\langle m|c^\dagger_{\mathbf{k}+\mathbf{q}\sigma}c_{\mathbf{k}\sigma}|n\rangle(e^{-\beta\bar{E}_n} - e^{-\beta\bar{E}_m})
\end{aligned}$$

Consider

$$\begin{aligned}
S_1 &= \sum_{nm} e^{-\beta\bar{E}_n}\langle n|c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}+\mathbf{q}\sigma}|m\rangle\langle m|c^\dagger_{\mathbf{k}+\mathbf{q}\sigma}c_{\mathbf{k}\sigma}|n\rangle \\
&= \sum_{n} e^{-\beta\bar{E}_n}\langle n|c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}+\mathbf{q}\sigma}c^\dagger_{\mathbf{k}+\mathbf{q}\sigma}c_{\mathbf{k}\sigma}|n\rangle
\end{aligned}$$

and

$$\begin{aligned}
S_2 &= \sum_{nm} e^{-\beta\bar{E}_m}\langle n|c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}+\mathbf{q}\sigma}|m\rangle\langle m|c^\dagger_{\mathbf{k}+\mathbf{q}\sigma}c_{\mathbf{k}\sigma}|n\rangle \\
&= \sum_{nm} e^{-\beta\bar{E}_m}\langle m|c^\dagger_{\mathbf{k}+\mathbf{q}\sigma}c_{\mathbf{k}\sigma}|n\rangle\langle n|c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}+\mathbf{q}\sigma}|m\rangle \\
&= \sum_{m} e^{-\beta\bar{E}_m}\langle m|c^\dagger_{\mathbf{k}+\mathbf{q}\sigma}c_{\mathbf{k}\sigma}c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}+\mathbf{q}\sigma}|m\rangle
\end{aligned}$$

Hence,

$$\begin{aligned}
C^R_{n_{\mathbf{q}}n_{-\mathbf{q}}}(\mathbf{q},\omega) = Z_G^{-1}\sum_{\mathbf{k}\sigma}&\frac{1}{\omega + (\bar{\epsilon}_{\mathbf{k}\sigma} - \bar{\epsilon}_{\mathbf{k}+\mathbf{q}\sigma})/\hbar + i0^+} \\
&\sum_{n} e^{-\beta\bar{E}_n}\langle n|c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}+\mathbf{q}\sigma}c^\dagger_{\mathbf{k}+\mathbf{q}\sigma}c_{\mathbf{k}\sigma} - c^\dagger_{\mathbf{k}+\mathbf{q}\sigma}c_{\mathbf{k}\sigma}c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}+\mathbf{q}\sigma}|n\rangle
\end{aligned}$$

Now consider

$$\begin{aligned}
c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}+\mathbf{q}\sigma}c^\dagger_{\mathbf{k}+\mathbf{q}\sigma}c_{\mathbf{k}\sigma} &= c^\dagger_{\mathbf{k}\sigma}(1 - c^\dagger_{\mathbf{k}+\mathbf{q}\sigma}c_{\mathbf{k}+\mathbf{q}\sigma})c_{\mathbf{k}\sigma} \\
&= c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma} - c^\dagger_{\mathbf{k}\sigma}c^\dagger_{\mathbf{k}+\mathbf{q}\sigma}c_{\mathbf{k}+\mathbf{q}\sigma}c_{\mathbf{k}\sigma}
\end{aligned}$$

and

$$\begin{aligned}
c^\dagger_{\mathbf{k}+\mathbf{q}\sigma}c_{\mathbf{k}\sigma}c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}+\mathbf{q}\sigma} &= c^\dagger_{\mathbf{k}+\mathbf{q}\sigma}(1 - c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma})c_{\mathbf{k}+\mathbf{q}\sigma} \\
&= c^\dagger_{\mathbf{k}+\mathbf{q}\sigma}c_{\mathbf{k}+\mathbf{q}\sigma} - c^\dagger_{\mathbf{k}+\mathbf{q}\sigma}c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}c_{\mathbf{k}+\mathbf{q}\sigma} \\
&= c^\dagger_{\mathbf{k}+\mathbf{q}\sigma}c_{\mathbf{k}+\mathbf{q}\sigma} - c^\dagger_{\mathbf{k}\sigma}c^\dagger_{\mathbf{k}+\mathbf{q}\sigma}c_{\mathbf{k}+\mathbf{q}\sigma}c_{\mathbf{k}\sigma}
\end{aligned}$$

In writing the above equations we have used

$$\{c_{\mathbf{k}\sigma}, c_{\mathbf{k}'\sigma'}\} = \{c^\dagger_{\mathbf{k}\sigma}, c^\dagger_{\mathbf{k}'\sigma'}\} = 0, \qquad \{c_{\mathbf{k}\sigma}, c^\dagger_{\mathbf{k}'\sigma'}\} = \delta_{\mathbf{k}\mathbf{k}'}\delta_{\sigma\sigma'}$$

Assembling the pieces together,

$$\begin{aligned}
C^R_{n_{\mathbf{q}}n_{-\mathbf{q}}}(\mathbf{q},\omega) &= Z_G^{-1}\sum_{\mathbf{k}\sigma}\frac{1}{\omega+(\bar{\epsilon}_{\mathbf{k}\sigma}-\bar{\epsilon}_{\mathbf{k}+\mathbf{q}\sigma})/\hbar+i0^+}\sum_n e^{-\beta\bar{E}_n}\langle n|c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}-c^\dagger_{\mathbf{k}+\mathbf{q}\sigma}c_{\mathbf{k}+\mathbf{q}\sigma}|n\rangle \\
&= \sum_{\mathbf{k}\sigma}\frac{1}{\omega+(\bar{\epsilon}_{\mathbf{k}\sigma}-\bar{\epsilon}_{\mathbf{k}+\mathbf{q}\sigma})/\hbar+i0^+}\langle c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}-c^\dagger_{\mathbf{k}+\mathbf{q}\sigma}c_{\mathbf{k}+\mathbf{q}\sigma}\rangle \\
&= \sum_{\mathbf{k}\sigma}\frac{f_{\mathbf{k}\sigma}-f_{\mathbf{k}+\mathbf{q}\sigma}}{\omega+(\bar{\epsilon}_{\mathbf{k}\sigma}-\bar{\epsilon}_{\mathbf{k}+\mathbf{q}\sigma})/\hbar+i0^+}
\end{aligned}$$

13. *Equation of motion.*

$$\bar{H}=\sum_{\mathbf{k}\sigma}\bar{\epsilon}_{\mathbf{k}\sigma}c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}+V=\bar{H}_0+V$$

For bosons,

$$G^R(\mathbf{k}\sigma,t)=-i\theta(t)\langle[c_{\mathbf{k}\sigma}(t),c^\dagger_{\mathbf{k}\sigma}(0)]\rangle$$

Taking the derivative with respect to t,

$$i\frac{\partial}{\partial t}G^R(\mathbf{k}\sigma,t)=\delta(t)\langle[c_{\mathbf{k}\sigma}(t),c^\dagger_{\mathbf{k}\sigma}(0)]\rangle+\theta(t)\langle[\frac{\partial}{\partial t}c_{\mathbf{k}\sigma}(t),c^\dagger_{\mathbf{k}\sigma}(0)]\rangle$$

The first term on the RHS is $\delta(t)\langle[c_{\mathbf{k}\sigma}(0),c^\dagger_{\mathbf{k}\sigma}(0)]\rangle=\delta(t)\langle 1\rangle=\delta(t)$. As for the second term,

$$\frac{\partial}{\partial t}c_{\mathbf{k}\sigma}(t)=\frac{i}{\hbar}[\bar{H},c_{\mathbf{k}\sigma}(t)]=\frac{i}{\hbar}[\bar{H}_0(t),c_{\mathbf{k}\sigma}(t)]+\frac{i}{\hbar}[V(t),c_{\mathbf{k}\sigma}(t)]$$

The first commutator is

$$\begin{aligned}
[\bar{H}_0,c_{\mathbf{k}\sigma}] &= \sum_{\mathbf{k}'\sigma'}\bar{\epsilon}_{\mathbf{k}'\sigma'}[c^\dagger_{\mathbf{k}'\sigma'}c_{\mathbf{k}'\sigma'},c_{\mathbf{k}\sigma}]=\sum_{\mathbf{k}'\sigma'}[c^\dagger_{\mathbf{k}'\sigma'},c_{\mathbf{k}\sigma}]c_{\mathbf{k}'\sigma'} \\
&= \sum_{\mathbf{k}'\sigma'}\bar{\epsilon}_{\mathbf{k}'\sigma'}(-\delta_{\mathbf{k}\mathbf{k}'}\delta_{\sigma\sigma'})c_{\mathbf{k}'\sigma'}=-\bar{\epsilon}_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}
\end{aligned}$$

Thus,

$$i\frac{\partial}{\partial t}c_{\mathbf{k}\sigma}(t)=-\frac{i}{\hbar}\bar{\epsilon}_{\mathbf{k}'\sigma'}c_{\mathbf{k}\sigma}(t)+\frac{i}{\hbar}[V(t),c_{\mathbf{k}\sigma}(t)]$$

The equation of motion for $G^R(\mathbf{k}\sigma,t)$ now becomes

$$i\hbar\frac{\partial}{\partial t}G^R(\mathbf{k}\sigma,t)=\hbar\delta(t)+\theta(t)(-i\bar{\epsilon}_{\mathbf{k}\sigma})\langle[c_{\mathbf{k}\sigma}(t),c^\dagger_{\mathbf{k}\sigma}(0)]\rangle+i\theta(t)\langle[[V(t),c_{\mathbf{k}\sigma}(t)],c^\dagger_{\mathbf{k}\sigma}(0)]\rangle$$

Rearranging terms,

$$(i\hbar\frac{\partial}{\partial t}-\bar{\epsilon}_{\mathbf{k}\sigma})G^R(\mathbf{k}\sigma,t)=\hbar\delta(t)-i\theta(t)\langle[-[V(t),c_{\mathbf{k}\sigma}(t)],c^\dagger_{\mathbf{k}\sigma}(0)]\rangle$$

This is the same equation as the one for fermions except that a commutator replaces an anticommutator.

14. *Mixed retarded function.*

The Hamiltonian is

$$H = \sum_{n\mathbf{k}\sigma} \epsilon_{n\mathbf{k}} c^\dagger_{n\mathbf{k}\sigma} c_{n\mathbf{k}\sigma} + \sum_{\sigma} \epsilon_d d^\dagger_\sigma d_\sigma + \sum_{n\mathbf{k}\sigma} V_{n\mathbf{k}d} c^\dagger_{n\mathbf{k}\sigma} d_\sigma + \sum_{n\mathbf{k}\sigma} V^*_{n\mathbf{k}d} d^\dagger_\sigma c_{n\mathbf{k}\sigma}$$

The mixed retarded function is

$$G^R(n\mathbf{k}d\sigma, t) = -i\theta(t)\langle\{c_{n\mathbf{k}\sigma}(t), d^\dagger_\sigma(0)\}\rangle$$

Its time-derivative is

$$i\frac{\partial}{\partial t}G^R(n\mathbf{k}d\sigma, t) = \delta(t)\langle\{c_{n\mathbf{k}\sigma}(t), d^\dagger_\sigma(0)\}\rangle + \theta(t)\langle\{\frac{\partial}{\partial t}c_{n\mathbf{k}\sigma}(t), d^\dagger_\sigma(0)\}\rangle$$

The first term on the RHS is equal to $\delta(t)\langle\{c_{n\mathbf{k}\sigma}(0), d^\dagger_\sigma(0)\}\rangle = 0$ since operators c and d anticommute. As for the second term,

$$\frac{\partial}{\partial t}c_{n\mathbf{k}\sigma}(t) = \frac{i}{\hbar}[\bar{H}, c_{n\mathbf{k}\sigma}]$$

Using $[AB, C] = A\{B, C\} - \{A, C\}B$, we find

$$\left[\sum_{n\mathbf{k}\sigma} \epsilon_{n\mathbf{k}} c^\dagger_{n\mathbf{k}\sigma} c_{n\mathbf{k}\sigma}, c_{n\mathbf{k}\sigma}\right] = -\epsilon_{n\mathbf{k}} c_{n\mathbf{k}\sigma}$$

$$\left[\sum_{\sigma} \epsilon_d d^\dagger_\sigma d_\sigma, c_{n\mathbf{k}\sigma}\right] = 0$$

$$\left[\sum_{n\mathbf{k}\sigma} V_{n\mathbf{k}d} c^\dagger_{n\mathbf{k}\sigma} d_\sigma, c_{n\mathbf{k}\sigma}\right] = -V_{n\mathbf{k}d} d_\sigma$$

$$\left[\sum_{n\mathbf{k}\sigma} V^*_{n\mathbf{k}d} d^\dagger_\sigma c_{n\mathbf{k}\sigma}, c_{n\mathbf{k}\sigma}\right] = 0$$

Hence,

$$\frac{\partial}{\partial t}c_{n\mathbf{k}\sigma} = -\frac{1}{\hbar}\epsilon_{n\mathbf{k}} c_{n\mathbf{k}\sigma} - \frac{1}{\hbar}V_{n\mathbf{k}d} d_\sigma$$

and

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}G^R(n\mathbf{k}d\sigma, t) &= -i\theta(t)\epsilon_{n\mathbf{k}}\langle\{c_{n\mathbf{k}\sigma}(t), d^\dagger_\sigma(0)\}\rangle - i\theta(t)V_{n\mathbf{k}d}\langle\{d_\sigma(t), d^\dagger_\sigma(0)\}\rangle \\ &= \epsilon_{n\mathbf{k}}G^R(n\mathbf{k}d\sigma, t) + V_{n\mathbf{k}d}G^R(dd\sigma, t) \end{aligned}$$

This is Eq. (6.15).

15. *Polarizability at zero temperature.*

$$\chi^0(\mathbf{q},\omega) = \frac{1}{V}\sum_{\mathbf{k}\sigma}\frac{f_{\mathbf{k}\sigma}-f_{\mathbf{k+q}\sigma}}{\hbar\omega+\bar{\epsilon}_{\mathbf{k}\sigma}-\bar{\epsilon}_{\mathbf{k+q}\sigma}+i0^+}$$
$$= \frac{1}{V}\sum_{\mathbf{k}\sigma}\frac{f_{\mathbf{k}\sigma}}{\hbar\omega+\bar{\epsilon}_{\mathbf{k}\sigma}-\bar{\epsilon}_{\mathbf{k+q}\sigma}+i0^+} - \frac{1}{V}\sum_{\mathbf{k}\sigma}\frac{f_{\mathbf{k+q}\sigma}}{\hbar\omega+\bar{\epsilon}_{\mathbf{k}\sigma}-\bar{\epsilon}_{\mathbf{k+q}\sigma}+i0^+}$$

In the second term, replace $\mathbf{k}$ with $-\mathbf{k}-\mathbf{q}$; then

$$f_{\mathbf{k+q}\sigma}\to f_{-\mathbf{k}\sigma}=f_{\mathbf{k}\sigma}, \quad \hbar\omega+\bar{\epsilon}_{\mathbf{k}\sigma}-\bar{\epsilon}_{\mathbf{k+q}\sigma}+i0^+ \to \hbar\omega+\epsilon_{-\mathbf{k}-\mathbf{q}}-\epsilon_{-\mathbf{k}}+i0^+ = \hbar\omega+\epsilon_{\mathbf{k+q}}-\epsilon_{\mathbf{k}}+i0^+$$

Therefore,

$$-(\hbar\omega+\bar{\epsilon}_{\mathbf{k}\sigma}-\bar{\epsilon}_{\mathbf{k+q}\sigma}+i0^+)\to -\hbar\omega+\bar{\epsilon}_{\mathbf{k}\sigma}-\bar{\epsilon}_{\mathbf{k+q}\sigma}-i0^+$$

The polarizability is thus given by

$$\chi^0(\mathbf{q},\omega) = \frac{1}{V}\sum_{\mathbf{k}\sigma}\frac{f_{\mathbf{k}\sigma}}{\hbar\omega+\bar{\epsilon}_{\mathbf{k}\sigma}-\bar{\epsilon}_{\mathbf{k+q}\sigma}+i0^+} + (\hbar\omega+i0^+\to-\hbar\omega-i0^+)$$

The denominator

$$\begin{aligned}\hbar\omega+\bar{\epsilon}_{\mathbf{k}\sigma}-\bar{\epsilon}_{\mathbf{k+q}\sigma}+i0^+ &= \hbar\omega+\hbar^2k^2/2m-\hbar^2(k^2+q^2+2\mathbf{k}.\mathbf{q})/2m+i0^+\\ &= \hbar\omega-\hbar^2q^2/2m-(\hbar^2kq/m)cos\theta+i0^+\\ &= \frac{\hbar^2 q}{m}\left(\frac{\omega}{\hbar q/m}-\frac{q}{2}-k\,cos\theta+i0^+\right)\\ &= \frac{\hbar^2 k_F q}{m}\left(\frac{\omega}{qv_F}-\frac{q}{2k_F}-\frac{k}{k_F}cos\theta+i0^+\right)\end{aligned}$$

where $v_F=\hbar k_F/m$ is the Fermi velocity and θ is the angle between $\mathbf{k}$ and $\mathbf{q}$. Thus

$$\chi^0(\mathbf{q},\omega) = \frac{m}{\hbar^2 V k_F q}\sum_{\mathbf{k}\sigma}\frac{f_{\mathbf{k}\sigma}}{(\omega/qv_F)-(q/2k_F)-(k/k_F)cos\theta+i0^+} + (\hbar\omega+i0^+\to-\hbar\omega-i0^+)$$

the sum over σ gives a factor of 2. At $T=0$, $f_{\mathbf{k}\sigma}=1$ if $k<k_F$, otherwise it is zero. The sum over $\mathbf{k}$ is replaced by an integral,

$$\sum_{\mathbf{k}}F(\mathbf{k}) = \frac{V}{(2\pi)^3}\int d^3kF(\mathbf{k}) = \frac{V}{(2\pi)^3}\int k^2dkd\Omega F(\mathbf{k})$$

Because of the presence of $f_{\mathbf{k}\sigma}$, which is equal to $\theta(k_F-k)$ at $T=0$, the integration over k ranges from 0 to k_F. Thus

$$\chi^0(\mathbf{q},\omega) = \frac{2m}{\hbar^2 V k_F q}\frac{V}{(2\pi)^3}\int_0^{k_F}k^2dk\int_{-1}^{1}cos\theta\int_0^{2\pi}d\phi\frac{1}{\omega/qv_F-q/2k_F-(k/k_F)cos\theta+i0^+}$$
$$+\,(\omega+i0^+\to-\omega-i0^+)$$

The integral over ϕ gives 2π. Let $x = k/k_F$. Then

$$\chi^0(\mathbf{q},\omega) = \frac{2mk_F^2}{(2\pi)^2\hbar^2 q}\int_0^1 x^2 dx \int_{-1}^1 \frac{d\,cos\theta}{\omega/qv_F - q/2k_F - x\,cos\theta + i0^+} + (\omega + i0^+ \to -\omega - i0^+)$$

Its real part is

$$\begin{aligned}
Re\,\chi^0(\mathbf{q},\omega) &= \frac{2mk_F^2}{(2\pi)^2\hbar^2 q}\int_0^1 x^2 dx \int_{-1}^1 \frac{d\,cos\theta}{\omega/qv_F - q/2k_F - x\,cos\theta} + (\omega \to -\omega) \\
&= \frac{-2mk_F^2}{(2\pi)^2\hbar^2 q}\int_0^1 x\,ln\left|\frac{\omega/qv_F - q/2k_F - x}{\omega/qv_F - q/2k_F + x}\right| dx + (\omega \to -\omega)
\end{aligned}$$

$$\begin{aligned}
\int_0^1 x\,ln\left|\frac{\omega/qv_F - q/2k_F - x}{\omega/qv_F - q/2k_F + x}\right| dx &= \int_0^1 x\,ln|x + (q/2k_F - \omega/qv_F)|dx \\
&\quad - \int_0^1 x\,ln|x - (q/2k_F - \omega/qv_F)|dx \\
&= \frac{1-z_-^2}{2} ln\left|\frac{1-z_-}{1+z_-}\right| - \frac{1}{4}(1+z_-)^2 + \frac{1}{4}(1-z_-)^2 \\
&= \frac{1-z_-^2}{2} ln\left|\frac{1-z_-}{1+z_-}\right| - z_-
\end{aligned}$$

Upon replacing ω by $-\omega$,

$$\begin{aligned}
z_+ &= \omega/qv_F + q/2k_F \to -\omega/qv_F + q/2k_F = -z_- \\
z_- &= \omega/qv_F - q/2k_F \to -\omega/qv_F - q/2k_F = -z_+
\end{aligned}$$

Hence

$$\begin{aligned}
Re\,\chi^0(\mathbf{q},\omega) &= \frac{-2mk_F}{(2\pi)^2\hbar^2}\left[1 + \frac{1-z_-^2}{2q/k_F}\,ln\left|\frac{1-z_-}{1+z_-}\right| - \frac{1-z_+^2}{2q/k_F}\,ln\left|\frac{1-z_+}{1+z_+}\right|\right] \\
&= \frac{-mk_F}{\pi^2\hbar^2}\left[\frac{1}{2} + \frac{1-z_-^2}{4q/k_F}\,ln\left|\frac{1-z_-}{1+z_-}\right| - \frac{1-z_+^2}{4q/k_F}\,ln\left|\frac{1-z_+}{1+z_+}\right|\right]
\end{aligned}$$

Replacing $mk_F/\pi^2\hbar^2$ by $d(\epsilon_F)$, the required answer is obtained.

As for the imaginary part of the polarizability,

$$\begin{aligned}
Im\,\chi^0(\mathbf{q},\omega) &= -\frac{\pi mk_F^2}{2\pi^2\hbar^2 q}\int_0^1 x^2 dx \int_{-1}^1 \delta(\omega/qv_F - q/2v_F - x\,cos\theta)d\,cos\theta - (\omega \to -\omega) \\
&= -\frac{\pi mk_F^2}{2\pi^2\hbar^2 q}\int_0^1 x dx \int_{-1}^1 \delta(z_-/x - cos\theta)d\,cos\theta - (z_- \to -z_+)
\end{aligned}$$

For this not to vanish, we must have $-1 < z_-/x < 1$. Since $max(x) = 1$, it follows that $-1 < z_- < 1$ and $x > z_-$. Hence,

$$Im\,\chi^0(\mathbf{q},\omega) = -\frac{\pi m k_F^2}{2\pi^2\hbar^2 q}\int_{z_-}^{1} x\,dx\,\theta(1-z_-^2) - (z_- \to -z_+)$$
$$= -\frac{\pi m k_F^2}{4\pi^2\hbar^2 q}\left[(1-z_-^2)\,\theta(1-z_-^2) - (1-z_+^2)\,\theta(1-z_+^2)\right]$$
$$= -d(\epsilon_F)\frac{\pi}{4q/k_F}\left[(1-z_-^2)\,\theta(1-z_-^2) - (1-z_+^2)\,\theta(1-z_+^2)\right]$$

16. *Polarizability.*

(a) 3D:

$$\omega = 0, \quad z_+ = q/2k_F, \quad z_- = -q/2k_F$$

Hence, $Im\,\chi^0(\mathbf{q},\omega) = 0$ (see the expression for $Im\,\chi^0(\mathbf{q},\omega)$ in the previous problem). Thus

$$\chi^0(\mathbf{q},\omega) = -d(\epsilon_F)\left[\frac{1}{2} + \frac{1-q^2/4k_F^2}{4q/k_F}\,ln\left|\frac{1+q/2k_F}{1-q/2k_F}\right| - \frac{1-q^2/4k_F^2}{4q/k_F}\,ln\left|\frac{1-q/2k_F}{1+q/2k_F}\right|\right]$$
$$= -d(\epsilon_F)\left[\frac{1}{2} - \frac{1-q^2/4k_F^2}{2q/k_F}\,ln\left|\frac{1-q/2k_F}{1+q/2k_F}\right|\right]$$
$$= -d(\epsilon_F)\left[\frac{1}{2} - \frac{1-q'^2/4}{2q'}\,ln\left|\frac{1-q'/2}{1+q'/2}\right|\right]$$
$$= -d(\epsilon_F)\left[\frac{1}{2} - \frac{4-q'^2}{8q'}\,ln\left|\frac{2-q'}{2+q'}\right|\right]$$

where $q' = q/2k_F$.

(b) 2D:

$$\chi^0(\mathbf{q},\omega) = \frac{1}{A}\sum_{\mathbf{k}\sigma}\frac{f_{\mathbf{k}\sigma}}{\hbar\omega + \bar{\epsilon}_{\mathbf{k}\sigma} - \bar{\epsilon}_{\mathbf{k}+\mathbf{q}\sigma} + i0^+} + (\omega + i0^+ \to -\omega - i0^+)$$

The sum over σ gives a factor of 2. Replacing the sum over $\mathbf{k}$ by an integral,

$$\chi^0(\mathbf{q},\omega) = \frac{2m}{A\hbar^2 k_F q}\frac{A}{(2\pi)^2}\int_0^{k_F} kdk\int_0^{2\pi}\frac{d\theta}{\omega/qv_F - q/2k_F - (k/k_F)cos\theta + i0^+} + (\omega + i0^+ \to -\omega - i0^+)$$
$$= \frac{2mk_F}{4\pi^2\hbar^2 q}\int_0^1 xdx\int_0^{2\pi}\frac{d\theta}{\omega/qv_F - q/2k_F - xcos\theta + i0^+} + (\omega + i0^+ \to -\omega - i0^+)$$

It is clear that when $\omega = 0$, $Im\,\chi^0(\mathbf{q},\omega) = 0$. Hence,

$$\chi^0(\mathbf{q},0) = -\frac{mk_F}{\pi^2\hbar^2 q}\int_0^1 xdx\int_0^{2\pi}\frac{d\theta}{q/2k_F + xcos\theta}$$

The integral over θ may be evaluated by changing variables: $t = tan(\theta/2)$ (or by the residue theorem upon setting $cos\theta = (z + 1/z)/2$, where $z = e^{i\theta}$),

$$t = tan(\theta/2) \Rightarrow cos\theta = (1 - t^2)/(1 + t^2), \quad d\theta = 2dt/(1 + t^2)$$

Then,

$$\begin{aligned}
I &= \int_0^{2\pi} \frac{d\theta}{q/2k_F + xcos\theta} \\
&= \int_0^{\pi} \frac{d\theta}{q/2k_F + xcos\theta} + \int_{\pi}^{2\pi} \frac{d\theta}{q/2k_F + xcos\theta} \\
&= 2\int_0^{\infty} \frac{dt}{(q/2k_F)(1 + t^2) + x(1 - t^2)} + 2\int_{-\infty}^{0} \frac{dt}{(q/2k_F)(1 + t^2) + x(1 - t^2)} \\
&= 2\int_0^{\infty} \frac{dt}{(q/2k_F + x) + (q/2k_F - x)t^2} + 2\int_{-\infty}^{0} \frac{dt}{(q/2k_F + x) + (q/2k_F - x)t^2}
\end{aligned}$$

First, consider the case when $q/2k_F > x$:

$$\begin{aligned}
I &= \frac{2}{\sqrt{(q/2k_F)^2 - x^2}} \left[tan^{-1}\sqrt{\frac{q/2k_F - x}{q/2k_F + x}}\, t \Big|_0^{\infty} + tan^{-1}\sqrt{\frac{q/2k_F - x}{q/2k_F + x}}\, t \Big|_{-\infty}^{0} \right] \\
&= \frac{2\pi}{\sqrt{(q/2k_F)^2 - x^2}}
\end{aligned}$$

Next we consider the case $q/2k_F < x$:
Let $q/2k_F + x = r^2,\ x - q/2k_F = s^2$. Then

$$I = \frac{2}{rs}\left[ln\left|\frac{r + st}{r - st}\right| \right]_0^{\infty} + \frac{2}{rs}\left[ln\left|\frac{r + st}{r - st}\right| \right]_{-\infty}^{0} = 0$$

Therefore,

$$\chi^0(\mathbf{q}, 0) = -\frac{2mk_F}{\pi\hbar^2 q}\int_0^1 \frac{xdx}{(q/2k_F)^2 - x^2}$$

Let $q' = q/k_F,\ u = q'^2/4 - x^2$; then $du = -2xdx$.
If $q'/2 < 1$, then

$$\begin{aligned}
\chi^0(\mathbf{q}, 0) &= \frac{m}{\pi\hbar^2 q'}\int u^{-1/2}du = \frac{2m}{\pi\hbar^2 q'}\sqrt{q'^2/4 - x^2}\Big|_{x=0}^{x=q'/2} \\
&= -\frac{2m}{\pi\hbar^2 q'}\frac{q'}{2} = -\frac{m}{\pi\hbar^2} = -d(\epsilon_F)
\end{aligned}$$

Recall that in two dimensions, the density of states per unit area is a constant given by $m.\pi\hbar^2$.

If $q'/2 > 1$, then

$$\chi^0(\mathbf{q},0) = \frac{2m}{\pi\hbar^2 q'} \left.\sqrt{q'^2/4 - x^2}\right|_0^1 = \frac{2m}{\pi\hbar^2 q'}(\sqrt{q'^2/4-1} - q'/2)$$
$$= -\frac{m}{\pi\hbar^2}\left[1 - \frac{2}{q'}\sqrt{q'^2/4-1}\right] = -d(\epsilon_F)(1 - \sqrt{q'^2-4}\,/q')$$

Hence,

$$\chi^0(\mathbf{q},0) = -d(\epsilon_F)\left[1 - \theta(q'-2)\frac{\sqrt{q'^2-4}}{q'}\right]$$

(c) 1D.
Clearly, $Im\,\chi^0(\mathbf{q},0) = 0$. Thus

$$\chi^0(\mathbf{q},0) = \frac{2}{L}\sum_{\mathbf{k}\sigma}\frac{f_{\mathbf{k}\sigma}}{\bar{\epsilon}_{\mathbf{k}\sigma} - \bar{\epsilon}_{\mathbf{k}+\mathbf{q}\sigma}}$$

Since

$$\bar{\epsilon}_{\mathbf{k}\sigma} - \bar{\epsilon}_{\mathbf{k}+\mathbf{q}\sigma} = \hbar^2 k^2/2m - (\hbar^2/2m)(k^2 + q^2 + 2kq) = -\hbar^2 q^2/2m - \hbar^2 kq/m\,,$$

it follows that

$$\chi^0(\mathbf{q},0) = \frac{4}{L}\sum_{\mathbf{k}}\frac{f_{\mathbf{k}}}{-\hbar^2 q^2/2m - \hbar^2 kq/m} = \frac{4m}{\hbar^2 Lq}\sum_{\mathbf{k}}\frac{f_{\mathbf{k}}}{-q/2-k}$$
$$= \frac{4m}{\hbar^2 Lq}\frac{L}{2\pi}\int_{-k_F}^{k_F}\frac{dk}{-q/2-k} = \frac{2m}{\pi\hbar^2 q}\int_{-1}^{1}\frac{dk}{-q/2k_F - k}$$
$$= \frac{2m}{\pi\hbar^2 q}\int_{-1}^{1}\frac{dk}{-q'/2-k} = -\frac{2m}{\pi\hbar^2 q}\int_{-1}^{1}\frac{dk}{q'/2+k} = -\frac{2m}{\pi\hbar^2 k_F q'}\;ln\left.|k+q'/2|\right|_{-1}^{1}$$
$$= -\frac{2m}{\pi\hbar^2 k_F q'}\,ln\left|\frac{1+q'/2}{1-q'/2}\right| = -\frac{2m}{\pi\hbar^2 k_F q'}\,ln\left|\frac{2+q'}{2-q'}\right|$$

In one dimension, $d(\epsilon_F) = 2m/(\pi\hbar^2 k_F)$. Therefore,

$$\chi^0(q,0) = -d(\epsilon_F)\left[\frac{1}{q'}\,ln\left|\frac{2+q'}{2-q'}\right|\right]$$

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7.1. $$H = \sum_{\vec{k}\sigma} \epsilon_{\vec{k}} c^{+}_{\vec{k}\sigma} c_{\vec{k}\sigma} + \epsilon \sum_{\sigma} d^{+}_{\sigma} d_{\sigma} + U n_{\uparrow} n_{\downarrow} + \sum_{\vec{k}\sigma} \left(V_{\vec{k}} c^{+}_{\vec{k}\sigma} d_{\sigma} + V^{*}_{\vec{k}} d^{+}_{\sigma} c_{\vec{k}\sigma} \right)$$

Note: from now on I will write $\vec{k}$ simply as k

$$G^{R}_{kd\sigma}(t) = -i\theta(t) \langle \{ c_{k\sigma}(t), d^{+}_{\sigma}(0) \} \rangle$$

$$i\hbar \frac{\partial}{\partial t} G^{R}_{kd\sigma}(t) = \hbar \delta(t) \langle \{ c_{k\sigma}(t), d^{+}_{\sigma}(0) \} \rangle + \hbar\theta(t) \langle \{ \tfrac{\partial}{\partial t} c_{k\sigma}(t), d^{+}_{\sigma}(0) \} \rangle$$

The first term on the RHS is $\hbar\delta(t)\langle \{ c_{k\sigma}(0), d^{+}_{\sigma}(0) \} \rangle = 0$ since c's and d's anticommute.

$$\hbar \frac{\partial}{\partial t} c_{k\sigma} = i[H, c_{k\sigma}] = i[H_e, c_{k\sigma}] + i[H_D, c_{k\sigma}] + i[H_T, c_{k\sigma}]$$

where

$$H_e = \sum_{k\sigma} \epsilon_k c^{+}_{k\sigma} c_{k\sigma}, \quad H_D = \epsilon \sum_{\sigma} d^{+}_{\sigma} d_{\sigma} + U n_{\uparrow} n_{\downarrow},$$

$$H_T = \sum_{k\sigma} \left(V_k c^{+}_{k\sigma} d_{\sigma} + V^{*}_k d^{+}_{\sigma} c_{k\sigma} \right)$$

Using $[AB, C] = A\{B, C\} - \{A, C\}B$, we find

$$[H_e, c_{k\sigma}] = \left[\sum_{k\sigma} \epsilon_k c^{+}_{k\sigma} c_{k\sigma}, c_{k\sigma} \right] = -\epsilon_k c_{k\sigma}$$

$$[H_D, c_{k\sigma}] = 0$$

$$[H_T, c_{k\sigma}] = -V_k d_{\sigma}$$

Therefore

$$\hbar \frac{\partial}{\partial t} c_{k\sigma}(t) = -i\epsilon_k c_{k\sigma} - iV_k d_{\sigma}$$

and

$$i\hbar \frac{\partial}{\partial t} G^{R}_{kd\sigma}(t) = -i\epsilon_k \theta(t) \langle \{ c_{k\sigma}(t), d^{+}_{\sigma}(0) \} \rangle - iV_k \theta(t) \langle \{ d_{\sigma}(t), d^{+}_{\sigma}(0) \} \rangle$$

$$= \epsilon_k G^{R}_{kd\sigma}(t) + V_k G^{R}_{d\sigma}(t)$$

7.2 Equation of motion for $\Gamma^R_{d\sigma}(t)$

$$\Gamma^R_{d\sigma}(t) = -i\theta(t)\langle\{n_{\bar\sigma}(t)d_\sigma(t), d^+_\sigma(0)\}\rangle$$

$$H = H_e + H_D + H_T$$

$$= \sum_{k\sigma}\epsilon_{k\sigma}C^+_{k\sigma}C_{k\sigma} + \epsilon\sum_\sigma d^+_\sigma d_\sigma + \omega n_\uparrow n_\downarrow + \sum_{k\sigma}(V_k C^+_{k\sigma}d_\sigma + V^*_k d^+_\sigma C_{k\sigma})$$

$$i\hbar\frac{\partial}{\partial t}\Gamma^R_{d\sigma}(t) = \hbar\delta(t)\langle\{n_{\bar\sigma}(0)d_\sigma(0), d^+_\sigma(0)\}\rangle + \hbar\theta(t)\langle\{\dot n_{\bar\sigma}(t)d_\sigma(t), d^+_\sigma(0)\}\rangle$$
$$+\hbar\theta(t)\langle\{n_{\bar\sigma}(t)\dot d_\sigma(t), d^+_\sigma(0)\}\rangle$$

Now consider the various terms on the RHS:

$$\{n_{\bar\sigma}d_\sigma, d^+_\sigma\} = d^+_{\bar\sigma}d_{\bar\sigma}d_\sigma d^+_\sigma + d^+_\sigma d^+_{\bar\sigma}d_{\bar\sigma}d_\sigma$$

In the second term on the RHS of the above equation, we move d^+_σ through $d^+_{\bar\sigma}$ then through $d_{\bar\sigma}$, each time producing a minus sign. Thus

$$\{n_{\bar\sigma}d_\sigma, d^+_\sigma\} = d^+_{\bar\sigma}d_{\bar\sigma}d_\sigma d^+_\sigma + d^+_{\bar\sigma}d_{\bar\sigma}d^+_\sigma d_\sigma$$
$$= n_{\bar\sigma}\{d_\sigma, d^+_\sigma\} = n_{\bar\sigma}$$

Next consider $\hbar\dot n_{\bar\sigma}$,

$$\hbar\dot n_{\bar\sigma} = i[H, n_{\bar\sigma}]$$

Note the following:

$$[H_e, n_{\bar\sigma}] = 0, \quad [\sum_\sigma d^+_\sigma d_\sigma, n_{\bar\sigma}] = [n_\sigma + n_{\bar\sigma}, n_{\bar\sigma}] = 0$$

$$[n_\uparrow n_\downarrow, n_{\bar\sigma}] = n_\uparrow[n_\downarrow, n_{\bar\sigma}] + [n_\uparrow, n_{\bar\sigma}]n_\downarrow$$

Whether $\bar\sigma = \uparrow$ or $\downarrow$, the above commutators vanish. Hence

$$[H_D, n_{\bar\sigma}] = 0$$

Now consider

$$[H_T, n_{\bar\sigma}] = [\sum_{k\sigma} V_k c^{+}_{k\sigma} d_\sigma + V_k^{*} d_\sigma^{+} c_{k\sigma}, n_{\bar\sigma}]$$

Since $c^{+}_{k\sigma}$, $c^{+}_{k\bar\sigma}$, $c_{k\sigma}$, $c_{k\bar\sigma}$, d_σ, and d^{+}_σ commute with $n_{\bar\sigma}$, we obtain

$$[H_T, n_{\bar\sigma}] = \sum_k V_k c^{+}_{k\bar\sigma} [d_{\bar\sigma}, n_{\bar\sigma}] + \sum_k V_k^{*} [d^{+}_{\bar\sigma}, n_{\bar\sigma}] c_{k\bar\sigma}$$

We evaluate the above commutators by use of $[A,BC] = \{A,B\}C - B\{A,C\}$:

$$[d_{\bar\sigma}, n_{\bar\sigma}] = [d_{\bar\sigma}, d^{+}_{\bar\sigma} d_{\bar\sigma}] = \{d_{\bar\sigma}, d^{+}_{\bar\sigma}\} d_{\bar\sigma} - d^{+}_{\bar\sigma}\{d_{\bar\sigma}, d_{\bar\sigma}\} = d_{\bar\sigma}$$

$$[d^{+}_{\bar\sigma}, n_{\bar\sigma}] = [d^{+}_{\bar\sigma}, d^{+}_{\bar\sigma} d_{\bar\sigma}] = \{d^{+}_{\bar\sigma}, d^{+}_{\bar\sigma}\} d_{\bar\sigma} - d^{+}_{\bar\sigma}\{d^{+}_{\bar\sigma}, d_{\bar\sigma}\} = -d^{+}_{\bar\sigma}$$

Therefore,

$$\hbar \dot n_{\bar\sigma} = i \sum_k V_k c^{+}_{k\bar\sigma} d_{\bar\sigma} - i \sum_k V_k^{*} d^{+}_{\bar\sigma} c_{k\bar\sigma}$$

Now we evaluate $\hbar \dot d_\sigma = i[H, d_\sigma]$:

$$[H_e, d_\sigma] = 0 \quad , \quad [\sum_\sigma d^{+}_\sigma d_\sigma, d_\sigma] = -d_\sigma$$

$$[n_\uparrow n_\downarrow, d_\sigma] = n_\uparrow [n_\downarrow, d_\sigma] + [n_\uparrow, d_\sigma] n_\downarrow$$

Suppose $\sigma = \uparrow$, then $[n_\uparrow n_\downarrow, d_\uparrow] = [d^{+}_\uparrow d_\uparrow, d_\uparrow] n_\downarrow = -d_\uparrow n_\downarrow = -n_\downarrow d_\uparrow$

Now suppose $\sigma = \downarrow$, then $[n_\uparrow n_\downarrow, d_\downarrow] = n_\uparrow [d^{+}_\downarrow d_\downarrow, d_\downarrow] = -n_\uparrow d_\downarrow$

Hence $[n_\uparrow n_\downarrow, d_\sigma] = -n_{\bar\sigma} d_\sigma$

Now consider

$$[H_T, d_\sigma] = [\sum_{k\sigma} V_k c^{+}_{k\sigma} d_\sigma, d_\sigma] + [\sum_{k\sigma} V_k^{*} d_\sigma^{+} c_{k\sigma}, d_\sigma]$$

$$= 0 - V_k^{*} c_{k\sigma}$$

Putting everything together, the equation of motion for $\Gamma^R_{d\sigma}(t)$ is obtained upon noting that

$$n_{\bar\sigma} n_{\bar\sigma} = d^{+}_{\bar\sigma} d_{\bar\sigma} d^{+}_{\bar\sigma} d_{\bar\sigma} = d^{+}_{\bar\sigma} (1 - d^{+}_{\bar\sigma} d_{\bar\sigma}) d_{\bar\sigma}$$

$$= d^{+}_{\bar\sigma} d_{\bar\sigma} - d^{+}_{\bar\sigma} d^{+}_{\bar\sigma} d_{\bar\sigma} d_{\bar\sigma} = d^{+}_{\bar\sigma} d_{\bar\sigma} = n_{\bar\sigma}$$

$$G^R_{d\sigma}(\omega) = \frac{\hbar\omega - \epsilon - U + \langle n_{\bar\sigma}\rangle U}{(\omega-\epsilon/\hbar)(\hbar\omega-\epsilon-U) - \Sigma^R(\omega)(\hbar\omega-\epsilon-U+\langle n_{\bar\sigma}\rangle U)}$$

Assume that Σ^R is independent of ω. Call the denominator $f(\omega)$. Then

$$\hbar f(\omega) = (\hbar\omega)^2 - (2\epsilon+U+\hbar\Sigma^R)\hbar\omega + \epsilon(\epsilon+U) + \hbar\Sigma^R(\epsilon+U-\langle n_{\bar\sigma}\rangle U)$$

The roots of $\hbar f(\omega)$ are

$$\begin{aligned}
\hbar\omega &= \epsilon + \tfrac{1}{2}(U+\hbar\Sigma^R) \pm \left\{[\epsilon+\tfrac{1}{2}(U+\hbar\Sigma^R)]^2 - \epsilon(\epsilon+U) - \hbar\Sigma^R[\epsilon+U-\langle n_{\bar\sigma}\rangle U]\right\}^{1/2} \\
&= \epsilon + \tfrac{1}{2}(U+\hbar\Sigma^R) \pm [(U+\hbar\Sigma^R)^2/4 - \hbar\Sigma^R U + \hbar\Sigma^R\langle n_{\bar\sigma}\rangle U]^{1/2} \\
&= \epsilon + \tfrac{1}{2}(U+\hbar\Sigma^R) \pm [(U-\hbar\Sigma^R)^2/4 + \hbar\Sigma^R\langle n_{\bar\sigma}\rangle U]^{1/2} \\
&= \epsilon + \tfrac{1}{2}(U+\hbar\Sigma^R) \pm \tfrac{1}{2}(U-\hbar\Sigma^R)\left[1 + \frac{4\hbar\Sigma^R\langle n_{\bar\sigma}\rangle U}{(U-\hbar\Sigma^R)^2}\right]^{1/2}
\end{aligned}$$

If $U \gg \hbar\Sigma^R$, then

$$\hbar\omega \simeq \epsilon + \tfrac{1}{2}(U+\hbar\Sigma^*) \pm \tfrac{1}{2}(U-\hbar\Sigma^R) \pm \frac{\hbar\Sigma^R\langle n_{\bar\sigma}\rangle U}{U} = \begin{cases} \epsilon + U + \hbar\Sigma^R\langle n_{\bar\sigma}\rangle \\ \epsilon + (1-\langle n_{\bar\sigma}\rangle)\hbar\Sigma^R \end{cases}$$

It is easy now to check that

$$G^R_{d\sigma}(\omega) \cong \frac{1-\langle n_{\bar\sigma}\rangle}{\omega - \epsilon/\hbar - (1-\langle n_{\bar\sigma}\rangle)\Sigma^R} + \frac{\langle n_{\bar\sigma}\rangle}{\omega - (\epsilon+U)/\hbar - \langle n_{\bar\sigma}\rangle\Sigma^R}$$

This result is obtained by neglecting ~~2n(n-1)Σ~~ $2\langle n_{\bar\sigma}\rangle(\langle n_{\bar\sigma}\rangle-1)\Sigma^R$ compared to $\langle n_{\bar\sigma}\rangle U$ since $\langle n_{\bar\sigma}\rangle$ ranges from 0 to 1.

The spin-resolved density of states is

$$\rho_\sigma = -\frac{1}{\pi\hbar}\,\mathrm{Im}\,G^R_{d\sigma}(\omega) = -\frac{1}{\pi\hbar}\Bigg[\frac{(1-\langle n_\sigma\rangle)^2\,\mathrm{Im}\,\Sigma^R}{[\omega-\epsilon/\hbar-(1-\langle n_{\bar\sigma}\rangle)\mathrm{Re}\,\Sigma^R]^2 + [(1-\langle n_{\bar\sigma}\rangle)\mathrm{Im}\,\Sigma^R]^2} + \frac{}{[(\omega-(\epsilon+U)/\hbar - \langle n_{\bar\sigma}\rangle\mathrm{Re}\,\Sigma^R]^2 + [\langle n_{\bar\sigma}\rangle\mathrm{Im}\,\Sigma^R]^2}\Bigg]$$

This is the sum of two Lorentzians. For the isolated quantum dot, the spin-resolved density of states consists of two delta-function peaks. We see that interactions shift the peaks and broaden them.

7.4. Tunneling current at $T=0$.

a) $$I(V,T) = +\frac{2e}{\hbar^2}\, \mathrm{Im}\, D^R_{AA}(\omega)\Big|_{\omega=-eV/\hbar}$$

where $$A = \sum_{kq\sigma} V_{kq}\, b^+_{q\sigma}\, c_{k\sigma}$$

$$D^R_{AA}(t) = -i\theta(t)\langle [A(t), A^+(0)]\rangle_0$$

The subscript "0" means that A evolves according to $\bar{H}_0 = H_L + H_R - \mu_L N_L - \mu_R N_R$.

$$D^R_{AA}(t) = -i\theta(t)\sum_{kq\sigma}\sum_{k'q'\sigma'} V_{kq} V^*_{k'q'} \langle [b^+_{q\sigma}(t)\, c_{k\sigma}(t),\, c^+_{k'\sigma'}(0)\, b_{q'\sigma'}(0)]\rangle_0$$

$$= \sum_{kq\sigma}\sum_{k'q'\sigma'} V_{kq} V^*_{k'q'}\, C^R(kk'qq'\sigma\sigma', t)$$

where

$$C^R(kk'qq'\sigma\sigma', t) = -i\theta(t)\langle [b^+_{q\sigma}(t)\, c_{k\sigma}(t),\, c^+_{k'\sigma'}(0)\, b_{q'\sigma'}(0)]\rangle_0$$

$$c_{k\sigma}(t) = e^{i\bar{H}_0 t/\hbar}\, c_{k\sigma}\, e^{-i\bar{H}_0 t/\hbar}$$

$$\dot{c}_{k\sigma} = \frac{i}{\hbar}[\bar{H}_0, c_{k\sigma}] = \frac{i}{\hbar}[\bar{H}_{0L} + \bar{H}_{0R}, c_{k\sigma}] = \frac{i}{\hbar}[H_{\alpha}, c_{k\sigma}]$$

$$= \frac{i}{\hbar}\Big[\sum_{k\sigma} \bar{\epsilon}_k\, c^+_{k\sigma} c_{k\sigma}, c_{k\sigma}\Big] = -\frac{i}{\hbar}\bar{\epsilon}_k\, c_{k\sigma}$$

$$\Rightarrow c_{k\sigma}(t) = e^{-i\bar{\epsilon}_k t/\hbar}\, c_{k\sigma}(0)$$

Hence $$c^+_{k\sigma}(t) = e^{i\epsilon_k t/\hbar}\, c^+_{k\sigma}(0)$$

Similarly,

$$b_{q\sigma}(t) = e^{-i\bar{\epsilon}_q t/\hbar}\, b_{q\sigma}(0), \quad b^+_{q\sigma}(t) = e^{i\bar{\epsilon}_q t/\hbar}\, b^+_{q\sigma}(0)$$

Therefore

$$C^R(kk'qq'\sigma\sigma', t) = -i\theta(t)\, e^{i(\bar{\epsilon}_q - \bar{\epsilon}_k)t/\hbar}\langle [b^+_{q\sigma} c_{k\sigma},\, c^+_{k'\sigma'} b_{q'\sigma'}]\rangle_0$$

Using

$$[AB, CD] = A\{B,C\}D - AC\{B,D\} + \{A,C\}DB - C\{A,D\}B$$

we find

$$\langle [b^+_{q\sigma} c_{k\sigma}, c^+_{k'\sigma'} b_{q\sigma}] \rangle_0 = \langle b^+_{q\sigma} \{ c_{k\sigma}, c^+_{k'\sigma'} \} b_{q'\sigma'} \rangle_0$$

$$- \langle b^+_{q\sigma} c^+_{k'\sigma'} \{ c_{k\sigma}, b_{q'\sigma'} \} \rangle + \langle \{ b^+_{q\sigma}, c^+_{k'\sigma'} \} b_{q\sigma} c_{k\sigma} \rangle_0 - \langle c^+_{k'\sigma'} \{ b^+_{q\sigma}, b_{q'\sigma'} \} c_{k\sigma} \rangle_0$$

Since c and b- operators anticommute,

$$\langle [b^+_{q\sigma} c_{k\sigma}, c^+_{k'\sigma'} b_{q\sigma}] \rangle_0 = \delta_{kk'} \delta_{\sigma\sigma'} \langle b^+_{q\sigma} b_{q'\sigma'} \rangle_0 - \delta_{qq'} \delta_{\sigma\sigma'} \langle c^+_{k'\sigma'} c_{k\sigma} \rangle_0$$

$$= \delta_{kk'} \delta_{\sigma\sigma'} \delta_{qq'} (f_q - f_k)$$

Hence

$$D^R_{AA}(t) = -i\theta(t) \sum_{kq\sigma} |V_{kq}|^2 (f_q - f_k) e^{i(\bar{\epsilon}_q - \bar{\epsilon}_k)t/\hbar}$$

and

$$D^R_{AA}(\omega) = \int_{-\infty}^{\infty} e^{i\omega t} D^R_{AA}(t) = -i \sum_{k\sigma q} |V_{k\sigma}|^2 (f_q - f_k) \int_0^\infty e^{i(\hbar\omega + \bar{\epsilon}_q - \bar{\epsilon}_k)t/\hbar} dt$$

$$= 2\hbar \sum_{kq} |V_{kq}|^2 (f_q - f_k) \frac{1}{\hbar\omega + \bar{\epsilon}_q - \bar{\epsilon}_k + i0^+}$$

The factor of 2 results from summing over σ. Thus

$$\mathrm{Im}\, D^R_{AA}(\omega) = -2\pi\hbar \sum_{kq} |V_{kq}|^2 (f_q - f_k) \delta(\hbar\omega + \bar{\epsilon}_q - \bar{\epsilon}_k)$$

where we used $1/(x+i0^+) = P(1/x) - i\pi\delta(x)$. The current is thus given by

$$I(V,T) = \frac{2e}{\hbar} \mathrm{Im}\, D^R_{AA}(\omega)\Big|_{\omega = -eV/\hbar} = -\frac{4\pi e}{\hbar} \sum_{kq} |V_{kq}|^2 (f_q - f_k) \delta(\bar{\epsilon}_q - \bar{\epsilon}_k - eV)$$

b) $$I(V, T=0) = -\frac{4\pi e}{\hbar} |\bar{V}|^2 D_L(0) D_R(0) \iint d\bar{\epsilon}_k \, d\bar{\epsilon}_q \, (f_q - f_k) \delta(\bar{\epsilon}_q - \bar{\epsilon}_k - eV)$$

$$= -\frac{4\pi e}{\hbar} |\bar{V}|^2 D_L(0) D_R(0) \int_{-eV}^{0} d\bar{\epsilon}_k \left[f(\bar{\epsilon}_k + eV) - f(\bar{\epsilon}_k) \right]$$

At $T=0$, for $-eV < \bar{\epsilon}_k < 0$, $f(\bar{\epsilon}_k + eV) = 0$, $f(\bar{\epsilon}_k) = 1$

$\Rightarrow$

$$I(V,T) = \frac{4\pi e^2 |V|^2}{\hbar} D_L(0) D_R(0) V = V/R$$

where

$$1/R = \frac{4\pi e^2}{\hbar} |\bar{V}|^2 D_L(0) D_R(0)$$

7.5 Magnetic impurity in a metal host.

a) $H = H_e + H_D + H_T$

$$H_e = \sum_{k\sigma} \epsilon_k c^+_{k\sigma} c_{k\sigma} \;, \quad H_D = \epsilon \sum_{\sigma} d^+_\sigma d_\sigma + U n_\uparrow n_\downarrow$$

$$H_T = \sum_{k\sigma} \left(V_k c^+_{k\sigma} d_\sigma + V_k^* d^+_\sigma c_{k\sigma} \right)$$

The retarded Green's function of the ~~dot~~ impurity

$$G^R_{d\sigma}(t) = -i\theta(t) \langle \{ d_\sigma(t), d^+_\sigma(0) \} \rangle$$

Its equation of motion is

$$i\hbar \frac{\partial}{\partial t} G^R_{d\sigma}(t) = -\hbar\delta(t) + \epsilon G^R_{d\sigma}(t) + U \Gamma^R_{d\sigma}(t) + \sum_k V_k^* G^R_{kd\sigma}(t)$$

where

$$G^R_{kd\sigma}(t) = -i\theta(t) \langle \{ c_{k\sigma}(t), d^+_\sigma(0) \} \rangle$$

and its equation of motion is

$$i\hbar \frac{\partial}{\partial t} G^R_{kd\sigma}(t) = \epsilon_k G^R_{kd\sigma}(t) + V_k G^R_{d\sigma}(t)$$

The term $\Gamma^R_{d\sigma}(t)$ is given by

$$\Gamma^R_{d\sigma}(t) = -i\theta(t) \langle \{ n_{\bar\sigma}(t) d_\sigma(t), d^+_\sigma(0) \} \rangle$$

All the above equations are derived in the text (Eqs. 7.16–19).

Applying the mean field approximation to $\Gamma^R_{d\sigma}(t)$, we find

$$\Gamma^R_{d\sigma}(t) \simeq \langle n_{\bar\sigma} \rangle G^R_{d\sigma}(t)$$

The equation of motion for $G^R_{d\sigma}(t)$ now becomes

$$i\hbar \frac{\partial}{\partial t} G^R_{d\sigma}(t) = \hbar\delta(t) + (\epsilon + \langle n_{\bar\sigma} \rangle U) G^R_{d\sigma}(t) + \sum_k V_k^* G^R_{kd\sigma}(t)$$

Writing

$$G^R_{d\sigma}(t) = \frac{1}{2\pi}\int e^{-i\omega t} G^R_{d\sigma}(\omega)d\omega \quad , \quad G^R_{kd\sigma}(t) = \frac{1}{2\pi}\int e^{-i\omega t} G^R_{kd\sigma}(\omega)d\omega$$

$$\delta(t) = \frac{1}{2\pi}\int e^{-i\omega t} d\omega \quad ,$$

we obtain

$$(\hbar\omega - \epsilon - \langle n_{\bar\sigma}\rangle U + i0^+)\, G^R_{d\sigma}(\omega) - \sum_k V_k^* G^R_{kd\sigma}(\omega) = \hbar$$

Similarly,

$$(\hbar\omega - \epsilon_k + i0^+)\, G^R_{kd\sigma}(\omega) = V_k G^R_{d\sigma}(\omega)$$

Solving the above two equations, we obtain

$$G^R_{d\sigma}(\omega) = \frac{\hbar}{\hbar\omega - \epsilon - \langle n_{\bar\sigma}\rangle U - \sum_k \frac{|V_k|^2}{\hbar\omega - \epsilon_k + i0^+}}$$

$$= \left[\omega - \epsilon/\hbar - \langle n_{\bar\sigma}\rangle U/\hbar - \Sigma^R\right]^{-1}$$

where

$$\Sigma^R = \frac{1}{\hbar}\sum_k \frac{|V_k|^2}{\hbar\omega - \epsilon_k + i0^+}$$

b) Ignoring $Re\,\Sigma$, and assuming that $\Delta = -\hbar\, Im\,\Sigma^R$ is independent of ω,

$$G^R_{d\sigma}(\omega) = \frac{\hbar}{\hbar\omega - \tilde\epsilon - i\hbar\, Im\,\Sigma} = \frac{\hbar}{\hbar\omega - \tilde\epsilon + i\Delta}$$

where

$$\tilde\epsilon = \epsilon + \langle n_{\bar\sigma}\rangle U$$

The spin-resolved density of states is

$$\rho_{d\sigma}(\omega) = -\frac{1}{\pi\hbar}\,\mathrm{Im}\,G^{R}_{d\sigma}(\omega) = \frac{1}{\pi}\,\frac{\Delta}{(\hbar\omega-\tilde{\epsilon})^2+\Delta^2}$$

$\langle n_\sigma\rangle$ is obtained by integrating $\rho_{d\sigma}$,

$$\langle n_\sigma\rangle = \frac{1}{\pi}\int_{-\infty}^{\epsilon_F}\frac{\Delta}{(\hbar\omega-\tilde{\epsilon})^2+\Delta^2}\,d(\hbar\omega) = \frac{1}{\pi}\cot^{-1}\frac{\tilde{\epsilon}-\epsilon_F}{\Delta}$$

That is

$$\langle n_\sigma\rangle = \frac{1}{\pi}\cot^{-1}\frac{\epsilon+\langle n_{\bar{\sigma}}\rangle U-\epsilon_F}{\Delta}$$

c)

$$\langle n_\uparrow\rangle = \frac{1}{\pi}\cot^{-1}\frac{\epsilon-\epsilon_F+\langle n_\downarrow\rangle U}{\Delta}$$

$$\langle n_\downarrow\rangle = \frac{1}{\pi}\cot^{-1}\frac{\epsilon-\epsilon_F+\langle n_\uparrow\rangle U}{\Delta}$$

Let $x = (\epsilon_F-\epsilon)/U$, $y = U/\Delta$

Then

$$\cot(\pi\langle n_\uparrow\rangle) = y(\langle n_\downarrow\rangle - x)$$

$$\cot(\pi\langle n_\downarrow\rangle) = y(\langle n_\uparrow\rangle - x)$$

Thus

$$\cot(\pi\langle n_\uparrow\rangle) - \cot(\pi\langle n_\downarrow\rangle) = -y(\langle n_\uparrow\rangle - \langle n_\downarrow\rangle)$$

Clearly, a nonmagnetic solution ($\langle n_\uparrow\rangle = \langle n_\downarrow\rangle$) satisfies the above equation. It is possible, however, for a magnetic solution to exist if $y \gg 1$. For example, if $\langle n_\downarrow\rangle = \alpha$ and $\langle n_\uparrow\rangle = 1-\alpha$, then the above equation reduces to

$$-2\cot(\pi\alpha) = -y(1-2\alpha)$$

and this equation has a solution when $\alpha \ll 1$ and $y \gg 1$.

Chapter 8

1. $\langle V \rangle$ and $\langle E \rangle$

$$\bar{H} = \sum_{\sigma_1} \int \psi^{\dagger}_{\sigma_1}(\vec{r}_1)\left(-\frac{\hbar^2}{2m}\nabla^2_{\vec{r}_1} - \mu\right)\psi_{\sigma}(\vec{r}_1)\, d^3r_1$$
$$+ \frac{1}{2}\sum_{\sigma_1\sigma_2} \int d^3r_1 \int d^3r_2\, \psi^{\dagger}_{\sigma_1}(\vec{r}_1)\psi^{\dagger}_{\sigma_2}(\vec{r}_2)\, v(\vec{r}_1-\vec{r}_2)\,\psi_{\sigma_2}(\vec{r}_2)\psi_{\sigma_1}(\vec{r}_1)$$
$$= \bar{H}_0 + V$$

$$\hbar\frac{\partial}{\partial t}\psi_{\sigma}(\vec{r}) = [\bar{H}, \psi_{\sigma}(\vec{r})]$$

$$[\bar{H}_0, \psi_{\sigma}(\vec{r})] = \sum_{\sigma_1}\int \left[\psi^{\dagger}_{\sigma_1}(\vec{r}_1)\left(-\frac{\hbar^2}{2m}\nabla^2_{\vec{r}_1} - \mu\right)\psi_{\sigma_1}(\vec{r}_1),\ \psi_{\sigma}(\vec{r})\right] d^3r_1$$

For the case of fermions, we use $[AB, C] = A\{B, C\} - \{A, C\}B$

where $A = \psi^{\dagger}_{\sigma_1}(\vec{r}_1)$, $B = \left(-\frac{\hbar^2}{2m}\nabla^2_{\vec{r}_1} - \mu\right)\psi_{\sigma_1}(\vec{r}_1)$

For the case of bosons, we use $[AB, C] = A[B, C] + [A, C]B$.

Using $[\psi_{\sigma_1}(\vec{r}_1), \psi_{\sigma}(\vec{r})]_{\mp} = 0$, $[\psi_{\sigma_1}(\vec{r}_1), \psi^{\dagger}_{\sigma}(\vec{r})]_{\mp} = \delta_{\sigma_1\sigma}\,\delta(\vec{r}-\vec{r}_1)$,

and noting that

$$\left[\left(-\frac{\hbar^2}{2m}\nabla^2_{\vec{r}_1} - \mu\right)\psi_{\sigma_1}(\vec{r}_1), \psi_{\sigma}(\vec{r})\right]_{\mp} = \left(-\frac{\hbar^2}{2m}\nabla^2_{\vec{r}_1} - \mu\right)[\psi_{\sigma_1}(\vec{r}_1), \psi_{\sigma}(\vec{r})]_{\mp} = 0,$$

we find

$$[\bar{H}_0, \psi_{\sigma}(\vec{r})] = -\sum_{\sigma_1}\delta_{\sigma_1\sigma}\int \delta(\vec{r}-\vec{r}_1)\left(-\frac{\hbar^2}{2m}\nabla^2_{\vec{r}_1} - \mu\right)\psi_{\sigma_1}(\vec{r}_1)\, d^3r_1$$
$$= \left(\frac{\hbar^2}{2m}\nabla^2 + \mu\right)\psi_{\sigma}(\vec{r})$$

Next we evaluate $[V, \psi_{\sigma}(\vec{r})]$. Since $[\psi_{\sigma_2}(\vec{r}_2)\psi_{\sigma_1}(\vec{r}_1), \psi_{\sigma}(\vec{r})] = 0$,

we obtain

$$[V, \psi_{\sigma}(\vec{r})] = \frac{1}{2}\sum_{\sigma_1\sigma_2}\int d^3r_1 \int d^3r_2\, [\psi^{\dagger}_{\sigma_1}(\vec{r}_1)\psi^{\dagger}_{\sigma_2}(\vec{r}_2), \psi_{\sigma}(\vec{r})]\, v(\vec{r}_1-\vec{r}_2)\psi_{\sigma_2}(\vec{r}_2)\psi_{\sigma_1}(\vec{r}_1)$$

For bosons,

$$[\psi^\dagger_{\sigma_1}(\vec r_1)\psi^\dagger_{\sigma_2}(\vec r_2),\psi_\sigma(\vec r)] = \psi^\dagger_{\sigma_1}(\vec r_1)[\psi^\dagger_{\sigma_2}(\vec r_2),\psi_\sigma(\vec r)] + [\psi^\dagger_{\sigma_1}(\vec r_1),\psi_\sigma(\vec r)]\psi^\dagger_{\sigma_2}(\vec r_2)$$

$$= -\delta_{\sigma_2\sigma}\,\delta(\vec r-\vec r_2)\psi^\dagger_{\sigma_1}(\vec r_1) - \delta_{\sigma_1\sigma}\,\delta(\vec r-\vec r_1)\psi^\dagger_{\sigma_2}(\vec r_2)$$

and

$$[V,\psi_\sigma(\vec r)] = -\frac{1}{2}\sum_{\sigma_1}\int d^3r_1\,\psi^\dagger_{\sigma_1}(\vec r_1)\,v(\vec r_1-\vec r)\,\psi_\sigma(\vec r)\psi_{\sigma_1}(\vec r_1)$$
$$-\frac{1}{2}\sum_{\sigma_2}\int d^3r_2\,\psi^\dagger_{\sigma_2}(\vec r_2)\,v(\vec r-\vec r_2)\,\psi_{\sigma_2}(\vec r_2)\psi_\sigma(\vec r)$$

since $v(\vec r_1-\vec r_2) = v(\vec r_2-\vec r_1)$, and for bosons $\psi_{\sigma_1}(\vec r_1)\psi_{\sigma_2}(\vec r_2) = \psi_{\sigma_2}(\vec r_2)\psi_{\sigma_1}(\vec r_1)$, it follows that

$$[V,\psi_\sigma(\vec r)] = -\frac{1}{2}\sum_{\sigma_1}\int d^3r_1\,\psi^\dagger_{\sigma_1}(\vec r_1)\,v(\vec r-\vec r_1)\,\psi_{\sigma_1}(\vec r_1)\psi_\sigma(\vec r)$$

For fermions,

$$[\psi^\dagger_{\sigma_1}(\vec r_1)\psi^\dagger_{\sigma_2}(\vec r_2),\psi_\sigma(\vec r)] = \psi^\dagger_{\sigma_1}(\vec r_1)\{\psi^\dagger_{\sigma_2}(\vec r_2),\psi_\sigma(\vec r)\} - \{\psi^\dagger_{\sigma_1}(\vec r_1),\psi_\sigma(\vec r)\}\psi^\dagger_{\sigma_2}(\vec r_2)$$

$$= \delta_{\sigma_2\sigma}\,\delta(\vec r-\vec r_2)\psi^\dagger_{\sigma_1}(\vec r_1) - \delta_{\sigma_1\sigma}\,\delta(\vec r-\vec r_1)\psi^\dagger_{\sigma_2}(\vec r_2)$$

Hence

$$[V,\psi_\sigma(\vec r)] = \frac{1}{2}\sum_{\sigma_1}\int\psi^\dagger_{\sigma_1}(\vec r_1)\,v(\vec r_1-\vec r)\,\psi_\sigma(\vec r)\psi_{\sigma_1}(\vec r_1)\,d^3r_1$$
$$-\frac{1}{2}\sum_{\sigma_2}\int\psi^\dagger_{\sigma_2}(\vec r_2)\,v(\vec r-\vec r_2)\,\psi_{\sigma_2}(\vec r_2)\psi_\sigma(\vec r)\,d^3r_2$$

For fermions, $\psi_\sigma(\vec r)\psi_{\sigma_1}(\vec r_1) = -\psi_{\sigma_1}(\vec r_1)\psi_\sigma(\vec r)$

Hence

$$[V,\psi_\sigma(\vec r)] = -\sum_{\sigma_1}\int\psi^\dagger_{\sigma_1}(\vec r_1)\,v(\vec r-\vec r_1)\,\psi_{\sigma_1}(\vec r_1)\psi_\sigma(\vec r)\,d^3r_1,$$

which is the same result as for bosons. Thus

$$\hbar\frac{\partial}{\partial\tau}\psi_\sigma(\vec r\tau) = \left[\frac{\hbar^2}{2m}\nabla^2+\mu-\sum_{\sigma_1}\int\psi^\dagger_{\sigma_1}(\vec r_1\tau)\,v(\vec r-\vec r_1)\,\psi_{\sigma_1}(\vec r_1\tau)\,d^3r_1\right]\psi_\sigma(\vec r\tau)$$

b) The above equation implies that

$$\sum_{\sigma_1} \int \psi^{+}_{\sigma_1}(\vec{r}_1\tau)\, v(\vec{r}-\vec{r}_1)\, \psi_{\sigma_1}(\vec{r}_1\tau)\, \psi_{\sigma}(\vec{r}\tau)\, d^3r_1 = \left[-\hbar\frac{\partial}{\partial\tau} + \frac{\hbar^2}{2m}\nabla^2 + \mu\right]\psi_\sigma(\vec{r}\tau)$$

Multiply on the left by $\psi^{+}_{\sigma}(\vec{r}\tau)$. On the LHS, the integration is over d^3r_1; hence $\psi^{+}_{\sigma}(\vec{r}\tau)$ can be moved inside the integral. On the RHS, we can move $\psi^{+}_{\sigma}(\vec{r}\tau)$ through the differential operator if we replace τ with τ' and take the limit $\tau' \to \tau^{+}$:

$$\sum_{\sigma_1} \int d^3r_1\, \psi^{+}_{\sigma}(\vec{r}\tau)\, \psi^{+}_{\sigma_1}(\vec{r}_1\tau)\, v(\vec{r}_1-\vec{r})\, \psi_{\sigma}(\vec{r}_1\tau)\, \psi_{\sigma}(\vec{r}\tau)$$

$$= \lim_{\vec{r}\,'\to\vec{r}}\ \lim_{\tau'\to\tau^{+}} \left[-\hbar\frac{\partial}{\partial\tau} + \frac{\hbar^2}{2m}\nabla^2 + \mu\right]\psi^{+}_{\sigma}(\vec{r}\,'\tau')\,\psi_{\sigma}(\vec{r}\tau)$$

Since

$$\psi^{+}_{\sigma}(\vec{r}\,'\tau^{+})\,\psi_{\sigma}(\vec{r}\tau) = \pm\langle T\psi_\sigma(\vec{r}\tau)\psi^{+}_{\sigma}(\vec{r}\,'\tau^{+})\rangle = \mp\, g(\vec{r}\sigma\tau, \vec{r}\,'\sigma\tau^{+}),$$

the desired result is obtained.

c) Take the limit $\vec{r}\,'\to\vec{r}$, sum over σ, multiply by $1/2$, and integrate over d^3r; we find

$$\langle V\rangle = \mp\frac{1}{2}\int d^3r \lim_{\vec{r}\,'\to\vec{r}}\ \lim_{\tau'\to\tau^{+}} \left(-\hbar\frac{\partial}{\partial\tau} + \frac{\hbar^2}{2m}\nabla^2 + \mu\right)\sum_\sigma g(\vec{r}\sigma\tau, \vec{r}\,'\sigma\tau')$$

d) The expression for the kinetic energy is given after Eq. (8.23),

$$\langle T\rangle = \mp\int d^3r \lim_{\vec{r}\,'\to\vec{r}} \sum_\sigma \left(-\frac{\hbar^2}{2m}\nabla^2\right) g(\vec{r}\sigma\tau, \vec{r}\,'\sigma\tau')$$

Adding this to $\langle V\rangle$, Eq. (8.25) is readily obtained.

8.2

a) $\bar{H}(\lambda) = H_0 - \mu N + \lambda V = \bar{H}_0 + \lambda V$

$$Z_{G\lambda} = \mathrm{Tr}\, e^{-\beta \bar{H}(\lambda)}$$

The thermodynamic potential is $\Omega_\lambda = -kT \ln Z_{G\lambda}$. Thus

$$\frac{\partial \Omega_\lambda}{\partial \lambda} = -kT Z_{G\lambda}^{-1} \frac{\partial Z_{G\lambda}}{d\lambda}$$

Expanding $e^{-\beta \bar{H}(\lambda)}$, we find

$$Z_{G\lambda} = \mathrm{Tr} \sum_{n=0}^{\infty} \frac{1}{n!} [-\beta \bar{H}(\lambda)]^n = \sum_{n=0}^{\infty} \frac{1}{n!} (-\beta)^n \mathrm{Tr}[(\bar{H}_0 + \lambda V)^n]$$

Hence

$$\frac{\partial Z_{G\lambda}}{\partial \lambda} = \sum_{n=1}^{\infty} \frac{1}{n!} (-\beta)^n \frac{\partial}{\partial \lambda} \mathrm{Tr}[(\bar{H}_0 + \lambda V)^n]$$

Note that

$$\frac{\partial}{\partial \lambda} \mathrm{Tr}[(\bar{H}_0 + \lambda V)^n] = \frac{\partial}{\partial \lambda} \sum_m \langle m | (\bar{H}_0 + \lambda V)(\bar{H}_0 + \lambda V) \cdots (\bar{H}_0 + \lambda V) | m \rangle$$

$$= \sum_m \langle m | V(\bar{H}_0 + \lambda V) \cdots (\bar{H}_0 + \lambda V) | m \rangle + \sum_m \langle m | (\bar{H}_0 + \lambda V) V (H_0 + \lambda V) \cdots (\bar{H}_0 + \lambda V) | m \rangle$$

$$+ \cdots + \sum_m \langle m | (\bar{H}_0 + \lambda V) \cdots (\bar{H}_0 + \lambda V) V | m \rangle$$

$$= \mathrm{Tr}[V(\bar{H}_0 + \lambda V)^{n-1}] + \mathrm{Tr}[(\bar{H}_0 + \lambda V) V (\bar{H}_0 + \lambda V)^{n-2}] + \cdots$$

$$+ \mathrm{Tr}[(\bar{H}_0 + \lambda V)^{n-1} V]$$

$$= n\, \mathrm{Tr}[(\bar{H}_0 + \lambda V)^{n-1} V]$$

In the last step we have used the cyclic permutation property of the trace: $\mathrm{Tr}(AB \cdots CD) = \mathrm{Tr}(DAB \cdots C)$

b) $$\frac{\partial Z_{G\lambda}}{\partial \lambda} = -\beta \sum_{n=1}^{\infty} \frac{1}{(n-1)!}(-\beta)^{n-1}\, Tr[(\bar{H}_0+\lambda V)^{n-1} V]$$

where we used the result from part (a). Hence

$$\frac{\partial Z_{G\lambda}}{\partial \lambda} = -\beta\, Tr\left[\sum_{n=0}^{\infty} \frac{(-\beta)^n}{n!}(\bar{H}(\lambda))^n V\right]$$

$$= -\beta\, Tr\left[e^{-\beta \bar{H}(\lambda)} V\right] = -\beta \frac{Tr[e^{-\beta\bar{H}(\lambda)}]\, Tr[e^{-\beta\bar{H}(\lambda)} V]}{Tr[e^{-\beta\bar{H}(\lambda)}]}$$

$$= -\beta Z_{G\lambda}\langle V\rangle_\lambda = -\beta e^{-\beta\Omega_\lambda}\langle V\rangle_\lambda$$

$$= -\frac{\beta}{\lambda} e^{-\beta\Omega_\lambda}\langle \lambda V\rangle_\lambda$$

where $\langle\cdots\rangle_\lambda$ is the ensemble average with respect to $\bar{H}(\lambda)$.

c) Using

$$\frac{\partial\Omega_\lambda}{\partial\lambda} = -kT Z_{G\lambda}^{-1}\frac{\partial Z_{G\lambda}}{\partial\lambda},$$

we find

$$\frac{\partial\Omega_\lambda}{\partial\lambda} = -kT Z_{G\lambda}^{-1}\left(-\frac{\beta}{\lambda}\right) Z_{G\lambda}\langle\lambda V\rangle_\lambda = \frac{1}{\lambda}\langle\lambda V\rangle_\lambda$$

d) $$\int_0^1 d\lambda\, \frac{\partial\Omega_\lambda}{\partial\lambda} = \Omega - \Omega_0 = \int_0^1 \frac{d\lambda}{\lambda}\langle\lambda V\rangle_\lambda$$

Using the result of problem 8.1, we can write

$$\langle\lambda V\rangle_\lambda = \mp\frac{1}{2}\int d^3r \lim_{\vec{r}'\to\vec{r}}\lim_{\tau'\to\tau^+}\left[-\hbar\frac{\partial}{\partial\tau}+\frac{\hbar^2\nabla^2}{2m}+\mu\right]\sum_\sigma \mathcal{G}^\lambda(\vec{r}\sigma\tau,\vec{r}'\sigma\tau')$$

$$\Rightarrow \Omega(T,V,\mu) = \Omega_0(T,V,\mu) \mp \frac{1}{2}\int_0^1\frac{d\lambda}{\lambda}\int d^3r \lim_{\vec{r}'\to\vec{r}}\lim_{\tau'\to\tau^+}\left[-\hbar\frac{\partial}{\partial\tau}+\frac{\hbar^2}{2m}\nabla^2+\mu\right]\sum_\sigma \mathcal{G}^\lambda(\vec{r}\sigma\tau,\vec{r}'\sigma\tau')$$

8.3 Discontinuity in g°.

The expression for $g^\circ(k\sigma,\tau)$ is given after Eq. (8.43b).

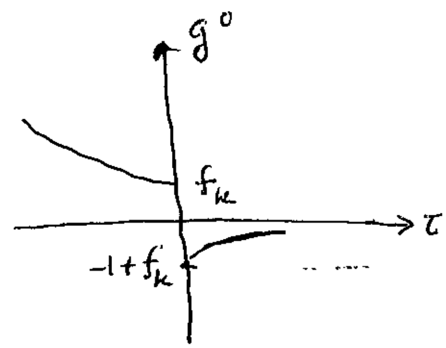
For fermions,

$$g^\circ(k\sigma,\tau) = \left[-\theta(\tau)(1-f_{k\sigma}) + \theta(-\tau) f_{k\sigma}\right] e^{-\bar{\epsilon}_k \tau/\hbar}$$

For $\tau<0$, $g^\circ(k\sigma,\tau) = f_{k\sigma}\, e^{-\bar{\epsilon}_k \tau/\hbar}$

For $\tau>0$, $g^\circ(k\sigma,\tau) = (-1+f_{k\sigma})\, e^{-\bar{\epsilon}_k \tau/\hbar}$

Hence, at $\tau=0$, the discontinuity is -1



8.4 Equation 8.66b.

Consider any interaction picture operator $\hat{B}$. Then

$$\langle\{\hat{c}^{\dagger}_{k\sigma}, \hat{B}\}\rangle_0 = Z^{-1}_{G,0}\, Tr\left[e^{-\beta\bar{H}_0}\, \hat{c}^{\dagger}_{k\sigma} \hat{B} + e^{-\beta\bar{H}_0} \hat{B}\, \hat{c}^{\dagger}_{k\sigma}\right]$$

$$= Z^{-1}_{G,0}\left(Tr\left[e^{-\beta\bar{H}_0}\, \hat{c}^{\dagger}_{k\sigma}\, \hat{B}\right] + Tr\left[\hat{c}^{\dagger}_{k\sigma} e^{-\beta\bar{H}_0}\, \hat{B}\right]\right)$$

Note that

$$[c^{\dagger}_{k\sigma}, \bar{H}_0] = -\epsilon_{k\sigma}\, c^{\dagger}_{k\sigma}$$

The same steps leading to Eq. (8.66a) are now followed, the only difference being that $c_{k\sigma} \to c^{\dagger}_{k\sigma}$ and $\epsilon_{k\sigma} \to -\epsilon_{k\sigma}$. Equation (8.66b) is then obtained.

5. Wick's theorem for bosons

We follow the same steps as in the case of fermions.

(a) First, Eqs. (8.63) and (8.64) are valid for bosons if the commutator replaces the anticommutator,

$$[\hat{c}_{k\sigma}(\tau_1), \hat{c}_{k'\sigma'}(\tau_2)] = [\hat{c}^{+}_{k\sigma}(\tau_1), \hat{c}^{+}_{k'\sigma'}(\tau_2)] = 0$$

$$[\hat{c}_{k\sigma}(\tau_1), \hat{c}^{+}_{k'\sigma'}(\tau_2)] = e^{\bar{\epsilon}_{k\sigma}(\tau_2-\tau_1)/\hbar}\,\delta_{kk'}\delta_{\sigma\sigma'}.$$

(b) Following the same steps leading to Eqs. (8.66a) and (8.66b), we obtain

$$\langle[\hat{c}_{k\sigma}, \hat{B}]\rangle_0 = (1-e^{-\beta\bar{\epsilon}_{k\sigma}})\langle\hat{c}_{k\sigma}\hat{B}\rangle_0$$

and

$$\langle[\hat{c}^{+}_{k\sigma}, \hat{B}]\rangle_0 = (1-e^{\beta\bar{\epsilon}_{k\sigma}})\langle\hat{c}^{+}_{k\sigma}\hat{B}\rangle_0$$

(c) Let $b_1, b_2, \dots, b_{2n}$ be boson operators in the interaction picture. We want to find $[b_1, b_2 b_3 \cdots b_{2n}]$. Consider the case $n=2$,

$$\begin{aligned}[b_1, b_2b_3b_4] &= b_1b_2b_3b_4 - b_2b_3b_4b_1 = [b_1, b_2]b_3b_4 \\ &\quad + b_2b_1b_3b_4 - b_2b_3b_4b_1 \\ &= [b_1, b_2]b_3b_4 + b_2[b_1, b_3]b_4 + b_2b_3b_1b_4 - b_2b_3b_4b_1 \\ &= [b_1, b_2]b_3b_4 + [b_1, b_3]b_2b_4 + b_2b_3[b_1, b_4]\end{aligned}$$

We can then prove by mathematical induction that

$$[b_1, b_2b_3\cdots b_{2n}] = \sum_{m=2}^{2n}[b_1, b_m]\prod_{k=2}^{2n}{}' b_k$$

where the prime on Π indicates that $k=m$ is excluded.

d) Wick's theorem is true for $m=1$. Assume it is true for $m=n-1$, i.e., assume that

$$\langle T \prod_{i=1}^{2n-2} a_i \rangle_0 = \sum \prod \langle T a_i a_j \rangle_0$$

and we show that it is true for $m=n$, i.e., we need to show that

$$\langle T \prod_{i=1}^{2n} a_i \rangle_0 = \sum \prod \langle T a_i a_j \rangle_0$$

The sum is over all possible ways of picking pairs.

First, let $b_1, b_2, \ldots, b_{2n}$ be a permutation of $a_1, a_2, \ldots, a_{2n}$ such that $b_1, b_2, \ldots, b_{2n}$ are arranged in descending time order from left to right. Then

$$\langle T \prod_{i=1}^{2n} a_i \rangle_0 = \langle \prod_{i=1}^{2n} b_i \rangle_0 = \langle b_1 \prod_{k=2}^{2n} b_k \rangle_0$$

Let $B = \prod_{k=2}^{2n} b_k$. Then

$$\langle \prod_{i=1}^{2n} a_i \rangle_0 = (1 - e^{\pm\beta \bar{\epsilon}_k})^{-1} \langle [b_1, \prod_{k=2}^{2n} b_k] \rangle_0$$

In the exponent, the $+(-)$ sign corresponds to $b_1 = c^{+}_{k\sigma}$ $(c_{k\sigma})$.

Using the result in (c) and the fact that the commutator of two interaction picture boson operators is a number, we obtain

$$\langle T \prod_{i=1}^{2n} a_i \rangle_0 = (1 - e^{\pm\beta \bar{\epsilon}_k})^{-1} \sum_{m=2}^{2n} [b_1, b_m] \langle {\prod_{k=2}^{2n}}' b_k \rangle_0$$

The prime on the product symbol means that the term $k=m$ is excluded. Since $[b_1, b_m]$ is a number, then we find upon using (b)

$$[b_1, b_m] = \langle [b_1, b_m] \rangle_0 = (1 - e^{\pm\beta \bar{\epsilon}_k}) \langle b_1 b_m \rangle_0$$
$$= (1 - e^{\pm\beta \bar{\epsilon}_k}) \langle T b_1 b_m \rangle_0$$

Hence,

$$\langle T \prod_{i=1}^{2n} a_i \rangle_0 = \sum_{m=2}^{2n} \langle T b_1 b_m \rangle_0 \langle \prod_{k=2}^{2n}{}' \, b_k \rangle_0$$

$$= \sum_{m=2}^{2n} \langle T b_1 b_m \rangle_0 \langle T \prod_{k=2}^{2n}{}' \, b_k \rangle_0 .$$

Note that $\langle T \prod_{k=2}^{2n}{}' \, b_k \rangle_0$ is the ensemble average of the time-ordered product of $2n-2$ operators. By assumption, Wick's theorem is true for such a product. That is, $\langle T \prod_{k=2}^{2n}{}' \, b_k \rangle_0$ is the sum over all contracted pairs that can be formed from the $2n-2$ operators. By summing over m in the above equation, we exhaust all pairs that can be formed from the $2n$ operators. Hence, Wick's theorem is true for $m=n$ if we assume that it is true for $m=n-1$.

8.6 Wick's Theorem

Let us assume that $\tau > \tau'$. Then

$$A = \langle \hat{N}(\tau)\hat{N}(\tau')\rangle_0 = \langle T\, \hat{N}(\tau)\hat{N}(\tau')\rangle_0$$

$$= \sum_{k\sigma}\sum_{k'\sigma'} \langle T\, \hat{c}^\dagger_{k\sigma}(\tau)\hat{c}_{k\sigma}(\tau)\hat{c}^\dagger_{k'\sigma'}(\tau')\hat{c}_{k'\sigma'}(\tau')\rangle_0$$

We now apply Wick's theorem

$$A = \sum_{k\sigma}\sum_{k'\sigma'} \langle T\hat{c}_{k\sigma}(\tau)\hat{c}^\dagger_{k\sigma}(\tau)\rangle_0 \langle T\hat{c}_{k'\sigma'}(\tau')\hat{c}^\dagger_{k'\sigma'}(\tau')\rangle_0$$

$$\pm \sum_{k\sigma}\sum_{k'\sigma'} \langle T\hat{c}_{k'\sigma'}(\tau')\hat{c}^\dagger_{k\sigma}(\tau)\rangle_0 \langle T\hat{c}_{k\sigma}(\tau)\hat{c}^\dagger_{k'\sigma'}(\tau')\rangle_0$$

The lower (upper) sign refers to the case when the c-operators are fermionic (bosonic). Thus

$$A = \sum_{k\sigma} g^0(k\sigma,0^-)\sum_{k'\sigma'} g^0(k'\sigma',0^-) \pm \sum_{k\sigma}\sum_{k'\sigma'}\delta_{kk'}\delta_{\sigma\sigma'}\, g^0(k\sigma,\tau'-\tau)\, g^0(k\sigma,\tau-\tau')$$

$$= \Big(\sum_{k\sigma} g^0(k\sigma,0^-)\Big)^2 \pm \sum_{k\sigma} g^0(k\sigma,\tau'-\tau)\, g^0(k\sigma,\tau-\tau')$$

We know that

$$g^0(\tau) = \left[-\theta(\tau)\begin{Bmatrix}1+n_{k\sigma}\\ 1-f_{k\sigma}\end{Bmatrix} \mp \theta(-\tau)\begin{Bmatrix}n_{k\sigma}\\ f_{k\sigma}\end{Bmatrix}\right] e^{-\bar{\epsilon}_{k\sigma}\tau/\hbar}$$

for $\tau > \tau'$,

$$g^0(\tau-\tau') = -\begin{Bmatrix}1+n_{k\sigma}\\ 1-f_{k\sigma}\end{Bmatrix} e^{-\bar{\epsilon}_{k\sigma}(\tau-\tau')/\hbar}$$

$$g^0(\tau'-\tau) = \mp\begin{Bmatrix}n_{k\sigma}\\ f_{k\sigma}\end{Bmatrix} e^{-\bar{\epsilon}_{k}(\tau'-\tau)/\hbar}$$

$$g^0(k\sigma,0^-) = \mp\begin{Bmatrix}n_{k\sigma}\\ f_{k\sigma}\end{Bmatrix}$$

Therefore, for fermions

$$A = \Big(\sum_{k\sigma} f_{k\sigma}\Big)^2 + \sum_{k\sigma} f_{k\sigma}(1-f_{k\sigma}),$$

while for bosons

$$A = \Big(\sum_{k\sigma} n_{k\sigma}\Big)^2 + \sum_{k\sigma} n_{k\sigma}(1+n_{k\sigma})$$

A is independent of τ and τ', as it should be since N commutes with $\bar{H}_0$ so that $\hat{N}(\tau) = e^{\bar{H}_0\tau/\hbar} N e^{-\bar{H}_0\tau/\hbar} = N e^{\bar{H}_0\tau/\hbar} e^{-\bar{H}_0\tau/\hbar} = N$

That is, $\hat{N}(\tau)$ is independent of τ, so A is also independent of τ and τ'. In fact, we could have used this observation to shorten the calculation a bit.

8.7 An equation for g°

a) $$g^\circ(\vec{r}-\vec{r}'\sigma, \tau-\tau') = -\langle T\psi_\sigma(\vec{r}\tau)\psi_\sigma^+(\vec{r}'\tau')\rangle_0$$
$$= -\theta(\tau-\tau')\langle\psi_\sigma(\vec{r}\tau)\psi_\sigma^+(\vec{r}'\tau')\rangle_0 \mp \theta(\tau'-\tau)\langle\psi_\sigma^+(\vec{r}'\tau')\psi_\sigma(\vec{r}\tau)\rangle_0$$

$$\hbar\frac{\partial}{\partial\tau}g^\circ(\vec{r}-\vec{r}'\sigma, \tau-\tau') = -\hbar\delta(\tau-\tau')\langle\psi_\sigma(\vec{r}\tau)\psi_\sigma^+(\vec{r}'\tau)\rangle_0$$
$$-\theta(\tau-\tau')\langle\hbar\frac{\partial}{\partial\tau}\psi_\sigma(\vec{r}\tau)\psi_\sigma^+(\vec{r}'\tau')\rangle_0$$
$$\pm\hbar\,\delta(\tau-\tau')\langle\psi_\sigma^+(\vec{r}'\tau)\psi_\sigma(\vec{r}\tau)\rangle_0 \mp\theta(\tau'-\tau)\langle\psi_\sigma^+(\vec{r}'\tau')\hbar\frac{\partial}{\partial\tau}\psi_\sigma(\vec{r}\tau)\rangle_0$$
$$= -\hbar\delta(\tau-\tau')\langle[\psi_\sigma(\vec{r}\tau), \psi_\sigma^+(\vec{r}'\tau)]_\mp\rangle_0$$
$$-\theta(\tau-\tau')\langle\hbar\frac{\partial}{\partial\tau}\psi_\sigma(\vec{r}\tau)\psi_\sigma^+(\vec{r}'\tau')\rangle_0$$
$$\mp\theta(\tau'-\tau)\langle\psi_\sigma^+(\vec{r}'\tau')\hbar\frac{\partial}{\partial\tau}\psi_\sigma(\vec{r}\tau)\rangle_0$$

Note that
$$[\psi_\sigma(\vec{r}\tau), \psi_\sigma^+(\vec{r}'\tau)]_\mp = \delta(\vec{r}-\vec{r}')$$
and
$$\hbar\frac{\partial}{\partial\tau}\psi_\sigma(\vec{r}\tau) = [\bar{H}, \psi_\sigma(\vec{r}\tau)]$$
Since we are interested in the equation for g°, we set $\bar{H} = \bar{H}_0$. Then,
$$[\bar{H}_0, \psi_\sigma(\vec{r}\tau)] = \left[\sum_\sigma\int\psi_\sigma^\dagger(\vec{r}\tau)\left(-\frac{\hbar^2}{2m}\nabla^2-\mu\right)\psi_\sigma(\vec{r}\tau)\,d^3r, \psi_\sigma(\vec{r}\tau)\right]$$
Using $[AB, C] = A[B, C]_\mp \pm [A, C]_\mp B$, we find
$$[\bar{H}_0, \psi_\sigma(\vec{r}\tau)] = \left(\frac{\hbar^2}{2m}\nabla^2+\mu\right)\psi_\sigma(\vec{r}\tau)$$

Therefore,

$$\hbar \frac{\partial}{\partial\tau} g^{\circ}(\vec{r}-\vec{r}'\sigma,\tau-\tau') = -\hbar\delta(\tau-\tau')\delta(\vec{r}-\vec{r}')$$

$$-\theta(\tau-\tau')\left(\frac{\hbar^2}{2m}\nabla^2+\mu\right)\langle\psi_\sigma(\vec{r}\tau)\psi_\sigma^\dagger(\vec{r}'\tau')\rangle_0$$

$$\mp\theta(\tau'-\tau)\left(\frac{\hbar^2}{2m}\nabla^2+\mu\right)\langle\psi_\sigma^\dagger(\vec{r}'\tau')\psi_\sigma(\vec{r}\tau)\rangle_0$$

$$= -\hbar\delta(\tau-\tau')\delta(\vec{r}-\vec{r}') - \left(\frac{\hbar^2}{2m}\nabla^2+\mu\right)\langle T\psi_\sigma(\vec{r}\tau)\psi_\sigma^\dagger(\vec{r}'\tau')\rangle_0$$

$$= -\hbar\delta(\tau-\tau')\delta(\vec{r}-\vec{r}') + \left(\frac{\hbar^2}{2m}\nabla^2+\mu\right)g^{\circ}(\vec{r}-\vec{r}'\sigma,\tau-\tau')$$

Hence,

$$\left(-\hbar\frac{\partial}{\partial\tau}+\frac{\hbar^2}{2m}\nabla^2+\mu\right)g^{\circ}(\vec{r}-\vec{r}'\sigma,\tau-\tau') = \hbar\delta(\tau-\tau')\delta(\vec{r}-\vec{r}')$$

b) $$g^{\circ}(\vec{r}-\vec{r}'\sigma,\tau-\tau') = \frac{1}{\beta\hbar V}\sum_{\vec{k}n} g^{\circ}(\vec{k}\sigma,\omega_n)e^{i\vec{k}\cdot(\vec{r}-\vec{r}')}e^{-i\omega_n(\tau-\tau')}$$

$$\delta(\vec{r}-\vec{r}') = \frac{1}{V}\sum_{\vec{k}} e^{i\vec{k}\cdot(\vec{r}-\vec{r}')} \quad , \quad \delta(\tau-\tau') = \frac{1}{\beta\hbar}\sum_{n=-\infty}^{\infty} e^{-i\omega_n(\tau-\tau')}$$

Thus

$$\frac{1}{\beta\hbar V}\sum_{\vec{k}n}\left(i\hbar\omega_n - \frac{\hbar^2k^2}{2m}+\mu\right)g^{\circ}(\vec{k}\sigma,\omega_n)\,e^{i\vec{k}\cdot(\vec{r}-\vec{r}')}e^{-i\omega_n(\tau-\tau')}$$

$$= \frac{\hbar}{\beta\hbar V}\sum_{\vec{k}n} e^{i\vec{k}\cdot(\vec{r}-\vec{r}')}e^{-i\omega_n(\tau-\tau')}$$

$$\Rightarrow \quad g^{\circ}(\vec{k}\sigma,\omega_n) = \frac{\hbar}{i\hbar\omega_n - \hbar^2k^2/2m+\mu} = \frac{1}{i\omega_n - \epsilon_{\vec{k}}/\hbar}$$

8.8 Analytic continuation

a)

$$C^R_{\tilde{A}\tilde{B}}(\omega) = Z_G^{-1} \sum_{nm} \frac{\langle n|\tilde{A}|m\rangle\langle m|\tilde{B}|n\rangle(e^{-\beta\bar{E}_n} \mp e^{-\beta\bar{E}_m})}{\omega - (\bar{E}_m - \bar{E}_n)/\hbar + i0^+}$$

Since $\tilde{A} = A - \langle A\rangle$, $\tilde{B} = B - \langle B\rangle$, it follows that

$$\langle n|\tilde{A}|m\rangle\langle m|\tilde{B}|n\rangle = \langle n|A|m\rangle\langle m|B|n\rangle - \langle A\rangle\langle n|m\rangle\langle m|B|n\rangle$$

$$- \langle n|A|m\rangle\langle m|n\rangle\langle B\rangle + \langle A\rangle\langle B\rangle\langle n|m\rangle\langle m|n\rangle$$

$$= \langle n|A|m\rangle\langle m|B|n\rangle - \delta_{nm}\langle A\rangle\langle n|B|n\rangle$$

$$- \delta_{nm}\langle B\rangle\langle n|A|n\rangle + \langle A\rangle\langle B\rangle\delta_{nm}$$

Therefore

$$C^R_{\tilde{A}\tilde{B}}(\omega) - C^R_{AB}(\omega)$$

$$= Z_G^{-1} \sum_n \frac{(e^{-\beta\bar{E}_n} \mp e^{-\beta\bar{E}_n})}{\omega + i0^+}\left[\langle A\rangle\langle B\rangle - \langle A\rangle\langle n|B|n\rangle - \langle B\rangle\langle n|A|n\rangle\right]$$

If A and B are bosonic operators, the right hand side vanishes $(e^{-\beta\bar{E}_n} - e^{-\beta\bar{E}_n} = 0)$. If A and B are fermionic operators, then $\langle A\rangle = \langle B\rangle = 0$, and the RHS vanishes. Thus

$$C^R_{\tilde{A}\tilde{B}}(\omega) = C^R_{AB}(\omega)$$

b)

$$C^T_{\tilde{A}\tilde{B}}(\tau) = -\langle T\tilde{A}(\tau)\tilde{B}(0)\rangle = -\left\langle T\left[A(\tau) - \langle A(\tau)\rangle\right]\left[B(0) - \langle B(0)\rangle\right]\right\rangle$$

Since $\bar{H}$ is time-independent, $\langle A(\tau)\rangle = \langle A(0)\rangle \equiv \langle A\rangle$. Thus

$$C^T_{\tilde{A}\tilde{B}}(\tau) = -\langle TA(\tau)B(0)\rangle + \langle A\rangle\langle B\rangle + \langle A\rangle\langle B\rangle - \langle A\rangle\langle B\rangle$$

$$= -\langle TA(\tau)B(0)\rangle + \langle A\rangle\langle B\rangle$$

$$= C^T_{AB}(\tau) + \langle A\rangle\langle B\rangle$$

$$\Rightarrow C^T_{AB}(\tau) = C^T_{\tilde{A}\tilde{B}}(\tau) - \langle A\rangle\langle B\rangle$$

$$C^T_{AB}(\omega_n) = C^T_{\tilde{A}\tilde{B}}(\omega_n) - \int_0^{\beta\hbar} e^{i\omega_n\tau} \langle A\rangle\langle B\rangle d\tau$$

If A and B are fermion creation or annihilation operators, then $\langle A\rangle = \langle B\rangle = 0$ and $C^T_{AB}(\omega_n) = C^T_{\tilde{A}\tilde{B}}(\omega_n)$.

If A and B are bosonic operators (an operators such as $c^\dagger c$ is considered bosonic even if c and $c^\dagger$ are fermionic), then $\langle A\rangle \neq 0$ and $\langle B\rangle \neq 0$ in general. Thus, for bosons

$$C^T_{AB}(\omega_n) = C^T_{\tilde{A}\tilde{B}}(\omega_n) - \beta\hbar \langle A\rangle\langle B\rangle \delta_{\omega_n,0}$$

c) $$C^R_{AB}(\omega) = C^R_{\tilde{A}\tilde{B}}(\omega) = Z_G^{-1} \sum_{i,j} \frac{\langle i|A|j\rangle\langle j|B|i\rangle(e^{-\beta\bar{E}_i} \mp e^{-\beta\bar{E}_j})}{\omega - (\bar{E}_j - \bar{E}_i)/\hbar + i0^+}$$

$$C^T_{AB}(\omega_n) = Z_G^{-1} \sum_{i,j} \frac{\langle i|A|j\rangle\langle j|B|i\rangle(e^{-\beta\bar{E}_i} \mp e^{-\beta\bar{E}_j})}{i\omega_n - (\bar{E}_j - \bar{E}_i)/\hbar}$$

same expression holds for $C^T_{\tilde{A}\tilde{B}}(\omega_n)$ if only we replace A by $\tilde{A}$ and B by $\tilde{B}$.

It looks like (i) $C^R_{AB}(\omega) = C^T_{AB}(\omega_n)\big|_{i\omega_n \to \omega + i0^+}$ and

(ii) $C^R_{\tilde{A}\tilde{B}}(\omega) = C^T_{\tilde{A}\tilde{B}}(\omega_n)\big|_{i\omega_n\to\omega+i0^+}$.

However, while $C^R_{AB}(\omega) = C^R_{\tilde{A}\tilde{B}}(\omega)$, we have seen that $C^T_{\tilde{A}\tilde{B}}(\omega_n)$ is not equal to $C^T_{AB}(\omega_n)$. Thus (i) and (ii) cannot be correct simultaneously. To resolve this, note that

* If $B(0)=1$ or $A(\tau)=1$ then $C^R_{AB}(\tau) = -i\theta(\tau)\langle[A(\tau),B(0)]\rangle = 0$.

However,

$$C^T_{AB}(\tau) = -\langle T A(\tau)B(0)\rangle = \begin{cases} -\langle A(\tau)\rangle & \text{if } B(0)=1 \\ -\langle B(0)\rangle & \text{if } A(\tau)=1 \end{cases}$$

Thus, if $B=1$, $C^R_{\tilde{A}\tilde{B}}(\omega)=0$ and $C^T_{\tilde{A}\tilde{B}}(\omega_n)=0$, but

$$C^T_{AB}(\omega_n) = -\langle A\rangle\delta_{\omega_n,0} \quad \text{and} \quad C^R_{AB}(\omega)=0$$

Thus $$C^T_{\tilde{A}\tilde{B}}(\omega_n)\big|_{i\omega_n\to\omega+i0^+} = C^R_{\tilde{A}\tilde{B}}(\omega)$$

Chapter 9

1. A vanishing sum

First for bosons:

$$\lim_{\delta\to 0^+} \sum_{n=-\infty}^{\infty} e^{i\omega_n\delta} = \lim_{\delta\to 0^+} \sum_{n=-\infty}^{0} e^{i2n\pi\delta/\beta\hbar} + \sum_{n=0}^{\infty} e^{i2n\pi\delta/\beta\hbar} - 1$$

$$= \lim_{\delta\to 0^+} \sum_{n=-\infty}^{0} \left(e^{2\pi i\delta/\beta\hbar}\right)^n + \lim_{\delta\to 0^+} \sum_{n=0}^{\infty} \left(e^{2\pi i\delta/\beta\hbar}\right)^n - 1$$

$$= \lim_{\delta\to 0^+} \sum_{n=0}^{\infty} \left(e^{-2\pi i\delta/\beta\hbar}\right)^n + \lim_{\delta\to 0^+} \sum_{n=0}^{\infty} \left(e^{2\pi i\delta/\beta\hbar}\right)^n - 1$$

$$= \lim_{\delta\to 0^+} \frac{1}{1-e^{-2\pi i\delta/\beta\hbar}} + \lim_{\delta\to 0^+} \frac{1}{1-e^{2\pi i\delta/\beta\hbar}} - 1$$

$$= \lim_{\delta\to 0^+} \frac{2-e^{2\pi i\delta/\beta\hbar}-e^{-2\pi i\delta/\beta\hbar}}{\left(1-e^{-2\pi i\delta/\beta\hbar}\right)\left(1-e^{2\pi i\delta/\beta\hbar}\right)} - 1$$

$$= \lim_{\delta\to 0^+} \frac{2\left[1-\cos(2\pi\delta/\beta\hbar)\right]}{2\left[1-\cos(2\pi\delta/\beta\hbar)\right]} - 1 = 0$$

For fermions,

$$\lim_{\delta\to 0^+} \sum_{n=-\infty}^{\infty} e^{i\omega_n\delta} = \lim_{\delta\to 0^+} \sum_{n} e^{i(2n+1)\pi\delta/\beta\hbar}$$

$$= \lim_{\delta\to 0^+} e^{\pi i\delta/\beta\hbar} \sum_{n=-\infty}^{\infty} e^{i2n\pi\delta/\beta\hbar} = (1)(0) = 0$$

2. Thermodynamic potential

Equation (8.26) reads

$$\Omega(T,V,\mu) = \Omega_0(T,V,\mu) \mp \frac{1}{2}\int_0^1 \frac{d\lambda}{\lambda}\int d^3r \lim_{\vec{r}'\to\vec{r}} \lim_{\tau'\to\tau^+} \left[-\hbar\frac{\partial}{\partial\tau} + \frac{\hbar^2}{2m}\nabla^2 + \mu\right]\sum_\sigma g^\lambda(\vec{r}\sigma\tau, \vec{r}'\sigma\tau')$$

Assuming a translationally invariant system,

$$g^\lambda(\vec{r}\sigma\tau, \vec{r}'\sigma\tau') = \frac{1}{V\beta\hbar}\sum_{\vec{k}}\sum_n e^{i\vec{k}\cdot(\vec{r}-\vec{r}')}\, e^{-i\omega_n(\tau-\tau')}\, g^\lambda(\vec{k}\sigma,\omega_n)$$

Thus

$$\Omega = \Omega_0 \mp \frac{1}{2V\beta\hbar}\int_0^1 \frac{d\lambda}{\lambda}\int d^3r \sum_{\vec{k}\sigma n} e^{i\omega_n 0^+}\left(i\hbar\omega_n - \frac{\hbar^2k^2}{2m} + \mu\right) g^\lambda(\vec{k}\sigma,\omega_n)$$

$$= \Omega_0 \mp \frac{1}{2\beta\hbar}\sum_{\vec{k}\sigma n}\int_0^1 \frac{d\lambda}{\lambda}\, e^{i\omega_n 0^+}\left(i\hbar\omega_n - \bar{\epsilon}_{\vec{k}\sigma}\right) g^\lambda(\vec{k}\sigma,\omega_n)$$

From Dyson's equations, we find

$$g^\lambda(\vec{k}\sigma,\omega_n) = \frac{1}{i\omega_n - \bar{\epsilon}_{\vec{k}\sigma}/\hbar - \Sigma^{*\lambda}(\vec{k}\sigma,\omega_n)}$$

Writing

$$i\hbar\omega_n - \bar{\epsilon}_{\vec{k}\sigma} = i\hbar\omega_n - \bar{\epsilon}_{\vec{k}\sigma} - \hbar\Sigma^{*\lambda}(\vec{k}\sigma,\omega_n) + \hbar\Sigma^{*\lambda}(\vec{k}\sigma,\omega_n),$$

we obtain

$$\Omega = \Omega_0 \mp \frac{1}{2\beta\hbar}\int_0^1 \frac{d\lambda}{\lambda}\sum_{\vec{k}\sigma n}\left[\hbar + \hbar\Sigma^{*\lambda}(\vec{k}\sigma,\omega_n)\, g^\lambda(\vec{k}\sigma,\omega_n)\right] e^{i\omega_n 0^+}$$

Using the result of the previous problem, we can write

$$\Omega = \Omega_0 \mp \frac{1}{2\beta}\int_0^1 \frac{d\lambda}{\lambda}\sum_{\vec{k}\sigma n} e^{i\omega_n 0^+}\,\Sigma^{*\lambda}(\vec{k}\sigma,\omega_n)\, g^\lambda(\vec{k}\sigma,\omega_n)$$

3. Frequency sums

(a) For bosons,

$$I = \lim_{\eta \to 0^+} \int_C \frac{e^{\eta z}}{z - \bar{\epsilon}/\hbar} \frac{dz}{e^{\beta\hbar z} - 1}$$

C is a circle of infinite radius centered at $z=0$.

$$I = 2\pi i \sum_j \mathrm{Res}(z_j)$$

where z_j's are the poles of the integrand.

$$\mathrm{Res}(\bar{\epsilon}/\hbar) = \frac{1}{e^{\beta\bar{\epsilon}} - 1} = n_{\bar{\epsilon}}$$

$$\mathrm{Res}(2n\pi i/\beta\hbar = i\omega_n) = \lim_{z \to i\omega_n} \frac{e^{z0^+}}{z - \bar{\epsilon}/\hbar} \frac{z - i\omega_n}{e^{\beta\hbar z} - 1}$$

$$= \frac{e^{i\omega_n 0^+}}{i\omega_n - \bar{\epsilon}/\hbar} \lim_{z \to i\omega_n} \frac{z - i\omega_n}{e^{\beta\hbar z} - 1}$$

The limit is evaluated using L'Hopital's rule,

$$\lim_{z \to i\omega_n} \frac{z - i\omega_n}{e^{\beta\hbar z} - 1} = \lim_{z \to i\omega_n} \frac{1}{\beta\hbar e^{\beta\hbar z}}$$

$$= \frac{1}{\beta\hbar e^{\beta\hbar i\omega_n}} = \frac{1}{\beta\hbar}$$

Hence,

$$0 = n_{\bar{\epsilon}} + \frac{1}{\beta\hbar} \sum_n \frac{e^{i\omega_n 0^+}}{i\omega_n - \bar{\epsilon}/\hbar}$$

$$\Rightarrow \sum_{n=-\infty}^{\infty} \frac{e^{i\omega_n 0^+}}{i\omega_n - \bar{\epsilon}/\hbar} = -\beta\hbar n_{\bar{\epsilon}}$$

b. For fermions,

$$I = \lim_{\eta\to 0^+} \int_c \frac{e^{\eta z}}{z-\bar{\epsilon}/\hbar}\,\frac{dz}{e^{\beta\hbar z}+1} = 0$$

Here,

$$Res(\bar{\epsilon}/\hbar) = f_{\bar{\epsilon}} \quad , \quad Res\left(i\omega_n = (2n+1)\pi i/\beta\hbar\right) = \frac{-e^{i\omega_n 0^+}}{\beta\hbar(i\omega_n - \bar{\epsilon}/\hbar)}$$

Hence,

$$\sum_{n=-\infty}^{\infty} \frac{e^{i\omega_n 0^+}}{i\omega_n - \bar{\epsilon}/\hbar} = \beta\hbar f_{\bar{\epsilon}}$$

4. An alternative method

$$g^0(\vec{k}\sigma, \tau) = -\langle T\, c_{\vec{k}\sigma}(\tau)\, c^+_{\vec{k}\sigma}(0)\rangle_0$$

Thus

$$\lim_{\tau\to 0^-} g^0(k\sigma,\tau) = \mp \lim_{\tau\to 0^-} \langle c^+_{k\sigma}(0)\, c_{k\sigma}(\tau)\rangle_0$$

(we have dropped the arrow sign over k). The above implies that

$$\langle c^+_{k\sigma} c_{k\sigma}\rangle_0 = \mp \lim_{\tau\to 0^-} g(k\sigma,\tau) = \mp \frac{1}{\beta\hbar} \lim_{\tau\to 0^-} \sum_{n=-\infty}^{\infty} g^0(k\sigma,\omega_n)\, e^{-i\omega_n \tau}$$

$$= \mp \frac{1}{\beta\hbar} \sum_{n=-\infty}^{\infty} \frac{e^{i\omega_n 0^+}}{i\omega_n - \bar{\epsilon}_{k\sigma}/\hbar}$$

Hence, for fermions

$$\sum_{n=-\infty}^{\infty} \frac{e^{i\omega_n 0^+}}{i\omega_n - \bar{\epsilon}_{k\sigma}/\hbar} = \beta\hbar \langle c^+_{k\sigma} c_{k\sigma}\rangle_0 = \beta\hbar f_{\bar{\epsilon}_{k\sigma}}$$

and for bosons

$$\sum_{n=-\infty}^{\infty} \frac{e^{i\omega_n 0^+}}{i\omega_n - \bar{\epsilon}_{k\sigma}/\hbar} = -\beta\hbar \langle c^+_{k\sigma} c_{k\sigma}\rangle_0 = -\beta\hbar\, n_{\bar{\epsilon}_{k\sigma}}$$

5. External potential

$$H = \sum_{k\sigma} \epsilon_{k\sigma} c^+_{k\sigma} c_{k\sigma} + \sum_{kq\sigma} v_q c^+_{k+q\sigma} c_{k\sigma}$$

a) To second order in the perturbation,

$$g(k\sigma,\tau) = g^0(k\sigma,\tau) + \delta g^{(1)}(k\sigma,\tau) + \delta g^{(2)}(k\sigma,\tau)$$

where

$$\delta g^{(1)}(k\sigma,\tau) = \frac{1}{\hbar}\int_0^{\beta\hbar} d\tau_1 \langle T c_{k\sigma}(\tau) c^+_{k\sigma}(0) V(\tau_1)\rangle_{0,c}$$

$$= \frac{1}{\hbar}\sum_{k_1 q \sigma_1} v_q \int_0^{\beta\hbar} d\tau_1 \langle T c_{k\sigma}(\tau) c^+_{k\sigma}(0) c^+_{k_1+q\sigma_1}(\tau_1) c_{k_1\sigma_1}(\tau_1)\rangle_{0,c}$$

All the operators in the above equation are interaction picture operators.

Using Wick's theorem,

$$\delta g^{(1)}(k\sigma,\tau) = \frac{1}{\hbar}\sum_{k_1 q\sigma_1} v_q \int_0^{\beta\hbar} d\tau_1 \, g^0(k\sigma,\tau-\tau_1) g^0_{k\sigma}(\tau_1)\, \delta_{\sigma_1\sigma}\delta_{q=0}\delta_{k_1,k}$$

$$= \frac{1}{\hbar} v_0 \int_0^{\beta\hbar} d\tau_1 \, g^0(k\sigma,\tau-\tau_1) g^0(k\sigma,\tau_1)$$

The second-order term is

$$\delta g^{(2)}(k\sigma,\tau) = -\frac{1}{2\hbar^2}\int_0^{\beta\hbar} d\tau_1 \int_0^{\beta\hbar} d\tau_2 \sum_{k_1 q_1\sigma_1}\sum_{k_2 q_2\sigma_2} v_{q_1} v_{q_2}$$

$$\langle T c_{k\sigma}(\tau) c^+_{k\sigma}(0) c^+_{k_1+q_1\sigma_1}(\tau_1) c_{k_1\sigma_1}(\tau_1) c^+_{k_2+q_2\sigma_2}(\tau_2) c_{k_2\sigma_2}(\tau_2)\rangle_{0,c}$$

$$= -\frac{1}{2\hbar^2}\int_0^{\beta\hbar} d\tau_1 \int_0^{\beta\hbar} d\tau_2 \sum_{k_1 q_1\sigma_1}\sum_{k_2 q_2\sigma_2} v_{q_1} v_{q_2}\, \delta_{\sigma_1\sigma}\delta_{\sigma_2\sigma}$$

$$\Big[-g^0(k\sigma,\tau-\tau_1) g^0(k_1\sigma_1,\tau_1-\tau_2) g^0(k\sigma,\tau_2)\, \delta_{k,k_1+q_1}\delta_{k_1,k_2+q_2}\delta_{k_2,k}$$
$$- g^0(k\sigma,\tau-\tau_2) g^0(k_2\sigma_2,\tau_2-\tau_1) g^0(k\sigma,\tau_1)\, \delta_{k,k_2+q_2}\delta_{k_2,k_1+q_1}\delta_{k_1,k}\Big]$$

The second term in the brackets is obtained from the first term by interchanging $(k_1\sigma_1 q_1 \tau_1) \longleftrightarrow (k_2\sigma_2 q_2 \tau_2)$. Since the spin and wave vector indices are summed over, and the times are integrated over, the second term gives the same contribution as the first term. Therefore, $(v_q v_{-q} = |v_q|^2)$

$$\delta g^{(2)}(k\sigma,\tau) = \frac{1}{\hbar^2}\int_0^{\beta\hbar} d\tau_1 \int_0^{\beta\hbar} d\tau_2 \sum_q |v_q|^2 g^0(k\sigma,\tau-\tau_1) g^0(k-q\sigma,\tau_1-\tau_2) g^0(k\sigma,\tau_2)$$

b) Fourier expanding the first-order term,

$$\frac{1}{\beta\hbar}\sum \delta g^{(1)}(k\sigma,\omega_n) e^{-i\omega_n\tau} =$$

$$\frac{1}{\hbar}\frac{v_0}{(\beta\hbar)^2}\sum_{n_1 n_2}\int d\tau_1\, g^0(k\sigma,\omega_{n_1}) g^0(k\sigma,\omega_{n_2}) e^{-i\omega_{n_1}(\tau-\tau_1)} e^{-i\omega_{n_2}\tau_1}$$

$$= \frac{v_0}{\hbar(\beta\hbar)^2}\sum_{n_1 n_2} g^0(k\sigma,\omega_{n_1}) g^0(k\sigma,\omega_{n_2}) e^{-i\omega_{n_1}\tau}\int_0^{\beta\hbar} d\tau_1\, e^{i(\omega_{n_1}-\omega_{n_2})\tau_1}$$

$$= \frac{v_0}{\hbar(\beta\hbar)^2}\sum_{n_1 n_2} g^0(k\sigma,\omega_{n_1}) g^0(k\sigma,\omega_{n_2}) e^{-i\omega_{n_1}\tau}\,\beta\hbar\,\delta_{n_1 n_2}$$

$$\Rightarrow \delta g^{(1)}(k\sigma,\omega_n) = \frac{v_0}{\hbar} g^0(k\sigma,\omega_n) g^0(k\sigma,\omega_n)$$

As for the second-order term,

$$\delta g^{(2)}(k\sigma,\tau) = \frac{1}{\beta\hbar}\sum_n e^{-i\omega_n\tau}\delta g^{(2)}(k\sigma,\omega_n)$$

$$= \frac{1}{\hbar^2}\frac{1}{(\beta\hbar)^3}\sum_q v_q v_{-q}\sum_{n_1 n_2 n_3}\int_0^{\beta\hbar} d\tau_1\int_0^{\beta\hbar} d\tau_2\, e^{-i\omega_{n_1}(\tau-\tau_1)} e^{-i\omega_{n_2}(\tau_1-\tau_2)} e^{-i\omega_{n_3}\tau_2}$$

$$g^0(k\sigma,\omega_{n_1}) g^0(k-q\sigma,\omega_{n_2}) g^0(k\sigma,\omega_{n_3})$$

$$= \frac{1}{\hbar^2}\frac{1}{\beta\hbar}\sum_q v_q v_{-q}\sum_{n_1 n_2 n_3}\delta_{n_1 n_2}\delta_{n_2 n_3} e^{-i\omega_{n_1}\tau} g^0(k\sigma,\omega_{n_1}) g^0(k-q\sigma,\omega_{n_2}) g^0(k\sigma,\omega_{n_2})$$

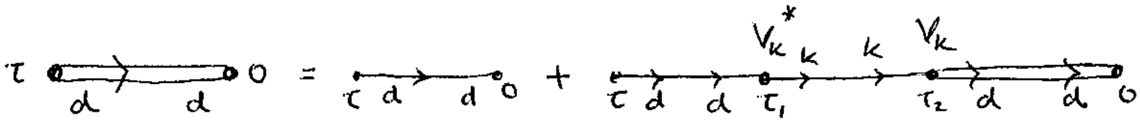
$$\Rightarrow \delta g^{(2)}(k\sigma,\omega_n) = \frac{1}{\hbar^2}\sum_q v_q v_{-q}\, g^0(k\sigma,\omega_n) g^0(k-q,\omega_n) g^0(k\sigma,\omega_n)$$

c) To write the n^{th} order correction $\delta g^{(n)}(k\sigma,\omega_n)$, note that there is only one connected, topologically distinct diagram with $n+1$ solid lines and n vertices. All the solid lines have the same frequency ω_n. The i^{th} vertex is assigned a wave vector q_i and matrix element v_{q_i}. The external lines are assigned wave vector k and frequency ω_n, and spin σ. At each interaction vertex, wave vector, frequency, and spin are conserved. To obtain $\delta g^{(n)}(k\sigma,\omega_n)$, multiply the $n+1$ g^0s and n v_q's, sum over all internal wave vector (there are $n-1$ internal wave vectors) and multiply the result by $1/\hbar^n$.

6. $$H_0 = \epsilon \sum_\sigma d_\sigma^+ d_\sigma + \sum_{k\sigma} \epsilon_{k\sigma} c^+_{k\sigma} c_{k\sigma}$$

$$H' = \sum_{k\sigma} \left(V_k c^+_{k\sigma} d_\sigma + V_k^* d_\sigma^+ c_{k\sigma} \right)$$

Dyson equation:



The algebraic equation is

$$g(d\sigma,\tau) = g^0(d\sigma,\tau) + \frac{1}{\hbar^2}\sum_k |V_k|^2 \int_0^{\beta\hbar} d\tau_1 \int_0^{\beta\hbar} d\tau_2 \; g^0(d\sigma,\tau-\tau_1) g^0(k\sigma,\tau_1-\tau_2) g(d\sigma,\tau_2)$$

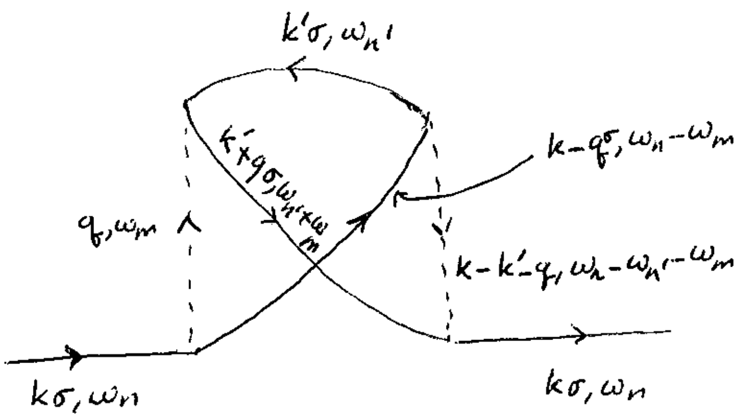
Fourier expanding, we find

$$g(d\sigma,\omega_n) = g^0(d\sigma,\omega_n) + g^0(d\sigma,\omega_n)\, \Sigma^*_\sigma(\omega_n)\, g(d\sigma,\omega_n)$$

where

$$\Sigma^*_\sigma(\omega_n) = \frac{1}{\hbar^2}\sum_k |V_k|^2 g^0(k\sigma,\omega_n) = \frac{1}{\hbar^2}\sum_k \frac{|V_k|^2}{i\omega_n - \epsilon_{k\sigma}/\hbar}$$

7.



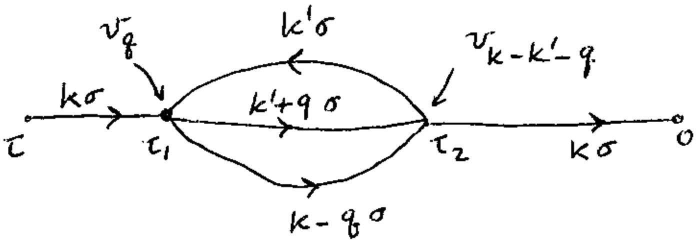
Using Feynman rules,

$$\delta g_J(k\sigma,\omega_n) = \left(\frac{-1}{\beta\hbar^2}\right)^2 \left[g^0(k\sigma,\omega_n)\right]^2 \sum_{k',q}\sum_{n,m} \left(\frac{V_q}{V}\right)\left(\frac{v_{k-k'-q}}{V}\right) g^0(k-q\sigma,\omega_n-\omega_m) \times$$

$$g^0(k'\sigma,\omega_{n'})\, g^0(k'+q\sigma,\omega_{n'}+\omega_m)$$

8. Time-ordered diagrams

We redraw the exchange diagram as follows



We see that this is the same diagram as 9.15 b except for

(i) σ' in Fig. 9.15 b is here replaced by σ

(ii) The vertex at τ_2 is now $v_{k-k'-q}$ instead of v_q.

Hence, the expression for $\delta g_J^{(2)}(k\sigma, \omega_n)$ is the same as that in Eq. (9.32) except that now there is no sum over σ' and $(v_q/V)^2 \longrightarrow (v_q/V)(v_{k-k'-q}/V)$.

9. A frequency sum

$$\delta g_R^{(2)}(k\sigma,\omega_n) = -\left(\frac{-1}{\beta\hbar}\right)^2 \sum_{qk'\sigma'} \left(\frac{v_q}{V}\right)^2 \sum_m \left[g^0(k\sigma,\omega_n)\right]^2 g^0(k-q\sigma,\omega_n-\omega_m)$$

$$\times \sum_{n'} g^0(k'\sigma',\omega_{n'})\, g^0(k'+q\sigma';\ \omega_{n'}+\omega_m)$$

$$S = \sum_{n'} g^0(k'\sigma',\omega_{n'})\, g^0(k'+q\sigma',\ \omega_{n'}+\omega_m)$$

$$= \sum_{n'} \frac{1}{i\omega_{n'} - \bar{\epsilon}_{k'\sigma'}/\hbar} \cdot \frac{1}{i\omega_{n'} + i\omega_m - \bar{\epsilon}_{k'+q\sigma'}/\hbar}$$

As $n' \to \pm\infty$, the summand $\longrightarrow -\frac{1}{\omega_{n'}^2} = \frac{-1}{(2n'+1)^2\pi^2/\beta^2\hbar^2}$

$\Rightarrow$ the series is convergent.

We are thus justified in introducing a convergence factor $e^{i\omega_n 0^+}$ into the sum.

$$S = \sum_{n'} \frac{e^{i\omega_{n'}0^+}}{(i\omega_{n'} - \bar{\epsilon}_{k'\sigma'}/\hbar)(i\omega_{n'} + i\omega_m - \bar{\epsilon}_{k'+q\sigma'}/\hbar)}$$

$$= \frac{1}{i\omega_m + (\bar{\epsilon}_{k'\sigma'} - \bar{\epsilon}_{k'+q\sigma'})/\hbar} \sum_{n'} \left[\frac{e^{i\omega_{n'}0^+}}{i\omega_{n'} - \bar{\epsilon}_{k'\sigma'}/\hbar} - \frac{e^{i\omega_{n'}0^+}}{i\omega_{n'} + i\omega_m - \bar{\epsilon}_{k'+q\sigma'}/\hbar} \right]$$

$$= \frac{1}{i\omega_m + (\bar{\epsilon}_{k\sigma} - \bar{\epsilon}_{k'+q\sigma'})/\hbar} \left[\sum_{n'} \frac{e^{i\omega_{n'}0^+}}{i\omega_{n'} - \bar{\epsilon}_{k'\sigma'}/\hbar} - e^{i\omega_m 0^+} \sum_{n''} \frac{e^{i\omega_{n''}0^+}}{i\omega_{n''} - \bar{\epsilon}_{k'+q\sigma'}/\hbar} \right]$$

In the last step we wrote $\omega_{n'} + \omega_m = \omega_{n''}$. Using Eq. (9.14),

$$S = \frac{\beta\hbar (f_{k'\sigma'} - e^{i\omega_m 0^+} f_{k'+q\sigma'})}{i\omega_m + (\bar{\epsilon}_{k'\sigma'} - \bar{\epsilon}_{k'+q\sigma'})/\hbar} = \frac{\beta\hbar (f_{k'\sigma'} - f_{k'+q\sigma'})}{i\omega_m + (\bar{\epsilon}_{k'\sigma'} - \bar{\epsilon}_{k'+q\sigma'})/\hbar}$$

10. From Eq. (9.9), the number of connected, topologically distinct diagrams of order n is

$$C_{TD}(n) = \frac{C(n)}{n!\,2^n}$$

Here we need to determine $C(n)$, the number of connected diagrams without loops. In Section 9.2 we considered the product

$$P_g = -\langle T c_{k\sigma}(\tau)\, c_1^+ c_1\, c_{1'}^+ c_{1'} \cdots c_n^+ c_n\, c_{n'}^+ c_{n'}\, c_{k\sigma}^+(0) \rangle_{0,c}$$

A diagram without loops is obtained by contracting every annihilation operator with the creation operator immediately on its right side. Other diagrams without loops are obtained by interchanging two internal vertices and following the same contraction procedure. Since there are $2n$ internal vertices, the number of their permutations is $(2n)!$. Hence

$$C_{TD,\,\text{no loops}}(n) = \frac{(2n)!}{n!\,2^n}$$

For example, for $n=1$, $C_{TD,\,\text{no loops}}(1) = \frac{2!}{1!\,2^1} = 1$

for $n=2$, $C_{TD,\,\text{no loops}}(2) = \frac{4!}{2!\,2^n} = 3$

Figure 9.3 indeed shows that there are three diagrams of second order with no loops.

10.1 First-order self energy

$$\sum\nolimits_1^*(\mathbf{k}\sigma,\omega_n) = -\frac{1}{\hbar V}\sum_{\mathbf{k}}\frac{4\pi e^2}{|\mathbf{k}-\mathbf{k}'|^2}f_{\mathbf{k}'}$$

$$As \quad T\to 0, f_{\mathbf{k}'}\to\theta(k_F-k')$$

$$\begin{aligned}
\sum\nolimits_1^*(\mathbf{k}\sigma,\omega_n) &= -\frac{1}{\hbar V}\frac{V}{(2\pi)^3}(4\pi e^2)\int\frac{\theta(k_F-k')}{|\mathbf{k}-\mathbf{k}'|^2}\mathrm{d}^3k' \\
&= -\frac{e^2}{2\pi\hbar}\int_0^{k_F}k'^2\mathrm{d}k'\int_0^{2\pi}\mathrm{d}\phi\int_{-1}^{1}\frac{\mathrm{d}cos\theta}{k'^2+k^2-2kk'cos\theta} \\
&= -\frac{e^2}{\pi\hbar}\int_0^{k_F}k'^2\mathrm{d}k'\int_{-1}^{1}\frac{\mathrm{d}x}{k'^2+k^2-2kk'x} \\
&= \frac{e^2}{\pi\hbar}\int_0^{k_F}\frac{k'^2\mathrm{d}k'}{2kk'}\int_{-1}^{1}\frac{\mathrm{d}x}{x-\frac{k'^2+k^2}{2kk'}} \\
&= \frac{e^2}{2\pi\hbar k}\int_0^{k_F}k'\mathrm{d}k'\left(ln\left|x-\frac{k'^2-k^2}{2kk'}\right|_{-1}^{1}\right) \\
&= \frac{e^2}{2\pi\hbar k}\int_0^{k_F}k'ln\left|\frac{(k'-k)^2}{(k'+k)^2}\right|\mathrm{d}k' \\
&= \frac{e^2}{\pi\hbar k}\int_0^{k_F}k'ln\left|\frac{k'-k}{k'+k}\right|\mathrm{d}k'
\end{aligned}$$

Let k'=k_Fy, $k=k_Fx$:

$$\begin{aligned}
\sum\nolimits_1^*(\mathbf{k}\sigma,\omega_n) &= -\frac{e^2}{\pi\hbar k_F x}\int_0^1 k_F y ln\left|\frac{y-x}{y+x}\right|k_F\mathrm{d}y \\
&= \frac{e^2k_F}{\pi\hbar x}\int_0^1 yln\left|\frac{y-x}{y+x}\right|\mathrm{d}y = -\frac{e^2k_F}{\pi\hbar x}\mathbf{I}
\end{aligned}$$

Where,

$$\mathbf{I} = \int_0^1 yln|y+x|\mathrm{d}y - \int_0^1 yln|y-x|\mathrm{d}y \equiv A(x)-A(-x)$$

$$A(x) = \int_0^1 yln|y+x|\mathrm{d}y = \left[\frac{y^2-x^2}{2}ln|y+x| - frac14(y-x)^2\right]_0^1$$

Thus,

$$\mathbf{I} = \frac{1-x^2}{2}ln\left|\frac{1+x}{1-x}\right|+x$$

Therefore,

$$\sum\nolimits_1^*(\mathbf{k}\sigma,\omega_n) = -\frac{e^2k_F}{\pi\hbar}\left[1+\frac{1-x^2}{2x}ln\left|\frac{1+x}{1-x}\right|\right]$$

10.2 Proper self energy in two dimentions

In 2D, The Coulomb interaction is $v_q = \frac{2\pi e^2}{q}$. Therefore,

$$\begin{aligned}
\sum\nolimits_1^* &= -\frac{1}{\hbar A}\sum_{\mathbf{k}'}\frac{2\pi e^2}{|\mathbf{k}-\mathbf{k}'|}f_{\mathbf{k}'} \\
&= -\frac{2\pi e^2}{\hbar A}\frac{A}{(2\pi)^2}\int_0^{k_F}k'\mathrm{d}k'\int_0^{2\pi}\frac{\mathrm{d}\theta}{(k'^2+k^2-2kk'cos\theta)^{1/2}}
\end{aligned}$$

Let $k' = k_F x$. Then,

$$\sum\nolimits_1^*(\mathbf{k}\sigma,\omega_n) = -\frac{e^2k_F}{2\pi\hbar}\int_0^1 x\mathrm{d}x\int_0^{2\pi}\frac{\mathrm{d}\theta}{(x^2+(\frac{k}{k_F})^2-2x(\frac{k}{k_F})cos\theta)^{1/2}}$$

The integral is difficult to do. We restrict ourselves to the case $k = k_F$, for which the integral becomes more manageable,

$$\sum\nolimits_1^*(\mathbf{k}\sigma,\omega_n) = -\frac{e^2k_F}{2\pi\hbar}\mathbf{I}$$

$$\mathbf{I} = \int_0^{2\pi}\mathrm{d}\theta\int_0^1\frac{x\mathrm{d}x}{(x^2-2xcos\theta+1)^{1/2}} = \int_0^{2\pi}J(\theta)\mathrm{d}\theta$$

The integral over x is tabulated:

$$\int\frac{x\mathrm{d}x}{\sqrt{ax^2+bx+c}} = \frac{1}{a}\sqrt{ax^2+bx+c}-\frac{b}{2a^{3/2}}ln\left|\frac{2ax+b}{\sqrt{a}}+2\sqrt{ax^2+bx+c}\right|$$

Thus,

$$\begin{aligned}
J(\theta) &= \left[\sqrt{x^2-2xcos\theta+1}+cos\theta ln\left|2x-2cos\theta+2\sqrt{x^2-2xcos\theta+1}\right|\right]_0^1 \\
&= \sqrt{2-2cos\theta}-1+cos\theta ln\left|\frac{2-2cos\theta+2\sqrt{2-2cos\theta}}{2-2cos\theta}\right| \\
&= 2sin\left(\frac{\theta}{2}\right)-1+cos\theta ln\left|1+\frac{1}{sin\left(\frac{\theta}{2}\right)}\right|
\end{aligned}$$

Thus,

$$\int_0^{2\pi}J(\theta)\mathrm{d}\theta = 8-2\pi+B$$

Where

$$B = \int_0^{2\pi} cos\theta ln\left|1 + \frac{1}{sin\left(\frac{\theta}{2}\right)}\right| \mathrm{d}\theta$$

Let u=$ln\left|1 + \frac{1}{sin\left(\frac{\theta}{2}\right)}\right|$, $\mathrm{d}v = cos\theta \mathrm{d}\theta$. Then

$$\begin{aligned} B &= -\int_0^{2\pi} \frac{sin\theta}{1 + \frac{1}{sin\left(\frac{\theta}{2}\right)}} \left(\frac{-\frac{1}{2}cos\left(\frac{\theta}{2}\right)}{sin^2\left(\frac{\theta}{2}\right)}\right) \mathrm{d}\theta \\ &= \frac{1}{2}\int_0^{2\pi} \frac{sin\theta cos\frac{\theta}{2}}{sin^2\frac{\theta}{2} sin\frac{\theta}{2}} \mathrm{d}\theta \\ &= \int_0^{2\pi} \frac{sin\frac{\theta}{2} cos^2\frac{\theta}{2}}{sin\frac{\theta}{2}(1 + sin\frac{\theta}{2})} \mathrm{d}\theta \\ &= 2\int_0^{\pi} \frac{cos^2 x}{sinx + 1} \mathrm{d}x \end{aligned}$$

In the last step, we have substituted $x = \theta/2$. Therefore,

$$B = 2\int_0^{\pi} \frac{1 - sin^2 x}{1 + sinx} \mathrm{d}x = 2\int_0^{2} (1 - sinx) \mathrm{d}x = 2\pi - 4$$

Hence,
$\mathbf{I} = 8 - 2\pi + 2\pi - 4$=4
We thus find

$$\sum\nolimits_1^* (\mathbf{k}\sigma, \omega_n) = -\frac{2e^2 k_F}{\pi\hbar}$$

10.3

$$\prod\nolimits^0 (\mathbf{q}, \omega) = \frac{2}{V}\sum_{\mathbf{k}} \frac{f_{\mathbf{k}} - f_{\mathbf{k+q}}}{\hbar\omega + \epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k+q}} + i0^+}$$

In the limit $\omega \rightarrow \infty$, $Im \prod^o (\mathbf{q}, \omega) = 0$ since it contains $\delta(\hbar\omega + \epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k+q}})$
Thus, as $\omega \rightarrow \infty$,

$$\begin{aligned} \prod\nolimits^0 (\mathbf{q}, \omega) = Re \prod\nolimits^o (\mathbf{q}, \omega) &= \frac{2}{V}\sum_{\mathbf{k}} \frac{f_{\mathbf{k}} - f_{\mathbf{k+q}}}{\hbar\omega + \epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k+q}}} \\ &= \frac{4}{V(\hbar\omega)^2}\sum_{\mathbf{k}} f_{\mathbf{k}}(\epsilon_{\mathbf{k+q}} - \epsilon_{\mathbf{k}}) \end{aligned}$$

(see the next problem 10.4)
Since $\epsilon_{\mathbf{k+q}} - \epsilon_{\mathbf{k}}$=$\frac{\hbar^2}{2m}(\mathbf{q}^2 + 2\mathbf{k} \cdot \mathbf{q})$,

$$\prod\nolimits^0 (\mathbf{q}, \omega) = \frac{4\hbar^2}{2mV(\hbar\omega)^2}\sum_{\mathbf{k}} (\mathbf{q}^2 + 2\mathbf{k} \cdot \mathbf{q}) f_{\mathbf{k}}$$

Since $f_{\mathbf{k}}$ depends only on $\epsilon_{\mathbf{k}} = \frac{\hbar^2 k^2}{2m}$, it follows that :

$$\sum_{\mathbf{k}} = (\mathbf{k}\cdot\mathbf{q})f_{\mathbf{k}} = 0$$

Therefore, as $\omega \rightarrow \infty$,

$$\prod^0(\mathbf{q},\omega) = \frac{2q^2}{mV\omega^2}\sum_{\mathbf{k}} f_{\mathbf{k}} = \frac{2q^2}{mV\omega^2}\frac{N}{2} = \frac{nq^2}{m\omega^2}$$

and

$$\begin{aligned}\epsilon(\mathbf{q},\omega\rightarrow\infty) &= 1 - v_{\mathbf{q}}\prod^0(\mathbf{q},\omega\rightarrow\infty) = 1 - \frac{4\pi e^2}{q^2}\frac{nq^2}{m\omega^2}\\ &= 1 - \frac{(4\pi e^2/m)}{\omega^2}\\ &= 1 - \frac{\omega_p^2}{\omega^2}\end{aligned}$$

10.4 An alternative derivation of the plasmon dispersion

a)

$$\begin{aligned}Re\prod^0(q,\omega) &= \frac{2}{V}\sum_k \frac{f_k - f_{k+q}}{\hbar\omega + \epsilon_k - \epsilon_{k+q}}\\ &= \frac{2}{V}\sum_k \frac{f_k}{\hbar\omega + \epsilon_k - \epsilon_{k+q}} - \frac{2}{V}\sum_k \frac{f_{k+q}}{\hbar\omega + \epsilon_k - \epsilon_{k+q}}\end{aligned}$$

We're dropping the arrow sign over the vectors. In the second sum, $k \rightarrow -k' - q$, then $\epsilon_{k'} \rightarrow \epsilon_{-k'-q} = \epsilon_{k'+q}$, $f_{k+q} \rightarrow f_{-k'} = f_{k'}$, $\epsilon_{k+q} \rightarrow \epsilon_{-k'} = \epsilon_{k'}$. Hence

$$\begin{aligned}Re\prod^0(q,\omega) &= \frac{2}{V}\sum_k \frac{f_k}{\hbar\omega + \epsilon_k - \epsilon_{k+q}} - \frac{2}{V}\sum_k \frac{f_k}{\hbar\omega - \epsilon_k + \epsilon_{k+q}}\\ &= \frac{2}{V}\sum_k f_k\left[\frac{1}{\hbar\omega + \epsilon_k - \epsilon_{k+q}} - \frac{1}{\hbar\omega - \epsilon_k + \epsilon_{k+q}}\right]\\ &= \frac{2}{V}\sum_k f_k\left[\frac{2\epsilon_{k+q} - 2\epsilon_k}{(\hbar\omega)^2 - (\epsilon_{k+q} - \epsilon_k)^2}\right]\\ &= \frac{4}{V}\sum_k \frac{f_k(\epsilon_{k+q} - \epsilon_k)}{(\hbar\omega)^2 - (\epsilon_{k+q} - \epsilon_k)^2}\end{aligned}$$

b) $\hbar\omega \ll \epsilon_{k+q} - \epsilon_k$

$$Re\prod^0(q,\omega) = \frac{4}{V(\hbar\omega)^2}\sum_k f_k(\epsilon_{k+q}-\epsilon_k)\left[1-\frac{(\epsilon_{k+q}-\epsilon_k)^2}{(\hbar\omega)^2}\right]^{-1}$$
$$= \frac{4}{V(\hbar\omega)^2}\sum_k f_k(\epsilon_{k+q}-\epsilon_k)\left[1+\frac{(\epsilon_{k+q}-\epsilon_k)^2}{(\hbar\omega)^2}+...\right]$$

c) T$\rightarrow 0$, $f_k \rightarrow \theta(k_F - k)$, $\epsilon_{k+q}-\epsilon_k{=}\frac{\hbar^2}{2m}(q^2+2\mathbf{k}\cdot\mathbf{q})$

$$\sum_k f_k(\epsilon_{k+q}-\epsilon_k) = \frac{\hbar^2 q^2}{2m}\sum_k f_k + \frac{\hbar^2}{m}\sum_k f_k \mathbf{k}\cdot\mathbf{q}$$

The sencond sum vanishes since f_k depends only on $|k|$. Thus,

$$\sum_k f_k(\epsilon_{k+q}-\epsilon_k) = \frac{\hbar^2 q^2}{2m}\frac{N}{2}$$

Where N is the total number of electrons.
Next, we need to evaluate

$$\sum_k f_k(\epsilon_{k+q}-\epsilon_k)^3 \equiv A$$

$$A = \left(\frac{\hbar^2}{2m}\right)^3 \sum_k f_k(q^2+2kqcos\theta)^3$$

Where θ is the angle between $\mathbf{k}$ and $\mathbf{q}$

$$A = \left(\frac{\hbar^2}{2m}\right)^3 \sum_k f_k(q^6+6kq^5cos\theta+12k^2q^4cos^2\theta+8k^3q^3cos^3\theta)$$
$$= \left(\frac{\hbar^2}{2m}\right)^3 q^6\frac{N}{2} + \left(\frac{\hbar^2}{2m}\right)^3 \frac{V}{(2\pi)^3}\int_0^{k_F} 2\pi k^2 \mathrm{d}k\int_{-1}^{1}\mathrm{d}cos\theta[6kq^5cos\theta+12k^2q^4cos^2\theta+8k^3q^3cos^3\theta]$$

Upon integrating over $cos\theta$, only the term proportional to $cos^2\theta$ gives a nonvanishing contribution,

$$A = \left(\frac{\hbar^2}{2m}\right)^3 q^6\frac{N}{2} + \left(\frac{\hbar^2}{2m}\right)^3 \frac{V}{(2\pi)^3}(12)\frac{2}{3}q^4\int_0^{k_F} k^4\mathrm{d}k$$
$$= \left(\frac{\hbar^2}{2m}\right)^3 q^6\frac{N}{2} + \left(\frac{\hbar^2}{2m}\right)^3 \frac{V}{(2\pi)^3}\frac{8}{5}q^4k_F^5$$

Therefore,

$$Re\prod^0(q,\omega) = \frac{n}{m}\left(\frac{q}{\omega}\right)^2 + \frac{4}{V(\hbar\omega)^4}\left(\frac{\hbar^2}{2m}\right)^3\frac{V}{(2\pi)^2}\frac{8}{5}q^4k_F^5 + ...$$
$$= \frac{n}{m}\left(\frac{q}{\omega}\right)^2 + \left(\frac{q}{\omega}\right)^4\frac{\hbar^2k_F^2}{m^2}\frac{k_F^3}{8m}\frac{8}{5}\frac{4}{(2\pi)^2}$$

Using k_F^3=$3\pi^2n$ (see Chapter 2),

$$Re\prod^0(q,\omega) = \frac{n}{m}\left(\frac{q}{\omega}\right)^2 + \frac{1}{5}\left(\frac{q}{\omega}\right)^4\frac{3n}{m}V_F^2 + ...$$
$$= \frac{n}{m}\left(\frac{q}{\omega}\right)^2\left[1 + \frac{3}{5}\left(\frac{qV_F}{\omega}\right)^2 + ...\right]$$

Which is Eq.(10.65);
The derivation of the plasmon dispersion now proceeds as in the text.

10.5 Thomas Fermi wave number in 2D

$$\prod^0(q,\omega) = \frac{1}{A}\sum_{k\sigma}\frac{f_k - f_{k+q}}{\hbar\omega + \epsilon_k - \epsilon_{k+q} + i0^+}$$

In the static case, Im$\prod^0$(q,ω=0)=0. Hence

$$\prod^0(q,\omega) = \frac{1}{A}\sum_{k\sigma}\frac{f_k - f_{k+q}}{\epsilon_k - \epsilon_{k+q}}$$

Now consider the long wavelength limit $q \to 0$,

$$\prod^0(q \to 0, \omega = 0) = \frac{1}{A}\sum_{k\sigma}\frac{\partial f}{\partial \epsilon_k}$$

At low temperature, $f_{\epsilon_k} \to \theta(\epsilon_F - \epsilon_k)$. Thus

$$\prod^0(q \to 0, \omega = 0) = -\frac{1}{A}\sum_{k\sigma}\delta(\epsilon_k - \epsilon_F) = -\mathrm{d}(\epsilon_F)$$

Where d(ϵ_F) is the density of states per unit area at the Fermi energy. To determine d(ϵ_F), consider the shell bounded by two constant energy surfaces ϵ and $\epsilon + \mathrm{d}\epsilon$. The number of states with energies between ϵ and $\epsilon + \mathrm{d}\epsilon$ is:

N$(\epsilon, \epsilon + \mathrm{d}\epsilon)$ = 2 (number of k-points in the shell)

The factor of 2 results from spin degeneracy. Since each **k**-point occupies an area in k-space given by $(2\pi)^2/A$.

$$(\epsilon, \epsilon + \mathrm{d}\epsilon) = 2\frac{2\pi k \mathrm{d}k}{(2\pi)^2/A} = \frac{Ak\mathrm{d}k}{\pi}$$

Since $\epsilon = \frac{\hbar^2 k^2}{2m}$, $\mathrm{d}\epsilon = \frac{\hbar^2}{m} k \mathrm{d}k$. Hence,

$$N(\epsilon, \epsilon + \mathrm{d}\epsilon) = \frac{Am}{\pi\hbar^2}\mathrm{d}\epsilon \equiv A\mathrm{d}(\epsilon)\mathrm{d}\epsilon$$
$$\Rightarrow \mathrm{d}(\epsilon) = \frac{m}{\pi\hbar^2} \Rightarrow \mathrm{d}(\epsilon_F) = \frac{m}{\pi\hbar^2}$$

The dielectric function,

$$\begin{aligned}\epsilon(q \to 0, \omega = 0) &= 1 - v_q \prod^0 (q \to 0, \omega = 0) \\ &= 1 + \frac{2\pi e^2}{q}\frac{m}{\pi\hbar^2} = 1 + \frac{2}{q}\frac{1}{(\hbar^2/me^2)} = 1 + \frac{2}{qa_0}\end{aligned}$$

The screened Coulomb interaction is thus,

$$V_{TF} = \frac{2\pi e^2/q}{1 + \frac{2}{qa_0}} = \frac{2\pi e^2}{q + 2/a_0}$$

10.6 Plasmon dispersion in 2D

Using the result of problem 10.4,

$$\begin{aligned} Re\prod^0(q,\omega) &= \frac{2}{A}\sum_k \frac{f_k - f_{k+q}}{\hbar\omega + \epsilon_k - \epsilon_{k+q}} \\ &= \frac{4}{A(\hbar\omega)^2}\sum_k f_k(\epsilon_{k+q} - \epsilon_k) + \frac{4}{A(\hbar\omega)^4}\sum_k f_k(\epsilon_{k+q} - \epsilon_k)^3 + ... \\ &= S_1 + S_2 \\ S_1 &= \frac{4}{A(\hbar\omega)^2}\sum_k f_k\left[\frac{\hbar^2}{2m}(\mathbf{q}^2 + 2\mathbf{k}\cdot\mathbf{q})\right] = \frac{4}{A(\hbar\omega)^2}\frac{\hbar^2 q^2}{2m}\sum_k f_k \\ &= \frac{4q^2}{2Am\omega^2}\frac{N}{2} = \frac{n}{m}\left(\frac{q}{\omega}\right)^2 \end{aligned}$$

Where $n = \frac{N}{A}$ is the number of electrons per unit area.

$$\begin{aligned} S_2 &= \frac{4}{A(\hbar\omega)^4}\sum_k f_k(\epsilon_{k+q} - \epsilon_k)^3 + ... \\ &= \frac{\hbar^2}{2Am^3\omega^4}\sum_k f_k(q^6 + 6kq^5 cos\theta + 12k^2q^4cos^2\theta + 8k^3q^3cos^3\theta + ...) \end{aligned}$$

Replacing

$$f_k \to \theta(k_F - k), \sum_k \to \frac{A}{(2\pi)^2} \int \mathrm{d}^2k = \frac{A}{(2\pi)^2} \int_0^{k_F} k\mathrm{d}k \int_0^{2\pi} \mathrm{d}\theta ...$$

The terms proportional to $cos\theta$ or $cos^3\theta$ vanish upon integration over θ. Also,

$$\int_0^{2\pi} cos^2\theta \mathrm{d}\theta = \pi$$

Hence,

$$S_2 = \frac{\hbar^2}{2Am^3\omega^4} 12\pi q^4 \frac{A}{(2\pi)^2} \int_0^{k_F} k^3\mathrm{d}k + ...$$

The terms represented by ... are of order q^6. In 2D,

$$N = \sum_{k\sigma} \theta(k_F - k) = 2\frac{A}{(2\pi)^2}\pi k_F^2 \Rightarrow n = \frac{N}{A} = \frac{k_F^2}{2\pi} \Rightarrow k_F^2 = 2\pi n$$

Thus,

$$\int_0^{k_F} k^3\mathrm{d}k = \frac{k_F^4}{4} = \frac{(2\pi n)^2}{4} = \pi^2 n^2$$

Thus,

$$S_2 = \frac{3\pi\hbar^2}{2m}\left(\frac{n}{m}\right)^2\left(\frac{q}{\omega}\right)^4 + ...$$

and

$$\begin{aligned} Re\prod{}^0(q,\omega) &= \left(\frac{n}{m}\right)^2\left(\frac{q}{\omega}\right)^2 + \frac{3\pi\hbar^2}{2m}\left(\frac{n}{m}\right)^2\left(\frac{q}{\omega}\right)^4 + ... \\ &= \left(\frac{n}{m}\right)^2\left(\frac{q}{\omega}\right)^2\left[1 + \frac{3\pi\hbar^2}{2m}\frac{n}{m}\left(\frac{q}{\omega}\right)^2 + ...\right] \end{aligned}$$

The plasmin frequency is the solution of $1 - v_q Re\prod^0(q,\omega) = 0$. In 2D, $v_q = \frac{2\pi e^2}{q}$. Thus

$$1 - \frac{2\pi n e^2 q}{m\omega^2}\left[1 + \frac{3\pi\hbar^2}{2m}\frac{n}{m}\left(\frac{q}{\omega}\right)^2 + ...\right] = 0$$

$$\begin{aligned} \Rightarrow \omega^2 &= \frac{2\pi n e^2 q}{m}\left[1 + \frac{3\pi\hbar^2}{2m}\frac{n}{m}\left(\frac{q}{\omega}\right)^2 + ...\right] \\ &= \frac{2\pi n e^2 q}{m}\left[1 + \frac{3\pi\hbar^2}{2m}\frac{n}{m}\frac{q^2}{2\pi n e^2 q)/m} + ...\right] \\ &= \frac{2\pi n e^2 q}{m}\left[1 + \frac{3\hbar^2 q}{4me^2} + ...\right] \end{aligned}$$

The Bohr radius $a_0 = \frac{\hbar^2}{me^2}$; hence

$$\omega^2 = \frac{2\pi ne^2 q}{m}\left[1 + \frac{3qa_0}{4} + ...\right]$$

$$\Rightarrow \omega = \sqrt{\frac{2\pi ne^2 q}{m}}\left[1 + \frac{3qa_0}{4} + ...\right]^{1/2}$$
$$= \sqrt{\frac{2\pi ne^2 q}{m}}\left[1 + \frac{3qa_0}{8} + ...\right]$$

1.

$$d^{0<}(\vec{q}\lambda,\tau) = -\langle \phi^{+}_{\vec{q}\lambda}(0)\,\phi_{\vec{q}\lambda}(\tau)\rangle_0$$

Replace ϕ by its form in terms of a and a^+,

$$d^{0<}(q\lambda,\tau) = -\langle (a^+_{q\lambda}(0) + a_{-q\lambda}(0))(a_{q\lambda}(\tau) + a^+_{-q\lambda}(\tau))\rangle_0$$

$$= -\langle a^+_{q\lambda}(0)\,a_{q\lambda}(\tau)\rangle_0 - \langle a^+_{q\lambda}(0)\,a^+_{-q\lambda}(\tau)\rangle_0 - \langle a_{-q\lambda}(0)\,a_{q\lambda}(\tau)\rangle_0$$

$$-\langle a_{-q\lambda}(0)\,a^+_{-q\lambda}(\tau)\rangle_0$$

I have dropped the arrow sign over q. From here on I will also drop λ; so q means $\vec{q}\lambda$ and $-q$ means $-\vec{q}\lambda$.

Using Eq. (11.58),

$$a_q(\tau) = e^{-\omega_q\tau} a_q\,,\quad a^+_{-q}(\tau) = e^{\omega_q\tau} a^+_{-q}\,,$$

and noting that terms such as $\langle a^+_q a^+_{-q}\rangle_0$ and $\langle a_{-q} a_q\rangle$ vanish, we can write

$$d^{0<}(q,\tau) = -e^{-\omega_q\tau}\langle a^+_q a_q\rangle_0 - e^{\omega_q\tau}\langle a_{-q} a^+_{-q}\rangle_0$$

The thermally averaged quantities are given by

$$\langle a^+_q a_q\rangle_0 = n_{\omega_q}\,,\quad \langle a_{-q} a^+_{-q}\rangle_0 = \langle 1 + a^+_{-q} a_{-q}\rangle = 1 + n_{\omega_q}$$

Thus

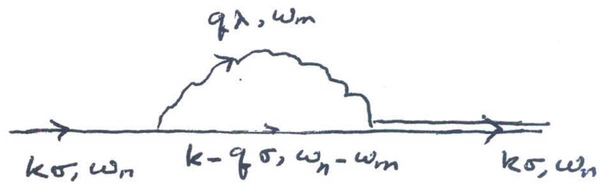
$$d^{0<}(q) = -n_{\omega_q} e^{-\omega_q\tau} - (1+n_{\omega_q}) e^{\omega_q\tau}$$

Since $1+n_{\omega_q} = -n_{-\omega_q}$, we obtain

$$d^{0<}(\vec{q}\lambda,\tau) = -n_{\omega_{\vec{q}\lambda}} e^{-\omega_{\vec{q}\lambda}\tau} + n_{-\omega_{\vec{q}\lambda}} e^{\omega_{\vec{q}\lambda}\tau}$$

2.

Here $n=1$. According to Feynman rules, the proper self energy contains the product of $g^0(k-q\sigma, \omega_n-\omega_m)$ with $|M_{q\lambda}|^2 d^0(q\lambda, \omega_m)$. The internal coordinates are



q, λ, and ω_m; these must be summed over. We should also multiply by the factor $(1/\hbar)^{2n}(-1/\beta\hbar)^n = (1/\hbar)^2(-1/\beta\hbar)$. Thus

$$\Sigma^* = -\frac{1}{\beta\hbar^3}\sum_{q\lambda}|M_{q\lambda}|^2\sum_m \frac{1}{i\omega_n - i\omega_m - \epsilon_{k-q}/\hbar} \cdot \frac{2\omega_{q\lambda}}{(i\omega_m)^2 - \omega_{q\lambda}^2}$$

To carry out the frequency summation, note that

$$\frac{2\omega_{q\lambda}}{(i\omega_m)^2 - \omega_{q\lambda}^2} = \frac{1}{i\omega_m - \omega_{q\lambda}} - \frac{1}{i\omega_m + \omega_{q\lambda}},$$

$$\frac{1}{(i\omega_n - i\omega_m - \bar{\epsilon}_{k+q}/\hbar)(i\omega_m - \omega_{q\lambda})} = \frac{\quad}{i\omega_n - \bar{\epsilon}_{k+q}/\hbar - \omega_{q\lambda}}\left[\frac{1}{i\omega_m - \omega_{q\lambda}} - \frac{1}{i\omega_m - i\omega_n + \bar{\epsilon}_{k+q}/\hbar}\right],$$

and

$$\frac{1}{(i\omega_n - i\omega_m - \bar{\epsilon}_{k+q}/\hbar)(i\omega_m + \omega_{q\lambda})} =$$

$$\frac{\quad}{i\omega_n - \bar{\epsilon}_{k+q}/\hbar + \omega_{q\lambda}}\left(\frac{1}{i\omega_m + \omega_{q\lambda}} - \frac{1}{i\omega_m - i\omega_n + \bar{\epsilon}_{k+q}/\hbar}\right)$$

Since the sum over m is convergent, we can introduce the convergence factor $e^{i\omega_m 0^+}$ and carry out the summation:

$$\sum_{m=-\infty}^{\infty} \frac{e^{i\omega_m 0^+}}{i\omega_m - \omega_{q\lambda}} = -\beta\hbar\, n_{\omega_{q\lambda}}$$

$$\sum_{m=-\infty}^{\infty} \frac{e^{i\omega_m 0^+}}{i\omega_m - i\omega_n + \bar{\epsilon}_{k+q}/\hbar} = \beta\hbar\, f_{-\bar{\epsilon}_{k+q}}$$

$$\sum_{m=-\infty}^{\infty} \frac{e^{i\omega_m 0^+}}{i\omega_m + \omega_{q\lambda}} = -\beta\hbar\, n_{-\omega_{q\lambda}}$$

Furthermore,

$$f_{-\bar{\epsilon}_{k+q}} = 1 - f_{\bar{\epsilon}_{k+q}} \equiv 1 - f_{\vec{k}+\vec{q}}$$

$$n_{-\omega_{q\lambda}} = -1 - n_{\omega_{q\lambda}}$$

Now the sum over m is carried out, and indeed Eq. (11.68) is obtained.

3.

a) $$d(q\lambda,\tau) = -\sum_{n=0}^{\infty} \frac{1}{n!}\left(\frac{1}{\hbar}\right)^n \int_0^{\beta\hbar} d\tau_1 \cdots \int_0^{\beta\hbar} d\tau_n \langle T\phi_{q\lambda}(\tau)\phi^+_{q\lambda}(0)V(\tau_1)\cdots V(\tau_n)\rangle_{0,c}$$

where

$$V = \sum_{kq}\sum_{q\lambda} M_{q\lambda} C^+_{k+q\sigma} C_{k\sigma}\phi_{q\lambda}, \quad \phi_{q\lambda} = a_{q\lambda} + a^+_{-q\lambda},$$

$$\phi^+_{q\lambda} = a^+_{q\lambda} + a_{-q\lambda} = \phi_{-q\lambda}$$

All operators are interaction-picture operators.

b) To second order in V (the first order vanishes)

$$d(q\lambda,\tau) = d^0(q\lambda,\tau) - \frac{1}{2!}\left(\frac{1}{\hbar}\right)^2 \sum_{k_1\sigma_1 q_1\lambda_1}\sum_{k_2\sigma_2 q_2\lambda_2} M_{q_1\lambda_1}M_{q_2\lambda_2}\int_0^{\beta\hbar} d\tau_1\int_0^{\beta\hbar} d\tau_2\, A$$

where

$$\bar{A} = \langle T\phi_{q\lambda}(\tau)\phi^+_{q\lambda}(0)C^+_{k_1+q_1\sigma_1}(\tau_1)C_{k_1\sigma_1}(\tau_1)\phi_{q_1\lambda_1}(\tau_1)C^+_{k_2+q_2\sigma_2}(\tau_2)C_{k_2\sigma_2}(\tau_2)\phi_{q_2\lambda_2}(\tau_2)\rangle_{0,c}$$

$$\equiv \mathcal{B}\mathcal{C}$$

$$\mathcal{B} = \langle T\phi_{q\lambda}(\tau)\phi^+_{q\lambda}(0)\phi_{q_1\lambda_1}(\tau_1)\phi_{q_2\lambda_2}(\tau_2)\rangle_0$$

$$\mathcal{C} = \langle T C^+_{k_1+q_1\sigma_1}(\tau_1)C_{k_1\sigma_1}(\tau_1)C^+_{k_2+q_2\sigma_2}(\tau_2)C_{k_2\sigma_2}(\tau_2)\rangle_0$$

To evaluate $\mathcal{B}$, we note that we cannot contract $\phi_{q\lambda}(\tau)$ with $\phi^+_{q\lambda}(0)$, for that would produce a disconnected diagram. Thus,

$$\mathcal{B} = \langle T\phi_{q\lambda}(\tau)\phi_{q_1\lambda_1}(\tau_1)\rangle_0 \langle T\phi_{q_2\lambda_2}(\tau_2)\phi^+_{q\lambda}(0)\rangle_0$$

$$+ \langle T\phi_{q\lambda}(\tau)\phi_{q_2\lambda_2}(\tau_2)\rangle_0 \langle T\phi_{q_1\lambda_1}(\tau_1)\phi^+_{q\lambda}(0)\rangle_0$$

$$= \langle T\phi_{q\lambda}(\tau)\phi^+_{-q_1\lambda_1}(\tau_1)\rangle_0 \langle T\phi_{q_2\lambda_2}(\tau_2)\phi^+_{q\lambda}(0)\rangle_0$$

$$+ \langle T\phi_{q\lambda}(\tau)\phi^+_{-q_2\lambda_2}(\tau_2)\rangle_0 \langle T\phi_{q_1\lambda_1}(\tau_1)\phi^+_{q\lambda}(0)\rangle_0$$

$$= d^0(q\lambda, \tau-\tau_1)\, d^0(q\lambda; \tau_2)\, \delta_{q_1,-q}\, \delta_{q_2,q}\, \delta_{\lambda_1\lambda}\, \delta_{\lambda_2\lambda}$$

$$+ d^0(q\lambda, \tau-\tau_2)\, d^0(q\lambda, \tau_1)\, \delta_{q_2,-q}\, \delta_{q_1,q}\, \delta_{\lambda_1\lambda}\, \delta_{\lambda_2\lambda}$$

To evaluate $\mathcal{C}$, note that we cannot contract $c^+_{k_1+q_1\sigma_1}(\tau_1)$ with $c_{k_1\sigma_1}(\tau_1)$, for that would imply that $q_1=0$, which in turn implies that $q=0$ (so that $\mathcal{B}$ is nonzero). But a phonon must have a nonzero wave vector. Thus

$$\mathcal{C} = -\langle T c_{k_1\sigma_1}(\tau_1)\, c^+_{k_2+q_2\sigma_2}(\tau_2)\rangle_0 \langle T c_{k_2\sigma_2}(\tau_2)\, c^+_{k_1+q_1\sigma_1}(\tau_1)\rangle_0$$

$$= -g^0(k_1\sigma_1, \tau_1-\tau_2)\, g^0(k_1+q_1\sigma_1, \tau_2-\tau_1)\, \delta_{\sigma_1\sigma_2}\, \delta_{k_2,k_1+q_1}\, \delta_{q_1,-q_2}$$

The product $\mathcal{B}\mathcal{C}$ thus consists of two terms. For both terms, $q_1 = -q_2 = \pm q$; hence $M_{q_1\lambda}M_{q_2\lambda_2}$ becomes equal to $M_{q\lambda}M_{-q\lambda} = |M_{q\lambda}|^2$.

Putting $\mathcal{B}$ and $\mathcal{C}$ into the expression for $d(q\lambda, \tau)$, it is seen that the second-order correction is the sum of two terms. It is easily verified that these two terms are equal. Hence,

$$d(q\lambda,\tau) = d^0(q\lambda,\tau) + \frac{|M_{q\lambda}|^2}{\hbar^2}\int_0^{\beta\hbar} d\tau_1 \int_0^{\beta\hbar} d\tau_2 \; d^0(q\lambda,\tau-\tau_2) \sum_{k\sigma} g^0(k\sigma,\tau_1-\tau_2)$$

$$\times\; g^0(k+q\sigma,\tau_2-\tau_1)\, d^0(q\lambda,\tau_1)$$

c) $$d(q\lambda,\tau) = \frac{1}{\beta\hbar}\sum_m e^{-i\omega_m\tau} d(q\lambda,\omega_m)$$

$$g^0(k\sigma,\tau) = \frac{1}{\beta\hbar}\sum_n e^{-i\omega_n\tau} g^0(k\sigma,\omega_n)$$

$$\frac{1}{\beta\hbar}\sum_m e^{-i\omega_m\tau} d(q\lambda,\omega_m) = \frac{1}{\hbar^2}\frac{1}{(\beta\hbar)^4}\sum_{k\sigma}\sum_{m_1 m_2 n_1 n_2} d^0(q\lambda,\omega_{m_1})\, g^0(k\sigma,\omega_{n_1})$$

$$\times\; g^0(k+q\sigma,\omega_{n_2})\, d^0(q\lambda,\omega_m)\, e^{-i\omega_{m_1}\tau}\int_0^{\beta\hbar} d\tau_1\int_0^{\beta\hbar} d\tau_2\; e^{i\omega_{m_1}\tau_2}\, e^{-i\omega_{n_1}(\tau_1-\tau_2)}\, e^{-i\omega_{n_2}(\tau_2-\tau_1)}\, e^{-i\omega_{m_2}\tau_1}$$

Doing the integrals over τ_1 and τ_2 gives:

$$\omega_{m_1} = \omega_{m_2}, \quad \omega_{n_2} = \omega_{n_1} + \omega_{m_1}$$

Thus

$$d(q\lambda,\omega_m) = d^0(q\lambda,\omega_m) + \frac{1}{\beta\hbar^3}\sum_{k\sigma n} |M_{q\lambda}|^2 d^0(q\lambda,\omega_m)\, g^0(k\sigma,\omega_n)\, g^0(k+q\sigma,\omega_n+\omega_m)$$

$$\times\; d^0(q\lambda,\omega_m)$$

$$= d^0(q\lambda,\omega_m) + \frac{|M_{q\lambda}|^2}{\hbar} d^0(q\lambda,\omega_m)\left[\frac{1}{\beta\hbar^2}\sum_{k\sigma n} g^0(k\sigma,\omega_n)\, g^0(k+q\sigma,\omega_n+\omega_m)\right] d^0(q\lambda,\omega_m)$$

4. The dressed phonon propagator is given by

$$d(q\lambda, \omega_m) = d^0(q, \omega_m) + \frac{V}{\hbar} |M_q|^2 d^0(q, \omega_m)\, \Pi(q, \omega_m)\, d(q, \omega_m)$$

$$\Rightarrow d(q, \omega_m) = \frac{d^0(q, \omega_m)}{1 - \frac{V}{\hbar}|M_q|^2 d^0(q, \omega_m)\Pi(q, \omega_m)}$$

$$= \frac{1}{d_0^{-1}(q, \omega_m) - \frac{V}{\hbar}|M_q|^2 \Pi(q, \omega_m)}$$

$$= \frac{1}{\frac{(i\omega_m)^2 - \Omega^2}{2\Omega} - \frac{V}{\hbar}|M_q|^2 \Pi(q, \omega_m)}$$

$$= \frac{2\Omega}{(i\omega_m)^2 - \Omega^2 - 2\frac{V}{\hbar}\Omega |M_q|^2 \Pi(q, \omega_m)}$$

$$|M_q|^2 = \frac{16\pi^2 Z^2 e^4}{V^2 q^2} \frac{N\hbar}{2M\Omega}$$

$$\Rightarrow \frac{2V}{\hbar}\Omega |M_q|^2 = \frac{16\pi^2 Z^2 e^4 n_i}{M q^2} = \frac{4\pi Z^2 e^2 n_i}{M} \cdot \frac{4\pi e^2}{q^2} = \Omega^2 V_q$$

where $V_q = 4\pi e^2/q^2$ is the Coulomb interaction. Replacing $\Pi(q, \omega_m)$ by $\Pi(q, 0)$, we obtain

$$d(q, \omega_m) = \frac{2\Omega}{(i\omega_m)^2 - \Omega^2[1 + V_q \Pi(q, 0)]}$$

$$1 + V_q \Pi(q, 0) = 1 + \frac{V_q \Pi^0(q, 0)}{1 - V_q \Pi^0(q, 0)} = \frac{1}{1 - V_q \Pi^0(q, 0)} = \frac{1}{\epsilon(q, 0)}$$

Hence,

$$d(q, \omega_m) = \frac{2\Omega}{(i\omega_m)^2 - \Omega^2/\epsilon(q, 0)}$$

The phonon frequency is thus given by

$$\omega = \frac{\Omega}{\sqrt{\epsilon(q, 0)}} \xrightarrow{q \to 0} \frac{\Omega}{\sqrt{1 + q_{TF}^2/q^2}} = \frac{\Omega q}{\sqrt{q^2 + q_{TF}^2}} \longrightarrow \frac{\Omega}{q_{TF}} q \equiv v q, \quad v = \frac{\Omega}{q_{TF}}$$

5.

a) $\vec{E}$ and $\vec{B}$ are defined in terms of ϕ and $\vec{A}$:

$$\vec{B} = \vec{\nabla} \times \vec{A} \quad , \quad \vec{E} = -\vec{\nabla}\phi - \frac{1}{c}\frac{\partial \vec{A}}{\partial t}$$

These lead to two of Maxwell's equations:

$$\vec{\nabla} \cdot \vec{B} = 0 \quad , \quad \vec{\nabla} \times \vec{E} + \frac{1}{c}\frac{\partial \vec{B}}{\partial t} = 0$$

There are two more Maxwell equations.

The Lagrangian density

$$\mathcal{L} = -\frac{1}{16\pi} F^{\alpha\beta} F_{\alpha\beta}$$

$$= -\frac{1}{16\pi} g^{\lambda\alpha} g^{\sigma\beta} (\partial_\lambda A_\sigma - \partial_\sigma A_\lambda)(\partial_\alpha A_\beta - \partial_\beta A_\alpha)$$

Here $g^{\mu\nu}$ is the standard metric,

$$x^\mu = g^{\mu\nu} x_\nu$$

and repeated indices are summed over (0 to 3).

$$\frac{\partial \mathcal{L}}{\partial(\partial_\mu A_\nu)} = -\frac{1}{16\pi} g^{\lambda\alpha} g^{\sigma\beta} [\delta_\mu^\lambda \delta_\nu^\sigma F_{\alpha\beta} - \delta_\mu^\sigma \delta_\nu^\lambda F_{\alpha\beta} + \delta_\mu^\alpha \delta_\nu^\beta F_{\lambda\sigma} - \delta_\mu^\beta \delta_\nu^\alpha F_{\lambda\sigma}]$$

$$= -\frac{1}{16\pi} [g^{\mu\alpha} g^{\nu\beta} F_{\alpha\beta} - g^{\nu\alpha} g^{\mu\beta} F_{\alpha\beta} + g^{\lambda\mu} g^{\sigma\nu} F_{\lambda\sigma} - g^{\lambda\nu} g^{\sigma\mu} F_{\lambda\sigma}]$$

$$= -\frac{1}{16\pi} [F^{\mu\nu} - F^{\nu\mu} + F^{\mu\nu} - F^{\nu\mu}] = -\frac{1}{4\pi} F^{\mu\nu}$$

$$\frac{\partial \mathcal{L}}{\partial A_\nu} = 0$$

Thus Lagrange's equations give:

$$\partial_\mu F^{\mu\nu} = 0$$

$$F^{00} = 0 \;, \quad F^{01} = \partial^0 A^1 - \partial^1 A^0 = \frac{1}{c}\frac{\partial}{\partial t} A_x + \frac{\partial}{\partial x}\phi = -E_x$$

$$F^{02} = -E_y \;, \quad F^{03} = -E_z$$

$$F^{10} = -F^{01} = E_x \;, \quad F^{11} = 0 ,$$

$$F^{12} = \partial^1 A^2 - \partial^2 A^1 = -\frac{\partial}{\partial x} A_y + \frac{\partial}{\partial y} A_x = -(\vec{\nabla}\times\vec{A})_z = -B_z \;, \ldots \text{etc.}$$

we find

$$F^{\mu\nu} = \begin{bmatrix} 0 & -E_x & -E_y & -E_z \\ E_x & 0 & -B_z & B_y \\ B_y & B_z & 0 & -B_x \\ E_z & -B_y & B_x & 0 \end{bmatrix}$$

Thus

$$\partial_\mu F^{\mu 0} = 0 \Rightarrow \vec{\nabla}\cdot\vec{E} = 0$$ (a Maxwell equation in free space)

and

$$\partial_\mu F^{\mu 1} = 0 \Rightarrow \frac{1}{c}\frac{\partial}{\partial t}E_x - \frac{\partial}{\partial y} B_z + \frac{\partial}{\partial z} B_y = 0$$

$$\Rightarrow \frac{1}{c}\frac{\partial}{\partial t} E_x = \frac{\partial}{\partial y} B_z - \frac{\partial}{\partial z} B_y = (\vec{\nabla}\times\vec{B})_x$$

Setting $\mu = 2, 3$, we thus obtain

$$\frac{1}{c}\frac{\partial \vec{E}}{\partial t} = \vec{\nabla}\times\vec{B}$$ (another maxwell equation in free space).

b) $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$

$$F_{00} = 0 \;, \quad F_{01} = \partial_0 A_1 - \partial_1 A_0 = E_x \;, \quad F_{02} = E_y \;, \quad F_{03} = E_z$$

$$F_{10} = -E_x \;, \quad F_{11} = 0 \;, \quad F_{12} = \partial_1 A_2 - \partial_2 A_1 = -\frac{\partial}{\partial x} A_y + \frac{\partial}{\partial y} A_x = -B_z \,.$$

$$F_{13} = -\frac{\partial}{\partial x} A_z + \frac{\partial}{\partial z} A_x = B_y \;, \; ---$$

We find

$$F_{\mu\nu} = F^{\mu\nu}(\vec{E} \rightarrow -\vec{E})$$

Thus

$$F_{\mu\nu}F^{\mu\nu} = 2(B^2 - E^2)$$

$$\Rightarrow \mathcal{L} = \frac{1}{8\pi}(E^2 - B^2)$$

c) From Eq. (11.80),

$$\vec{E} = -\sqrt{\frac{4\pi}{V}} \sum_{q\lambda} \dot{A}_{q\lambda} \vec{\epsilon}_\lambda(\vec{q}) e^{i\vec{q}\cdot\vec{r}}, \quad \vec{B} = i\sqrt{\frac{4\pi c^2}{V}} \sum_{q\lambda} A_{q\lambda} \vec{q}\times\vec{\epsilon}_\lambda(\vec{q}) e^{i\vec{q}\cdot\vec{r}}$$

Since $\vec{E}$ and $\vec{B}$ are real, we may write

$$E^2 = \vec{E}\cdot\vec{E}^*, \quad B^2 = \vec{B}\cdot\vec{B}^*$$

$$\frac{1}{8\pi}\int E^2 d^3r = \frac{1}{8\pi}\cdot\frac{4\pi}{V}\sum_{q\lambda}\sum_{q'\lambda'} \dot{A}_{q\lambda}\dot{A}^*_{q'\lambda'} \vec{\epsilon}_\lambda(\vec{q})\cdot\vec{\epsilon}^{\,*}_{\lambda'}(\vec{q}\,')\int e^{i(\vec{q}-\vec{q}\,')\cdot\vec{r}} d^3r$$

Since

$$\int e^{i(\vec{q}-\vec{q}\,')\cdot\vec{r}} d^3r = V\delta_{\vec{q},\vec{q}\,'},$$

we find

$$\frac{1}{8\pi}\int E^2 d^3r = \frac{1}{2}\sum_{\vec{q}\lambda\lambda'} \dot{A}_{\vec{q}\lambda}\dot{A}^*_{\vec{q}\lambda} \vec{\epsilon}_\lambda(\vec{q})\cdot\vec{\epsilon}_{\lambda'}(\vec{q})$$

$$= \frac{1}{2}\sum_{q\lambda} \dot{A}_{q\lambda}\dot{A}^*_{\vec{q}\lambda} = \frac{1}{2}\sum_{q\lambda} \dot{A}_{\vec{q}\lambda}\dot{A}_{-\vec{q}\lambda}$$

$$\frac{1}{8\pi}\int B^2 d^3r = \frac{1}{8\pi}\cdot\frac{4\pi c^2}{V}\sum_{\vec{q}\lambda}\sum_{\vec{q}\,'\lambda'} A_{\vec{q}\lambda}A^*_{\vec{q}\,'\lambda'} \vec{q}\times\epsilon_\lambda(\vec{q})\cdot(\vec{q}\,'\times\vec{\epsilon}_{\lambda'}(\vec{q}\,'))\int e^{i(\vec{q}-\vec{q}\,')\cdot\vec{r}} d^3r$$

$$= \frac{c^2}{2}\sum_{\vec{q}\lambda\lambda'} A_{\vec{q}\lambda}A^*_{\vec{q}\lambda}(\vec{q}\times\epsilon_\lambda(\vec{q}))\cdot(\vec{q}\times\vec{\epsilon}_{\lambda'}(\vec{q}))$$

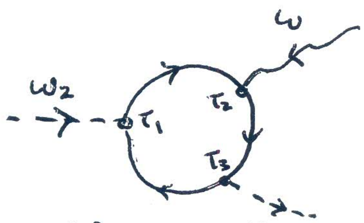
$$= \frac{c^2}{2}\sum_{\vec{q}\lambda\lambda'} A_{\vec{q}\lambda}A^*_{\vec{q}\lambda} q^2 \delta_{\lambda\lambda'}$$

$$= \frac{1}{2}\sum_{\vec{q}\lambda} \omega_q^2 A_{\vec{q}\lambda}A_{-\vec{q}\lambda}$$

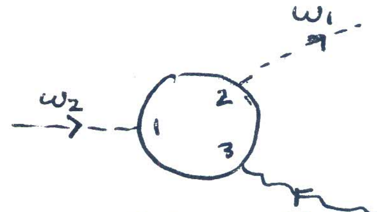
Hence

$$L = \frac{1}{2}\sum_{\vec{q}\lambda}\left(\dot{A}_{\vec{q}\lambda}\dot{A}_{-\vec{q}\lambda} - \omega_q^2 A_{\vec{q}\lambda}A_{-\vec{q}\lambda}\right)$$

6.

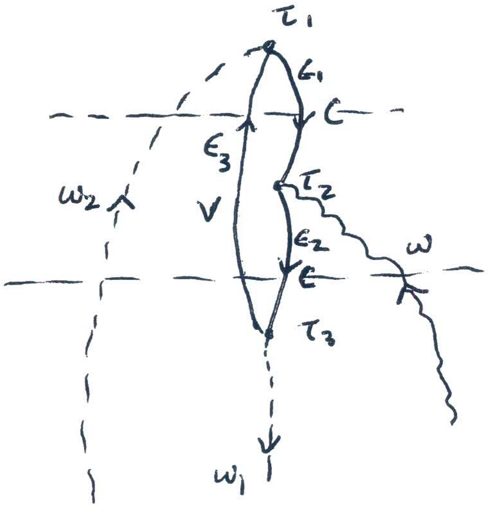


(1)



(2)

Each figure gives 6 time ordered diagrams (since we have three times τ_1, τ_2, and τ_3). Let us consider the following time-ordered diagram, obtained from Fig. 1



In this diagram, electron scattering by phonon emission takes place in the conduction band.

The expression for this diagram is

$$D_1 = \sum_{\vec{k}\sigma} \int \frac{d\epsilon_1}{2\pi} \int \frac{d\epsilon_2}{2\pi} \int \frac{d\epsilon_3}{2\pi} \frac{\rho^{0>}(c\vec{k}\sigma,\epsilon_1)\, \rho^{0>}(c\vec{k}\sigma,\epsilon_2)\, \rho^{0<}(v\vec{k}\sigma,\epsilon_3) P_k^{cv}(\lambda_2) M_{q\lambda}^{cc} P_k^{vc}(\lambda_1)}{(-\omega_2+\epsilon_1-\epsilon_3)(-\omega_2-\omega+\epsilon_2-\epsilon_3)}$$

$$\rho^{0>}(c\vec{k}\sigma,\epsilon_1) = -A^0(ck\sigma,\epsilon_1) = -2\pi\,\delta(\epsilon_1 - \epsilon_{c\vec{k}\sigma}/\hbar)$$

$$\rho^{0>}(c\vec{k}\sigma,\epsilon_2) = -2\pi\,\delta(\epsilon_2 - \epsilon_{c\vec{k}\sigma}/\hbar)$$

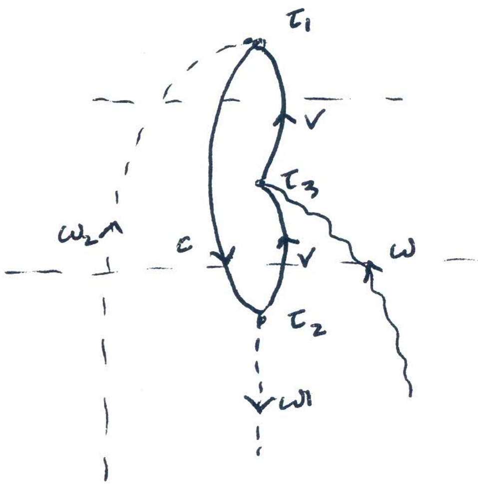
$$\rho^{0<}(vk\sigma,\epsilon_3) = 2\pi\,\delta(\epsilon_3 - \epsilon_{v\vec{k}\sigma}/\hbar)$$

Thus we get

$$D = \sum_{k\sigma} \frac{P_{\vec{k}}^{cv}(\lambda_2)\, M_{\vec{q}\lambda}^{cc}\, P_{\vec{k}}^{vc}(\lambda_1)}{(E_g/\hbar-\omega_2)(E_g/\hbar-\omega_2-\omega)}$$

where $E_g = \epsilon_{c\vec{k}} - \epsilon_{v\vec{k}}$ (assuming the bands are dispersionless)

Now consider the following time-ordered diagram arising from Fig. 2.



Here, the incident photon creates an electron-hole pair, and the hole is then scattered by phonon emission. The interaction matrix element is $M_{\text{hole-phonon}}$.

The time-ordered diagram rules give

$$D_2 = \sum_{k\sigma} \frac{-p_k^{cv}(\lambda_2)\, M_{q\lambda}^{h-p}\, p_k^{vc}(\lambda_1)}{(E_g/\hbar\omega - \omega_2)(E_g/\hbar - \omega_2 - \omega)}$$

The electron-phonon matrix element depends on the sign of the charge. For hole-phonon scattering, $M^{h-p} = -M^{e-p}$. Then the two expression D_1 and D_2 add up to one of the six terms in the expression for Γ given in the text. The other five terms are obtained in a similar way.

Chapter 12

1.

$$S = \sum_{k\sigma}\sum_{q\lambda} M_{q\lambda} c^+_{k+q\sigma} c_{k\sigma}\left(\frac{a_{q\lambda}}{\epsilon_k - \epsilon_{k+q} + \hbar\omega_{q\lambda}} + \frac{a^+_{-q\lambda}}{\epsilon_k - \epsilon_{k+q} - \hbar\omega_{q\lambda}}\right)$$

$$H_0 = \sum_{k\sigma} \epsilon_k c^+_{k\sigma} c_{k\sigma} + \sum_{q\lambda} \hbar\omega_{q\lambda}(a^+_{q\lambda} a_{q\lambda} + 1/2) = H_{0e} + H_{0p}$$

Using the formulas

$$[AB, CD] = A\{B, C\}D - AC\{B, D\} + \{A, C\}DB - C\{A, D\}B,$$

$$\{c_{k\sigma}, c_{k'\sigma'}\} = \{c^+_{k\sigma}, c^+_{k'\sigma'}\} = 0, \text{ and } \{c_{k\sigma}, c^+_{k'\sigma'}\} = \delta_{kk'}\delta_{\sigma\sigma'},$$

we find

$$[c^+_{k+q\sigma} c_{k\sigma}, c^+_{k'\sigma'} c_{k'\sigma'}] = \delta_{\sigma\sigma'}(\delta_{kk'} - \delta_{k',k+q}) c^+_{k+q} c_{k\sigma}$$

Hence

$$[S, H_{0e}] = \sum_{k\sigma}\sum_{q\lambda}\sum_{k'\sigma'} \epsilon_{k'} M_{q\lambda}\left(\frac{a_{q\lambda}}{\epsilon_k - \epsilon_{k+q} + \hbar\omega_{q\lambda}} + \frac{a^+_{-q\lambda}}{\epsilon_k - \epsilon_{k+q} - \hbar\omega_{q\lambda}}\right)$$

$$\times\ \delta_{\sigma\sigma'}(\delta_{kk'} - \delta_{k',k+q}) c^+_{k+q\sigma} c_{k\sigma}$$

$$= \sum_{k\sigma}\sum_{q\lambda} M_{q\lambda} c^+_{k+q} c_{k\sigma}\left[\frac{(\epsilon_k - \epsilon_{k+q}) a_{q\lambda}}{\epsilon_k - \epsilon_{k+q} + \hbar\omega_{q\lambda}} + \frac{(\epsilon_k - \epsilon_{k+q}) a^+_{-q\lambda}}{\epsilon_k - \epsilon_{k+q} - \hbar\omega_{q\lambda}}\right]$$

Next, we note that

$$[a_{q\lambda}, a^+_{q'\lambda'} a_{q'\lambda'}] = \delta_{qq'}\delta_{\lambda\lambda'} a_{q\lambda},\quad [a^+_{-q\lambda}, a^+_{q'\lambda'} a_{q'\lambda'}] = -\delta_{\lambda\lambda'}\delta_{qq'} a^+_{-q\lambda}$$

It follows that

$$[S, H_{0p}] = \sum_{k\sigma}\sum_{q\lambda} M_{q\lambda} c^+_{k+q\sigma} c_{k\sigma}\left[\frac{\hbar\omega_{q\lambda} a_{q\lambda}}{\epsilon_k - \epsilon_{k+q} + \hbar\omega_{q\lambda}} + \frac{-\hbar\omega_{q\lambda} a^+_{-q\lambda}}{\epsilon_k - \epsilon_{k+q} - \hbar\omega_{q\lambda}}\right]$$

Therefore,

$$[S, H_0] = [S, H_{0e}] + [S, H_{0p}]$$

$$= \sum_{k\sigma}\sum_{q\lambda} M_{q\lambda} c^+_{k+q\sigma} c_{k\sigma}(a_{q\lambda} + a^+_{-q\lambda}) = H'$$

2. Ground state energy

$$H = \sum_k \epsilon_k (c_{k\uparrow}^+ c_{k\uparrow} + c_{k\downarrow}^+ c_{k\downarrow}) + \sum_{kk'} \omega_{kk'} c_{k'\uparrow}^+ c_{-k'\downarrow}^+ c_{-k\downarrow} c_{k\uparrow}$$

$$= H_0 + H'$$

$$|\psi_0\rangle = \prod_k (u_k + v_k c_{k\uparrow}^+ c_{-k\downarrow}^+)|0\rangle$$

$$E = \langle\psi_0|H|\psi_0\rangle = \langle\psi_0|H_0|\psi_0\rangle + \langle\psi_0|H'|\psi_0\rangle$$

$$\langle\psi|H_0|\psi\rangle = \sum_k \epsilon_k \langle\psi_0|c_{k\uparrow}^+ c_{k\uparrow}|\psi_0\rangle + \sum_k \epsilon_k \langle\psi_0|c_{k\downarrow}^+ c_{k\downarrow}|\psi_0\rangle$$

$$= P + Q$$

$$P = \sum_k \epsilon_k \langle\psi_0|c_{k\uparrow}^+ c_{k\uparrow}|\psi_0\rangle$$

$$= \sum_k \epsilon_k \quad \langle 0|\prod_p (u_p + v_p c_{-p\downarrow} c_{p\uparrow}) c_{k\uparrow}^+ c_{k\uparrow} \prod_q (u_q + v_q c_{q\uparrow}^+ c_{-q\downarrow}^+)|0\rangle$$

$$= \sum_k \epsilon_k \langle 0|ABD|0\rangle$$

where

$$A = \prod_{p\neq k} (u_p + v_p c_{-p\downarrow} c_{p\uparrow}), \quad B = \prod_{q\neq k} (u_q + v_q c_{q\uparrow}^+ c_{-q\downarrow}^+)$$

$$D = (u_k + v_k c_{-k\downarrow} c_{k\uparrow}) c_{k\uparrow}^+ c_{k\uparrow} (u_k + v_k c_{k\uparrow}^+ c_{-k\downarrow}^+)$$

$$D|0\rangle = u_k^2 c_{k\uparrow}^+ c_{k\uparrow}|0\rangle + u_k v_k c_{k\uparrow}^+ c_{k\uparrow} c_{k\uparrow}^+ c_{-k\downarrow}^+ |0\rangle$$

$$+ u_k v_k c_{-k\downarrow} c_{k\uparrow} c_{k\uparrow}^+ c_{k\uparrow}|0\rangle + v_k^2 c_{-k\downarrow} c_{k\uparrow} c_{k\uparrow}^+ c_{k\uparrow} c_{k\uparrow}^+ c_{-k\downarrow}^+ |0\rangle$$

Note that $c_{k\uparrow}|0\rangle = 0$ and that $c_{k\sigma} c_{k\sigma}^+|0\rangle = (1 - c_{k\sigma}^+ c_{k\sigma})|0\rangle = |0\rangle$.

It follows that

$$D|0\rangle = u_k v_k c_{k\uparrow}^+ c_{-k\downarrow}^+ |0\rangle + v_k^2 |0\rangle$$

The bra $\langle 0|AB$ corresponds to a state with no particles with wave vector k; hence

$$\langle 0|AB\, u_k v_k c_{k\uparrow}^+ c_{-k\downarrow}^+|0\rangle = 0$$

Thus

$$P = \sum_k v_k^2 \epsilon_k \langle 0 | A B | 0 \rangle$$

$$= \sum_k v_k^2 \epsilon_k \prod_{p \neq k} (u_p^2 + v_p^2) = \sum_k v_k^2 \epsilon_k$$

Similarly, $Q = \sum_k v_k^2 \epsilon_k$

Now consider $\langle \psi_0 | H' | \psi_0 \rangle$,

$$\langle \psi_0 | H' | \psi_0 \rangle = \sum_{kk'} U_{kk'} \langle 0 | A' B' D' | 0 \rangle$$

where

$$A' = \prod_{p \neq k, k'} (u_p + v_p c_{-p\downarrow} c_{p\uparrow})$$

$$B' = \prod_{q \neq k, k'} (u_q + v_q c^+_{q\uparrow} c^+_{-q\downarrow})$$

$$D' = (u_k + v_k c_{-k\downarrow} c_{k\uparrow})(u_{k'} + v_{k'} c_{-k'\downarrow} c_{k'\uparrow}) c^+_{k'\uparrow} c^+_{-k'\downarrow} c_{-k\downarrow} c_{k\uparrow}$$

$$\times (u_k + v_k c^+_{k\uparrow} c^+_{-k\downarrow})(u_{k'} + v_{k'} c^+_{k'\uparrow} c^+_{-k'\downarrow})$$

The arguments used in calculating P can be used again. The only terms in $D'|0\rangle$ that will yield nonvanishing contribution to $\langle 0 | A' B' D' | 0 \rangle$ correspond to terms in D' with equal number of annihilation and creation operators. Since $c_{k\uparrow}|0\rangle = 0$, there are only two terms that can possibly contribute to $\langle 0 | A' B' D' | 0 \rangle$. One term is

$$v_k^2 v_{k'}^2 c_{-k\downarrow} c_{k\uparrow} c_{-k'\downarrow} c_{k'\uparrow} c^+_{k'\uparrow} c^+_{-k'\downarrow} c_{-k\downarrow} c_{k\uparrow} c^+_{k\uparrow} c^+_{-k\downarrow} c^+_{k'\uparrow} c^+_{-k'\downarrow} |0\rangle$$

Now consider $c^+_{k'\uparrow} c^+_{-k'\downarrow} c_{-k\downarrow}$. Using the anticommutation relations,

$$c^+_{k'\uparrow} c^+_{-k'\downarrow} c_{-k\downarrow} = c^+_{k'\uparrow} (\delta_{kk'} - c_{-k\downarrow} c^+_{-k'\downarrow}) = c^+_k \delta_{kk'} + c_{-k\downarrow} c^+_{k'\uparrow} c^+_{-k'\downarrow}$$

However,

$$c_{-k\downarrow} c_{k\uparrow} c_{-k'\downarrow} c_{k'\uparrow} c_{-k\downarrow} = 0$$

since we can move $c_{-k\downarrow}$ all the way to the left and $c_{-k\downarrow} c_{-k\downarrow} = 0$.
Furthermore, when $k = k'$, $c_{-k\downarrow} c_{k\uparrow} c_{-k'\downarrow} c_{k'\uparrow} = 0$ since

$$c_{-k\downarrow} c_{k\uparrow} = - c_{k\uparrow} c_{-k\downarrow} \text{ and } c_{-k\downarrow} c_{-k'\downarrow} = 0 \text{ when } k = k'.$$

Therefore, this term with 6 annihilation and 6 creation operators gives a vanishing contribution to $\langle 0 | A' B' D' | 0 \rangle$. The only other term in $D|0\rangle$ that may give a nonvanishing contribution is the following

3. The anomalous Green's function

$$\bar{H} = \sum_{k\sigma} \bar{\epsilon}_k c^+_{k\sigma} c_{k\sigma} + \sum_{kk'} W_{kk'} c^+_{k'\uparrow} c^+_{-k'\downarrow} c_{-k\downarrow} c_{k\uparrow}$$

$$\frac{\partial}{\partial \tau} F^+(k,\tau) = -\langle T \frac{\partial}{\partial \tau} c^+_{-k\downarrow}(\tau) c^+_{k\uparrow}(0) \rangle$$

(See the equation before Eq. (12.76) and the sentence following that equation).

$$\frac{\partial}{\partial \tau} c^+_{-k\downarrow} = \frac{1}{\hbar} [\bar{H}, c^+_{-k\downarrow}] = \frac{1}{\hbar} [\bar{H}_0, c^+_{-k\downarrow}] + \frac{1}{\hbar} [H', c^+_{-k\downarrow}]$$

$$[\bar{H}_0, c^+_{-k\downarrow}] = \sum_{k_1\sigma} \bar{\epsilon}_{k_1} [c^+_{k_1\sigma} c_{k_1\sigma}, c^+_{-k\downarrow}]$$

$$= \sum_{k_1\sigma} \bar{\epsilon}_{k_1} \left(c^+_{k_1\sigma} \{c_{k_1\sigma}, c^+_{-k\downarrow}\} - \{c^+_{k_1\sigma}, c^+_{-k\downarrow}\} c_{k\sigma} \right)$$

$$= \sum_{k_1\sigma} \bar{\epsilon}_{k_1} (\delta_{k_1,-k} \delta_{\sigma\downarrow} c^+_{k_1\sigma} - 0) = \bar{\epsilon}_{-k} c^+_{-k\downarrow} = \bar{\epsilon}_k c^+_{-k\downarrow}$$

$$[H', c^+_{-k\downarrow}] = \sum_{k_1k_2} W_{k_1k_2} [c^+_{k_2\uparrow} c^+_{-k_2\downarrow} c_{-k_1\downarrow} c_{k_1\uparrow}, c^+_{-k\downarrow}]$$

$$= \sum_{k_1k_2} W_{k_1k_2} c^+_{k_2\uparrow} c^+_{-k_2\downarrow} [c_{-k_1\downarrow} c_{k_1\uparrow}, c^+_{-k\downarrow}]$$

since $[c^+_{k_2\uparrow} c^+_{-k_2\downarrow}, c^+_{-k\downarrow}] = 0$

Using $[AB, C] = A\{B, C\} - \{A, C\} B$,

$$[c_{-k_1\downarrow} c_{k_1\uparrow}, c^+_{-k\downarrow}] = c_{-k_1\downarrow} \{c_{k_1\uparrow}, c^+_{-k\downarrow}\} - \{c_{k_1\downarrow}, c^+_{-k\downarrow}\} c_{k_1\uparrow}$$

$$= 0 - \delta_{k_1,k} c_{k_1\uparrow}$$

Thus

$$[H', c^+_{-k\downarrow}] = -\sum_{k'} W_{kk'} c^+_{k'\uparrow} c^+_{-k'\downarrow} c_{k\uparrow}$$

Therefore

$$\frac{\partial}{\partial\tau} F^{+}(k,\tau) = -\frac{\epsilon_k}{\hbar} \langle T c^{+}_{-k\downarrow}(\tau)\, c^{+}_{k\uparrow}(0)\rangle$$

$$+ \frac{1}{\hbar} \sum_{k'} U_{kk'} \langle T c^{+}_{k'\uparrow}(\tau)\, c^{+}_{-k'\downarrow}(\tau)\, c_{k\uparrow}(\tau)\, c^{+}_{k\uparrow}(0)\rangle$$

Recall that $F^{+}(k,\tau) = -\langle T c_{-k\downarrow}(\tau)\, c^{+}_{k\uparrow}(0)\rangle$.

Following the discussion in Sec. 12.7, we write

$$\langle T c^{+}_{k'\uparrow}(\tau)\, c^{+}_{-k'\downarrow}(\tau)\, c_{k\uparrow}(\tau)\, c^{+}_{k\uparrow}(0)\rangle$$

$$\cong \langle T c^{+}_{k'\uparrow}(\tau)\, c^{+}_{-k'\downarrow}(\tau)\rangle \langle T c_{k\uparrow}(\tau)\, c^{+}_{k\uparrow}(0)\rangle$$

$$= -\langle T c^{+}_{-k'\downarrow}(\tau)\, c^{+}_{k'\uparrow}(\tau)\rangle \langle T c_{k\uparrow}(\tau)\, c^{+}_{k\uparrow}(0)\rangle$$

$$= - F(k',0)\, g(k\uparrow,\tau)$$

The approximation made is the mean field approximation. Thus

$$(\partial/\partial\tau - \bar{\epsilon}_k/\hbar)\, F^{+}(k,\tau) = -\frac{1}{\hbar}\sum_{k'} U_{kk'}\, F^{+}(k',0)\, g(k\uparrow,\tau)$$

$$\Delta_k = -\sum_{k'} U_{k'k}\, F(k',0) \Rightarrow \Delta_k^{*} = -\sum_{k'} U^{*}_{k'k}\, F^{+}(k',0)$$

$$= -\sum_{k'} U_{kk'}\, F^{+}(k',0)$$

Hence

$$(\partial/\partial\tau - \bar{\epsilon}_k/\hbar)\, F^{+}(k,\tau) = \frac{\Delta_k^{*}}{\hbar}\, g(k\uparrow,\tau)$$

4. Dirac-delta function

Consider

$$S = \sum_{n=-\infty}^{\infty} e^{-i\omega_n \tau} \quad , \quad -\beta\hbar < \tau < \beta\hbar$$

For $\tau = 0$, $S = \infty$

For $\tau \neq 0$,

$$S = \sum_{n=-\infty}^{\infty} e^{-i(2n+1)\pi\tau/\beta\hbar} = e^{-i\pi\tau/\beta\hbar} \sum_{n=-\infty}^{\infty} e^{-2n\pi i\tau/\beta\hbar}$$

$$= e^{-i\pi\tau/\beta\hbar} \sum_{n=-\infty}^{\infty} e^{-i\alpha n} = e^{-i\pi\tau/\beta\hbar} S' \quad , \quad \alpha = 2\pi\tau/\beta\hbar$$

$$S' = \sum_{n=-\infty}^{\infty} e^{-i\alpha n} = \sum_{n=-\infty}^{0} e^{-i\alpha n} + \sum_{n=0}^{\infty} e^{-i\alpha n} - 1$$

$$= \sum_{n=0}^{\infty} e^{i\alpha n} + \sum_{n=0}^{\infty} e^{-i\alpha n} - 1$$

$$= \frac{1}{1-e^{i\alpha}} + \frac{1}{1-e^{-i\alpha}} - 1 = \frac{2-2\cos\alpha}{2-2\cos\alpha} - 1 = 0$$

since $\cos\alpha \neq 1$ $(\alpha \neq 0)$.

Next, consider the integral $(\epsilon \to 0)$

$$I = \int_{-\epsilon}^{\epsilon} S\, d\tau = \sum_{n=-\infty}^{\infty} \int_{0^-}^{0^+} e^{-i\omega_n \tau} d\tau = \sum_{n=-\infty}^{\infty} \frac{e^{-i\omega_n \tau}}{-i\omega_n} \Bigg|_{0^-}^{0^+}$$

$$= \sum_{n=-\infty}^{\infty} \frac{e^{-i\omega_n 0^+}}{-i\omega_n} - \sum_{n=-\infty}^{\infty} \frac{e^{-i\omega_n 0^-}}{-i\omega_n}$$

$$= \sum_{n=-\infty}^{\infty} \frac{e^{-i\omega_n 0^+}}{-i\omega_n} + \sum_{n=-\infty}^{\infty} \frac{e^{i\omega_n 0^+}}{i\omega_n}$$

From Eq. (9.14), $\displaystyle\sum_{n=-\infty}^{\infty} \frac{e^{i\omega_n 0^+}}{i\omega_n - \epsilon} = \beta\hbar f_\epsilon \Rightarrow \sum_{n=-\infty}^{\infty} \frac{e^{i\omega_n 0^+}}{i\omega_n} = \beta\hbar f_{\epsilon=0} = \beta\hbar/2$

Taking complex conjugate of the above $\Rightarrow \displaystyle\sum_{n=-\infty}^{\infty} \frac{e^{-i\omega_n 0^+}}{-i\omega_n} = \beta\hbar/2$

Therefore,

$$I = \beta\hbar$$

We now have the following,

$$S = \begin{cases} 0 & \tau \neq 0 \\ \infty & \tau = 0 \end{cases}$$

and

$$\int_{-\epsilon}^{\epsilon} S\, d\tau = \beta\hbar$$

$$\Rightarrow \quad S = \beta\hbar\, \delta(\tau)$$

$$\Rightarrow \quad \delta(\tau) = \frac{1}{\beta\hbar} \cdot \sum_{n=-\infty}^{\infty} e^{-i\omega_n \tau} \quad , \qquad -\beta\hbar < \tau < \beta\hbar$$

5. Equation of motion

$$\bar{H}_{MF} = \sum_{k\sigma} \bar{\epsilon}_k c^+_{k\sigma} c_{k\sigma} - \sum_k \Delta^*_k c_{-k\downarrow} c_{k\uparrow} - \sum_k \Delta_k c^+_{k\uparrow} c^+_{-k\downarrow} + \sum_k \Delta_k \langle c^+_{k\uparrow} c^+_{-k\downarrow} \rangle$$

$$= \bar{H}_0 + H'$$

Equation (12.71) reads

$$\frac{\partial}{\partial\tau} g(k\uparrow, \tau) = -\delta(\tau) - \langle T \tfrac{\partial}{\partial\tau} c_{k\uparrow}(\tau) c^+_{k\uparrow}(0) \rangle$$

$$\frac{\partial}{\partial\tau} c_{k\uparrow}(\tau) = \frac{1}{\hbar} [\bar{H}_0, c_{k\uparrow}(\tau)] + \frac{1}{\hbar} [H', c_{k\uparrow}(\tau)]$$

$$[\bar{H}_0, c_{k\uparrow}] = -\bar{\epsilon}_k c_{k\uparrow}$$

$$[H', c_{k\uparrow}] = -\sum_{k'} \Delta^*_{k'} [c_{-k'\downarrow} c_{k'\uparrow}, c_{k\uparrow}] - \sum_{k'} \Delta_{k'} [c^+_{k'\uparrow} c^+_{-k'\downarrow}, c_{k\uparrow}]$$

$$+ \sum_{k'} \Delta_{k'} \langle c^+_{k'\uparrow} c^+_{-k'\downarrow} \rangle [1, c_{k\uparrow}] = 0 - \sum_{k'} \Delta_{k'} [c^+_{k'\uparrow} c^+_{-k'\downarrow}, c_{k\uparrow}] + 0$$

$$= + \sum_{k'} \Delta_{k'} \{ c^+_{k'\uparrow}, c_{k\uparrow} \} c^+_{-k'\downarrow} = \sum_{k'} \Delta_{k'} \delta_{k'k} c^+_{-k'\downarrow} = \Delta_k c^+_{-k\downarrow}$$

Thus

$$\frac{\partial}{\partial\tau} g(k\uparrow, \tau) = -\delta(\tau) - (\Delta_k/\hbar) \langle T c^+_{-k\downarrow}(\tau) c^+_{k\uparrow}(0) \rangle = -\delta(\tau) + (\Delta_k/\hbar) F^+(k, \tau)$$

As for $F^+(k,\tau)$,

$$\frac{\partial}{\partial\tau} F^+(k,\tau) = -\langle T \tfrac{\partial}{\partial\tau} c^+_{-k\downarrow}(\tau) c^+_{k\uparrow}(0) \rangle$$

$$\frac{\partial}{\partial\tau} c^+_{-k\downarrow}(\tau) = (1/\hbar) [\bar{H}_0, c^+_{-k\downarrow}] + (1/\hbar) [H', c^+_{-k\downarrow}]$$

$$[\bar{H}_0, c^+_{-k\downarrow}] = \bar{\epsilon}_k c^+_{-k\downarrow}$$

$$[H', c^+_{-k\downarrow}] = -\sum_{k'} \Delta^*_{k'} [c_{-k'\downarrow} c_{k'\uparrow}, c^+_{-k\downarrow}] = \sum_{k'} \Delta^*_{k'} \{ c_{-k'\downarrow}, c^+_{-k\downarrow} \} c_{k'\uparrow}$$

$$= \sum_{k'} \Delta^*_{k'} \delta_{k'k} c_{k'\uparrow} = \Delta^*_k c_{k\uparrow}$$

Therefore,

$$\frac{\partial}{\partial\tau} F^+(k,\tau) = -(\bar{\epsilon}_k/\hbar) \langle T c^+_{-k\downarrow}(\tau) c^+_{k\uparrow}(0) \rangle - (\Delta^*_k/\hbar) \langle T c_{k\uparrow}(\tau) c^+_{k\uparrow}(0) \rangle$$

$$= (\bar{\epsilon}_k/\hbar) F^+(k,\tau) + (\Delta^*_k/\hbar) g(k\uparrow, \tau)$$

$$\Rightarrow (\partial/\partial\tau - \bar{\epsilon}_k/\hbar) F^+(k,\tau) = (\Delta^*_k/\hbar) g(k\uparrow, \tau)$$

6. Perturbation due to an electromagnetic field

$$T = \frac{1}{2m} \sum_\sigma \int \psi_\sigma^+(\vec{r}) (-i\hbar\vec{\nabla} + e\vec{A}/c)^2 \psi_\sigma(\vec{r}) d^3r$$

$$\frac{1}{2m}(-i\hbar\vec{\nabla} + e\vec{A}/c)^2 = -\frac{\hbar^2\nabla^2}{2m} + \frac{e^2}{2mc^2}A^2 - \frac{ie\hbar}{2mc}(\vec{\nabla}\cdot\vec{A} + \vec{A}\cdot\vec{\nabla})$$

Thus

$$T = \frac{1}{2m} \sum_\sigma \int \psi_\sigma^+(\vec{r}) \left(-\frac{\hbar^2}{2m}\nabla^2\right) \psi_\sigma(\vec{r}) d^3r + \frac{e^2}{2mc^2} \sum_\sigma \int A^2(\vec{r},t) \psi_\sigma^+(\vec{r}) \psi_\sigma(\vec{r}) d^3r$$

$$- \frac{ie\hbar}{2mc} \sum_\sigma \int \psi_\sigma^+(\vec{r}) [\vec{\nabla}\cdot\vec{A} + \vec{A}\cdot\vec{\nabla}] \psi_\sigma(\vec{r}) d^3r$$

$$= T_{A=0} + \frac{e^2}{2mc^2} \int A^2(\vec{r},t) n(\vec{r}) d^3r + T'$$

$$T' = \frac{-ie\hbar}{2mc} \sum_\sigma \int \psi_\sigma^+(\vec{r}) [\vec{\nabla}\cdot\vec{A} + \vec{A}\cdot\vec{\nabla}] \psi_\sigma(\vec{r}) d^3r$$

$$= \frac{-ie\hbar}{2mc} \sum_\sigma \left[\int \psi_\sigma^+(\vec{r}) \vec{\nabla}\cdot\vec{A} \psi_\sigma(\vec{r}) d^3r + \int \psi_\sigma^+(\vec{r}) \vec{A}\cdot\vec{\nabla} \psi_\sigma(\vec{r}) d^3r \right]$$

Integrating by parts the first term,

$$T' = -\frac{ie\hbar}{2mc} \sum_\sigma \left[-\int (\vec{\nabla}\psi_\sigma^+(\vec{r}))\cdot\vec{A} \psi_\sigma(\vec{r}) d^3r + \int \psi_\sigma^+(\vec{r}) \vec{A}\cdot\vec{\nabla} \psi_\sigma(\vec{r}) d^3r \right]$$

$$= -\frac{ie\hbar}{2mc} \sum_\sigma \left\{ \int [\psi_\sigma^+(\vec{r}) \vec{\nabla}\psi_\sigma(\vec{r}) - (\vec{\nabla}\psi_\sigma^+(\vec{r})) \psi_\sigma(\vec{r})] \cdot \vec{A}(\vec{r},t) d^3r \right.$$

$$= -\frac{1}{c} \int \vec{J}^P(\vec{r}) \cdot \vec{A}(\vec{r},t) d^3r$$

7. $D_{\alpha\beta}(q,0)$

In Eq. (12.24) set $\omega_m = 0$ [Eq. (124) should have no sum over n]

$$D_{\alpha\beta}(q,0) = \frac{\hbar^2 e^2}{4m^2 V} \sum_k (2k_\alpha + q_\alpha)(2k_\beta + q_\beta)\, I$$

$$I = \int_{-\infty}^{\infty} \frac{d\epsilon_1}{\pi} \int_{-\infty}^{\infty} \frac{d\epsilon_2}{\pi} \frac{f_{\epsilon_1} - f_{\epsilon_2}}{\epsilon_1 - \epsilon_2} \mathrm{Tr}\left[\mathrm{Im}\,\tilde{G}^R(k,\epsilon_1)\,\mathrm{Im}\,\tilde{G}^R(k+q,\epsilon_2)\right)$$

$$\mathrm{Tr}\left[\mathrm{Im}\,\tilde{G}^R(k,\epsilon_1)\,\mathrm{Im}\,\tilde{G}^R(k+q,\epsilon_2)\right) = \pi^2\hbar^2\left[\delta(\epsilon_1 - E_k/\hbar) - \delta(\epsilon_1 + E_k/\hbar)\right]$$

$$\times\left[\delta(\epsilon_2 - E_{k+q}/\hbar) - \delta(\epsilon_2 + E_{k+q}/\hbar)\right) \frac{\epsilon_1\epsilon_2 + \bar{\epsilon}_k\bar{\epsilon}_{k+q}/\hbar^2 + \Delta^2/\hbar^2}{2E_k E_{k+q}}$$

Let $$J(\epsilon_1,\epsilon_2) = \frac{f_{\epsilon_1} - f_{\epsilon_2}}{\epsilon_1 - \epsilon_2}\,\frac{\epsilon_1\epsilon_2 + \bar{\epsilon}_k\bar{\epsilon}_{k+q}/\hbar^2 + \Delta^2/\hbar^2}{2E_k E_{k+q}}$$

Then

$$I = \hbar^2\left[J(E_k/\hbar, E_{k+q}/\hbar) + J(-E_k/\hbar, -E_{k+q}/\hbar) - J(E_k/\hbar, -E_{k+q}/\hbar)\right.$$
$$\left. - J(-E_k/\hbar, E_{k+q}/\hbar)\right)$$

$$J(E_k/\hbar, E_{k+q}/\hbar) = \frac{f_{E_k} - f_{E_{k+q}}}{(E_k - E_{k+q})/\hbar}\,\frac{E_kE_{k+q} + \bar{\epsilon}_k\bar{\epsilon}_{k+q} + \Delta^2}{2\hbar^2 E_k E_{k+q}}$$

$$J(-E_k/\hbar, -E_{k+q}/\hbar) = \frac{f_{-E_k} - f_{-E_{k+q}}}{-(E_k - E_{k+q})/\hbar}\,\frac{E_kE_{k+q} + \bar{\epsilon}_k\bar{\epsilon}_{k+q} + \Delta^2}{2\hbar^2 E_k E_{k+q}}$$

Since $f_{-E_k} = 1 - f_k$, it follows that

$$\frac{f_{-E_k} - f_{-E_{k+q}}}{-(E_k - E_{k+q})/\hbar} = \frac{1 - f_{E_k} - 1 + f_{E_{k+q}}}{-(E_k - E_{k+q})/\hbar} = \frac{f_{E_k} - f_{E_{k+q}}}{(E_k - E_{k+q})/\hbar}$$

$$\Rightarrow J(-E_k/\hbar, -E_{k+q}/\hbar) = J(E_k/\hbar, E_{k+q}/\hbar)$$

Next,

$$J(E_k/\hbar, -E_{k+q}/\hbar) = \frac{f_{E_k} - f_{-E_{k+q}}}{(E_k + E_{k+q})/\hbar}\cdot\frac{-E_kE_{k+q} + \bar{\epsilon}_k\bar{\epsilon}_{k+q} + \Delta^2}{2\hbar^2 E_k E_{k+q}}$$

$$= \frac{f_{E_k} + f_{E_{k+q}} - 1}{(E_k + E_{k+q})/\hbar}\cdot\frac{-E_kE_{k+q} + \bar{\epsilon}_k\bar{\epsilon}_{k+q} + \Delta^2}{2\hbar^2 E_k E_{k+q}}$$

and

$$J(-E_k/\hbar, E_{k+q}/\hbar) = \frac{f_{-E_k} - f_{E_{k+q}}}{-(E_k + E_{k+q})/\hbar} \; \frac{-E_k E_{k+q} + \bar{\epsilon}_k \bar{\epsilon}_{k+q} + \Delta^2}{2\hbar^2 E_k E_{k+q}}$$

since

$$f_{-E_k} - f_{E_{k+q}} = -(f_{E_k} + f_{E_{k+q}} - 1),$$

we obtain

$$J(-E_k/\hbar, E_{k+q}/\hbar) = J(E_k/\hbar, -E_{k+q}/\hbar)$$

Putting all these term into I, the expression for $D_{\alpha\beta}(q,0)$, as given in Eq. (12.27), is readily obtained.

8. Pair fluctuations in the ground state

$$\chi = \frac{1}{V}\sum_k c_{-k\downarrow}c_{k\uparrow}$$

$$\langle\chi\rangle = \langle\Psi_0|\chi|\Psi_0\rangle = \frac{1}{V}\sum_k \langle 0|\prod_p (u_p + v_p c_{-p\downarrow}c_{p\uparrow})\, c_{-k\downarrow}c_{k\uparrow}\prod_q (u_q + v_q c^+_{q\uparrow}c^+_{-q\downarrow})|0\rangle$$

$$= \frac{1}{V}\langle 0|ABD|0\rangle$$

where

$$A = \prod_{p\neq k}(u_p + v_p c_{-p\downarrow}c_{p\uparrow}), \quad B = \prod_{q\neq k}(u_q + v_q c^+_{q\uparrow}c^+_{-q\downarrow})$$

$$D = (u_k + v_k c_{-k\downarrow}c_{k\uparrow})\, c^+_{-k\downarrow}c_{k\uparrow}\,(u_k + v_k c^+_{k\uparrow}c^+_{-k\downarrow})$$

Using

$$c_{k\uparrow}|0\rangle = 0,$$

$$c_{-k\downarrow}c_{k\uparrow}c^+_{k\uparrow}c^+_{-k\downarrow}|0\rangle = c_{-k\downarrow}(1 - c^+_{k\uparrow}c_{k\uparrow})c^+_{-k\downarrow}|0\rangle$$

$$= c_{-k\downarrow}c^+_{-k\downarrow}|0\rangle + c_{-k\downarrow}c^+_{k\uparrow}c^+_{-k\downarrow}c_{k\uparrow}|0\rangle$$

$$= (1 - c^+_{-k\downarrow}c_{-k\downarrow})|0\rangle + 0 = |0\rangle,$$

~~we~~ find

$$\langle\chi\rangle = \frac{1}{V}\sum_k u_k v_k \langle 0|AB|0\rangle = \frac{1}{V}\sum_k u_k v_k \prod_{p\neq k}(u_p^2 + v_p^2)$$

$$= \frac{1}{V}\sum_k u_k v_k$$

This has the same value as $(1/V)\sum_k \langle 0|D|0\rangle$ (as if operators A and B are replaced by 1). With this in mind, we can write.

$$\langle\chi^2\rangle = \langle\Psi_0|\chi^2|\Psi_0\rangle = \frac{1}{V^2}\sum_{kk'}\langle\Psi_0|c_{-k'\downarrow}c_{k'\uparrow}c_{-k\downarrow}c_{k\uparrow}|0\rangle$$

$$= \frac{1}{V^2}\sum_{kk'}\langle 0|(u_{k'} + v_{k'}c_{-k'\downarrow}c_{k'\uparrow})(u_k + v_k c_{-k\downarrow}c_{k\uparrow})\,c_{-k'\downarrow}c_{k'\uparrow}c_{-k\downarrow}c_{k\uparrow}$$

$$\times\,(u_{k'} + v_{k'}c^+_{k'\uparrow}c^+_{-k'\downarrow})(u_k + v_k c^+_{k\uparrow}c^+_{-k\downarrow})|0\rangle$$

Clearly, the only terms that survive are those having equal number of annihilation and creation operators,

$$\langle \chi^2 \rangle = \frac{1}{V^2}\sum_{kk'} u_{k'}u_k v_{k'}v_k \langle 0| c_{-k'\downarrow} c_{k'\uparrow} c_{-k\downarrow} c_{k\uparrow} c^+_{k'\uparrow} c^+_{-k'\downarrow} c^+_{k\uparrow} c^+_{-k\downarrow}|0\rangle$$

If $k = k'$, then

$$c^+_{-k'\downarrow} c_{k\uparrow} c^+_{-k\downarrow} = c^+_{-k\downarrow} c^+_{k\uparrow} c^+_{-k\downarrow} = -c^+_{k\uparrow} c^+_{-k\downarrow} c^+_{-k\downarrow} = 0$$

since $c^+_{-k\downarrow} c^+_{k\uparrow} = -c^+_{k\uparrow} c^+_{-k\downarrow}$ and $(c^+_{-k\downarrow})^2 = 0$.

Hence, only terms with $k \neq k'$ survive. When $k \neq k'$, then using the anticommutation property of the c-operators, we can rearrange the operators and write

$$\langle \chi^2 \rangle = \frac{1}{V^2}\sum_{\substack{k,k' \\ k\neq k'}} u_k v_k u_{k'} v_{k'} \langle 0| c_{k'\uparrow} c^+_{k'\uparrow} c_{-k'\downarrow} c^+_{-k'\downarrow} c_{k\uparrow} c^+_{k\uparrow} c_{-k\downarrow} c^+_{-k\downarrow}|0\rangle$$

Noting that $c_{p\sigma} c^+_{p\sigma}|0\rangle = (1 - c^+_{p\sigma} c_{p\sigma})|0\rangle = |0\rangle$, we obtain

$$\langle \chi^2 \rangle = \frac{1}{V^2}\sum_{\substack{k,k' \\ k\neq k'}} u_k v_k u_{k'} v_{k'} = \frac{1}{V^2}\sum_{k,k'} u_{k'}v_{k'}u_k v_k - \frac{1}{V^2}\sum_k u_k^2 v_k^2$$

$$= \langle \chi \rangle^2 - \frac{1}{V^2}\sum_k u_k^2 v_k^2 \Rightarrow \langle \chi^2 \rangle - \langle \chi \rangle^2 = -\frac{1}{V^2}\sum_k u_k^2 v_k^2$$

From Eq. (12.44),

$$u_k^2 = \frac{1}{2}\left[1 + \frac{\bar{\epsilon}_k}{\sqrt{\bar{\epsilon}_k^2 + \Delta_k^2}}\right], \quad v_k^2 = \frac{1}{2}\left[1 - \frac{\bar{\epsilon}_k}{\sqrt{\bar{\epsilon}_k^2 + \Delta_k^2}}\right]$$

$$\Rightarrow u_k^2 v_k^2 = \frac{1}{4}\left[1 - \frac{\bar{\epsilon}_k^2}{\bar{\epsilon}_k^2 + \Delta_k^2}\right] = \frac{1}{4}\cdot\frac{\bar{\epsilon}_k^2}{\bar{\epsilon}_k^2 + \Delta_k^2}$$

In the BCS model, Δ_k is nonzero for $-\hbar\omega_D < \bar{\epsilon}_k < \hbar\omega_D$. Taking Δ_k as a constant Δ, we obtain

$$\langle \chi^2 \rangle - \langle \chi \rangle^2 = -\frac{1}{4V^2}\sum_k \frac{\Delta^2}{\bar{\epsilon}_k^2 + \Delta^2} = -\frac{1}{4V^2} D(\epsilon_F)\int_{-\hbar\omega_D}^{\hbar\omega_D} \frac{\Delta^2}{\Delta^2 + \epsilon^2}\, d\epsilon$$

The integral is independent of V, while the density of states at the Fermi energy $D(\epsilon_F)$ is proportional to V. Hence, as $V \to \infty$, $\langle \chi^2 \rangle - \langle \chi \rangle^2 \to 0$.

9.

H is time-independent, so we may set $\tau' = 0$.

$$g(\vec{r}\uparrow\tau, \vec{r}'\uparrow 0) = -\langle T\psi_\uparrow(\vec{r}\tau)\psi_\uparrow^+(\vec{r}'0)\rangle$$

$$= -\theta(\tau)\langle\psi_\uparrow(\vec{r}\tau)\psi_\uparrow^+(\vec{r}'0)\rangle + \theta(-\tau)\langle\psi_\uparrow^+(\vec{r}'0)\psi_\uparrow(\vec{r}\tau)\rangle$$

$$\frac{\partial}{\partial\tau}g(\vec{r}\uparrow\tau, \vec{r}'\uparrow 0) = -\delta(\tau)\langle\psi_\uparrow(\vec{r})\psi_\uparrow^+(\vec{r}') - \delta(\tau)\langle\psi_\uparrow^+(\vec{r})\psi_\uparrow(\vec{r})\rangle$$

$$-\langle T\frac{\partial}{\partial\tau}\psi_\uparrow(\vec{r}\tau)\psi_\uparrow^+(\vec{r}'0)\rangle$$

The first two terms on the RHS give

$$-\delta(\tau)\langle\{\psi_\uparrow(\vec{r}), \psi_\uparrow^+(\vec{r}')\}\rangle = -\delta(\tau)\langle\delta(\vec{r}-\vec{r}')\rangle = -\delta(\tau)\delta(\vec{r}-\vec{r}')$$

$$\frac{\partial}{\partial\tau}\psi_\uparrow(\vec{r}\tau) = -\frac{1}{\hbar}[\psi_\uparrow(\vec{r}\tau), \bar{H}]$$

$$= -\frac{1}{\hbar}[\psi_\uparrow(\vec{r}\tau), \bar{H}_0] - \frac{1}{\hbar}[\psi_\uparrow(\vec{r}\tau), H']$$

$$[\psi_\uparrow(\vec{r}\tau), \bar{H}_0] = [\psi_\uparrow(\vec{r}\tau), \sum_\sigma\int d^3r'\,\psi_\sigma^+(\vec{r}'\tau)\left(\frac{1}{2m}\left(-i\hbar\nabla' + \frac{e\vec{A}(\vec{r}')}{c}\right)^2\right.$$

$$\left.-\mu\right)\psi_\sigma(\vec{r}'\tau)]$$

Using $[A, BC] = \{A, B\}C - B\{A, C\}$

and

$$\{\psi_\uparrow(\vec{r}\tau), \psi_\sigma^+(\vec{r}'\tau)\} = \delta_{\sigma\uparrow}\delta(\vec{r}-\vec{r}')$$

$$\{\psi_\uparrow(\vec{r},\tau), \psi_\sigma(\vec{r}'\tau)\} = 0$$

we obtain

$$[\psi_\uparrow(\vec{r}\tau), \bar{H}_0] = \left\{\frac{1}{2m}\left[-i\hbar\vec{\nabla} + \frac{e\vec{A}(\vec{r})}{c}\right]^2 - \mu\right\}\psi_\uparrow(\vec{r}\tau)$$

Next,

$$[\psi_\uparrow(\vec r\tau), H'] = [\psi_\uparrow(\vec r\tau), -W_0\int d^3r'\,\psi_\uparrow^+(\vec r'\tau)\psi_\downarrow^+(\vec r'\tau)\psi_\downarrow(\vec r'\tau)\psi_\uparrow(\vec r'\tau)]$$

Dropping the τ argument for now,

$$[\psi_\uparrow(\vec r), H'] = -W_0\int d^3r'\,[\psi_\uparrow(\vec r), \psi_\uparrow^+(\vec r')\psi_\downarrow^+(\vec r')\psi_\downarrow(\vec r')\psi_\uparrow(\vec r')]$$

$$= -U_0\int d^3r'\,\{\psi_\uparrow(\vec r), \psi_\uparrow^+(\vec r')\}\psi_\downarrow^+(\vec r')\psi_\downarrow(\vec r')\psi_\uparrow(\vec r')\}$$

Note that in evaluating the commutator, which is of the form

$$[A, BCDE] = [A, BC]DE + BC[A, DE]$$

the commutator $[A, DE] = [\psi_\uparrow(\vec r), \psi_\downarrow(\vec r')\psi_\uparrow(\vec r')]$ vanishes

by the formula $[A, DE] = \{A, D\}E - D\{A, E\}$

As for $[A, BC]$, it is equal to $\{A, B\}C - B\{A, C\}$

and $\{A, C\} = \{\psi_\uparrow(\vec r), \psi_\downarrow^+(\vec r')\} = 0$

Thus

$$[\psi_\uparrow(\vec r\tau), H'] = -W_0\,\psi_\downarrow^+(\vec r\tau)\psi_\downarrow(\vec r\tau)\psi_\uparrow(\vec r\tau)$$

and

$$\frac{\partial}{\partial\tau}\psi_\uparrow(\vec r\tau) = \frac{1}{\hbar}\left\{\frac{\hbar^2}{2m}\left[\vec\nabla + \frac{ie}{\hbar c}A(\vec r)\right]^2 + \mu\right\}\psi_\uparrow(\vec r\tau)$$

$$+ \frac{W_0}{\hbar}\psi_\downarrow^+(\vec r\tau)\psi_\downarrow(\vec r\tau)\psi_\uparrow(\vec r\tau)$$

Therefore

$$\frac{\partial}{\partial\tau} g(\vec r\uparrow\tau, \vec r'\uparrow 0) = -\delta(\tau)\delta(\vec r - \vec r')$$

$$-\frac{1}{\hbar}\left\{\frac{\hbar^2}{2m}\left[\vec\nabla + \frac{ie}{\hbar c}\vec A(\vec r)\right]^2 + \mu\right\}\langle T\psi_\uparrow(\vec r\tau)\psi_\uparrow^+(\vec r'0)\rangle$$

$$-\frac{W_0}{\hbar}\langle T\psi_\downarrow^+(\vec r\tau)\psi_\downarrow(\vec r\tau)\psi_\uparrow(\vec r\tau)\psi_\uparrow^+(\vec r'0)\rangle$$

The last term on the RHS is factored as follows

$$\langle T\psi_\downarrow^+(\vec r\tau)\psi_\downarrow(\vec r\tau)\psi_\uparrow(\vec r\tau)\psi_\uparrow^+(\vec r'0)\rangle =$$

$$= -\langle T\psi_\uparrow(\vec r\tau)\psi_\downarrow(\vec r\tau)\rangle\langle T\psi_\downarrow^+(\vec r\tau)\psi_\uparrow^+(\vec r'0)\rangle$$

$$= -F(\vec r\tau,\vec r\tau)F^+(\vec r\tau,\vec r'0)$$

We thus find

$$\hbar\frac{\partial}{\partial\tau}g(\vec r\uparrow\tau,\vec r'\uparrow0) = -\hbar\delta(\tau)\delta(\vec r-\vec r')$$
$$+\left\{\frac{\hbar^2}{2m}\left[\vec\nabla+\frac{ie}{\hbar c}\vec A(\vec r)\right]^2+\mu\right\}g(\vec r\uparrow\tau,\vec r'\uparrow0)+\Delta(\vec r)F^+(\vec r\tau,\vec r'0)$$

Writing

$$g(\vec r\uparrow\tau,\vec r'\uparrow0) = \frac{1}{\beta\hbar}\sum_{n=-\infty}^{\infty}e^{-i\omega_n\tau}g_\uparrow(\vec r,\vec r',\omega_n),$$

$$\delta(\tau) = \frac{1}{\beta\hbar}\sum_{n=-\infty}^{\infty}e^{-i\omega_n\tau},$$

and similarly for $F^+(\vec r\tau,\vec r'0)$, the required equation is obtained.

As for $F^+(\vec r\tau,\vec r'0) = -\langle T\psi_\downarrow^+(\vec r\tau)\psi_\uparrow^+(\vec r'0)\rangle$, we have

$$\frac{\partial F^+}{\partial\tau} = -\langle T\frac{\partial}{\partial\tau}\psi_\downarrow^+(\vec r\tau)\psi_\uparrow^+(\vec r'0)\rangle$$

The derivative of $\psi_\downarrow^+(\vec r\tau)$ is found by calculating the commutator of $\psi_\downarrow^+$ and H. This calculation is very much similar to the one above, and we will not go through it.

So the final results are

$$\left\{i\hbar\omega_n + \frac{\hbar^2}{2m}\left[\vec{\nabla} + \frac{ie}{\hbar c}\vec{A}(\vec{r})\right]^2 + \mu\right\} g(\vec{r},\vec{r}',\omega_n) + \Delta(\vec{r}) F^{\dagger}(\vec{r},\vec{r}',\omega_n) = \hbar\delta(\vec{r}-\vec{r}')$$

$$\left\{-i\hbar\omega_n + \frac{\hbar^2}{2m}\left[\vec{\nabla} - \frac{ie}{\hbar c}\vec{A}(\vec{r})\right]^2 + \mu\right\} F^{\dagger}(\vec{r},\vec{r}',\omega_n) - \Delta^{*}(\vec{r})\, g(\vec{r},\vec{r}',\omega_n) = 0$$

b) Let us define the operators B and C as

$$B = i\hbar\omega_n + \frac{\hbar^2}{2m}\left[\vec{\nabla} + \frac{ie}{\hbar c}\vec{A}(\vec{r})\right]^2 + \mu$$

$$C = -i\hbar\omega_n + \frac{\hbar^2}{2m}\left[\vec{\nabla} - \frac{ie}{\hbar c}\vec{A}(\vec{r})\right]^2 + \mu$$

Then

$$B g(\vec{r},\vec{r}',\omega_n) = \hbar\delta(\vec{r}-\vec{r}') - \Delta(\vec{r}) F^{\dagger}(\vec{r},\vec{r}',\omega_n)$$

$$C F^{\dagger}(\vec{r},\vec{r}',\omega_n) - \Delta^{*}(\vec{r})\, g(\vec{r},\vec{r}',\omega_n) = 0$$

$\tilde{g}^{\circ}(\vec{r},\vec{r}',\omega_n)$ is Green's function for the normal metal in the presence of the vector potential $\vec{A}(\vec{r})$; hence

$$B\,\tilde{g}^{\circ}(\vec{r},\vec{r}',\omega_n) = \hbar\delta(\vec{r}-\vec{r}')$$

To see that

$$g(\vec{r},\vec{r}',\omega_n) = \tilde{g}^{\circ}(\vec{r},\vec{r}',\omega_n) - \frac{1}{\hbar}\int d^3l\, \tilde{g}^{\circ}(\vec{r},l,\omega_n)\Delta(l) F^{\dagger}(l,\vec{r}',\omega_n)$$

let us apply B to the RHS

$$B\left[\tilde{g}^{\circ}(\vec{r},\vec{r}',\omega_n) - \frac{1}{\hbar}\int d^3l\, \tilde{g}^{\circ}(\vec{r},\vec{l},\omega_n)\Delta(\vec{l}) F^{\dagger}(\vec{l},\vec{r}',\omega_n)\right]$$

$$= \hbar\delta(\vec{r}-\vec{r}') - \frac{1}{\hbar}\int d^3l\, \hbar\delta(\vec{r}-\vec{l})\Delta(\vec{l}) F^{\dagger}(\vec{l},\vec{r}',\omega_n)$$

$$= \hbar\delta(\vec{r}-\vec{r}') - \Delta(\vec{r}) F^{\dagger}(\vec{r},\vec{r}',\omega_n)$$

$\Rightarrow$ $\tilde{g}^{\circ}(\vec{r},\vec{r}',\omega_n) - \frac{1}{\hbar}\int d^3l\, \tilde{g}^{\circ}(\vec{r},\vec{l},\omega_n)\Delta(\vec{l}) F^{\dagger}(\vec{l},\vec{r}',\omega_n)$ satisfies the same equation as $g(\vec{r},\vec{r}',\omega_n)$. In the normal state, $\Delta = 0$ and g reduces to $\tilde{g}^{o}$.

Now we show that if we set

$$F^{+}(\vec{r},\vec{r}',\omega_n) = \frac{1}{\hbar}\int d^3 l \; \tilde{g}^{o}(\vec{l},\vec{r},-\omega_n)\, g(\vec{l},\vec{r}',\omega_n)\, \Delta^{*}(\vec{l}),$$

then the equation

$$C F^{+}(\vec{r},\vec{r}',\omega_n) = \Delta^{*}(\vec{r})\, g(\vec{r},\vec{r}',\omega_n)$$

will be satisfied.

Starting with

$$g_{\sigma}(\vec{r}\tau,\vec{r}'0) = -\langle T \psi_{\sigma}(\vec{r}\tau)\psi_{\sigma}^{+}(\vec{r}'0)\rangle$$

$$= -\theta(\tau)\langle \psi_{\sigma}(\vec{r}\tau)\psi_{\sigma}^{+}(\vec{r}'0)\rangle + \theta(-\tau)\langle \psi_{\sigma}^{+}(\vec{r}'0)\psi_{\sigma}(\vec{r}\tau)\rangle$$

we write

$$\psi_{\sigma}(\vec{r}\tau) = e^{\bar{H}\tau/\hbar}\,\psi_{\sigma}(\vec{r}0)\,e^{-\bar{H}\tau/\hbar}$$

$$\Rightarrow [\psi_{\sigma}(\vec{r}\tau)]^{\dagger} = e^{-\bar{H}\tau/\hbar}\,\psi_{\sigma}^{+}(\vec{r}0)\,e^{\bar{H}\tau/\hbar} = \psi_{\sigma}^{+}(\vec{r},-\tau)$$

[Recall that in the imaginary-time formalism, $\psi_{\sigma}^{+}(\vec{r}\tau)$ is not the hermitian conjugate of $\psi_{\sigma}(\vec{r}\tau)$]

Hence

$$g^{*}(\vec{r}\tau,\vec{r}'0) = -\theta(\tau)\langle \psi_{\sigma}(\vec{r}'0)\,\psi_{\sigma}^{+}(\vec{r},-\tau)\rangle + \theta(-\tau)\langle \psi_{\sigma}^{+}(\vec{r},-\tau)\psi_{\sigma}(\vec{r}'0)\rangle$$

$$= -\langle T\psi_{\sigma}(\vec{r}'0)\,\psi_{\sigma}^{+}(\vec{r},-\tau)\rangle$$

$$= -\langle T\psi_{\sigma}(\vec{r}'\tau)\,\psi_{\sigma}^{+}(\vec{r}0)\rangle$$

In the last step we used the time translational invariance property.

Therefore,

$$g^*(\vec{r}\tau, \vec{r}'0) = g(\vec{r}'\tau, \vec{r}0)$$

We have

$$g(\vec{r}\tau, \vec{r}'0) = \frac{1}{\beta\hbar}\sum_n g(\vec{r}, \vec{r}', \omega_n)\, e^{-i\omega_n\tau}$$

$$\Rightarrow g^*(\vec{r}\tau, \vec{r}'0) = \frac{1}{\beta\hbar}\sum_n g^*(\vec{r}, \vec{r}', \omega_n)\, e^{i\omega_n\tau}$$

$$= g(\vec{r}'\tau, \vec{r}0) = \frac{1}{\beta\hbar}\sum_n g(\vec{r}', \vec{r}, \omega_n)\, e^{-i\omega_n\tau}$$

$$= \frac{1}{\beta\hbar}\sum_n g(\vec{r}', \vec{r}, -\omega_n)\, e^{i\omega_n\tau}$$

Hence,

$$g^*(\vec{r}, \vec{r}', \omega_n) = g(\vec{r}', \vec{r}, -\omega_n)$$

The equation for $\tilde{g}^{\circ}(\vec{r}, \vec{r}', \omega_n)$ is

$$B\tilde{g}^{\circ}(\vec{r}, \vec{r}', \omega_n) = \hbar\,\delta(\vec{r}-\vec{r}')$$

$$\Rightarrow B^*\,\tilde{g}^{\circ *}(\vec{r}, \vec{r}', \omega_n) = \hbar\,\delta(\vec{r}-\vec{r}')$$

Noting that

$$B^* = C, \quad \text{and} \quad \tilde{g}^{\circ *}(\vec{r}, \vec{r}', \omega_n) = \tilde{g}^{\circ}(\vec{r}', \vec{r}, -\omega_n),$$

we find

$$C\tilde{g}^{\circ}(\vec{r}', \vec{r}, -\omega_n) = \hbar\,\delta(\vec{r}-\vec{r}')$$

Thus

$$C\,\frac{1}{\hbar}\int d^3l\; \tilde{g}^{\circ}(\vec{l}, \vec{r}, -\omega_n)\, g(l, \vec{r}', \omega_n)\, \Delta^*(\vec{l})$$

$$= \int d^3l\; \delta(\vec{r}-\vec{l})\, g(\vec{l}, \vec{r}', \omega_n)\, \Delta^*(\vec{l})$$

$$= g(\vec{r}, \vec{r}', \omega_n)\, \Delta^*(\vec{r}),$$

which indicates that $\frac{1}{\hbar}\int d^3l\; \tilde{g}^{\circ}(\vec{l}, \vec{r}, -\omega_n)\, g(\vec{l}, \vec{r}', \omega_n)\, \Delta^*(\vec{l})$ does indeed satisfy the same equation as $F^{+}(\vec{r}, \vec{r}', \omega_n)$.

Of course, we could write

$$F^+(\vec{r},\vec{r}',\omega_n) = \frac{1}{\hbar}\int d^3l\, \tilde{g}^0(\vec{l},\vec{r},-\omega_n)\, g(\vec{l},\vec{r}',\omega_n)\, \Delta^*(\vec{l}) + R(\vec{r},\vec{r}',\omega_n)$$

where R is a function satisfying the equation

$$C\, R(\vec{r},\vec{r}',\omega_n) = 0$$

However, $F^+ = 0$ when $\Delta^* = 0$, so we set $R = 0$.

c)

$$\Delta^* = \frac{V_0}{\beta\hbar} \sum_n F^+(\vec{r},\vec{r},\omega_n)$$

$$= \frac{V_0}{\beta\hbar} \sum_n \int d^3l\, \tilde{g}^0(\vec{l},\vec{r},-\omega_n)\, g(\vec{l},\vec{r},\omega_n)\, \Delta^*(\vec{l})$$

As the magnetic field approaches the critical field, $\Delta \to 0$ and $g \to \tilde{g}^0$; thus

$$\Delta^* = \frac{V_0}{\beta\hbar} \sum_n \int d^3l\, \tilde{g}^0(\vec{l},\vec{r},-\omega_n)\, \tilde{g}^0(\vec{l},\vec{r},\omega_n)\, \Delta^*(\vec{l})$$

$\tilde{g}^0(\vec{r},\vec{r}',\omega_n)$ satisfies the equation for $g(\vec{r},\vec{r}',\omega_n)$ with $\Delta = 0$,

$$\left\{ i\hbar\omega_n + \frac{\hbar^2}{2m}\left[\vec{\nabla} + \frac{ie}{\hbar c}\vec{A}(\vec{r})\right]^2 + \mu \right\} \tilde{g}^0(\vec{r},\vec{r}',\omega_n) = \hbar\,\delta(\vec{r}-\vec{r}')$$

In the absence of a magnetic field, $\tilde{g}^0 \to g^0$, so g^0 satisfies the equation

$$\left[i\hbar\omega_n + \frac{\hbar^2}{2m}\nabla^2 + \mu \right] g^0(\vec{r},\vec{r}',\omega_n) = \hbar\,\delta(\vec{r}-\vec{r}')$$

It follows that

$$\tilde{g}^0(\vec{r},\vec{r}',\omega_n) = g^0(\vec{r},\vec{r}',\omega_n)\, e^{\frac{ie}{\hbar c}\int_{\vec{r}}^{\vec{r}'} \vec{A}(\vec{s})\cdot d\vec{s}}$$

To show this, let $C(\vec{r},\vec{r}') = e^{(ie/\hbar c)\int_{\vec{r}}^{\vec{r}'} \vec{A}(\vec{s})\cdot d\vec{s}}$

Then,

$$\vec{\nabla}\tilde{g}^{\circ}(\vec{r},\vec{r}',\omega_n) = \vec{\nabla}[g^{\circ}C] = (\vec{\nabla}g^{\circ})C + g^{\circ}\vec{\nabla}C$$

$$= (\nabla g^{\circ})C - \frac{ie}{\hbar c}g^{\circ}C\vec{A}(\vec{r})$$

$$= (\nabla g^{\circ})C - \frac{ie}{\hbar c}\tilde{g}^{\circ}$$

Hence

$$(\vec{\nabla} + \frac{ie}{\hbar c}\vec{A})\tilde{g}^{\circ} = (\nabla g^{\circ})C$$

Next consider,

$$(\vec{\nabla} + \frac{ie}{\hbar c}\vec{A})^2\tilde{g}^{\circ} = (\vec{\nabla} + \frac{ie}{\hbar c}\vec{A})\cdot[(\nabla g^{\circ})C]$$

$$= (\nabla^2 g^{\circ})C + (\vec{\nabla}g^{\circ})\cdot(\vec{\nabla}C) + \frac{ie}{\hbar c}\vec{A}\cdot(\nabla g^{\circ})C$$

$$= (\nabla^2 g^{\circ})C$$

since $\vec{\nabla}C = -\frac{ie}{\hbar c}\vec{A}C$

Therefore $g^{\circ}(\vec{r},\vec{r}',\omega_n)\exp\left[\frac{ie}{\hbar c}\int_{\vec{r}}^{\vec{r}'}\vec{A}(s)\cdot d\vec{s}\right]$ does indeed satisfy the equation for $\tilde{g}^{\circ}(\vec{r},\vec{r}',\omega_n)$.

The required expression for Δ^* immediately follows.

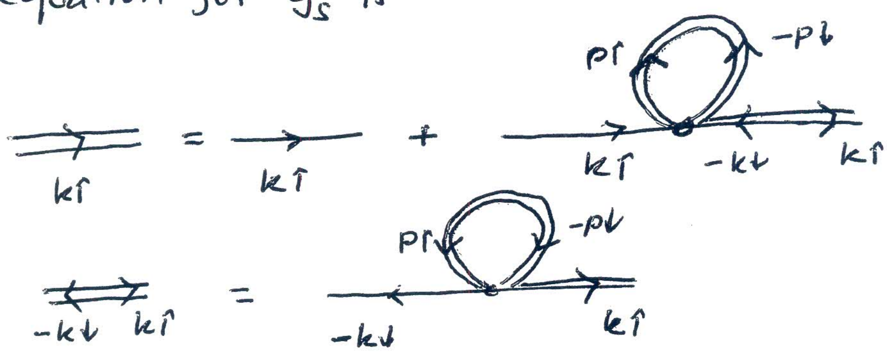
12.10

$$H = \sum_{k\sigma} \bar{\epsilon}_k c^+_{k\sigma} c_{k\sigma} + \sum_{p\sigma} \bar{\xi}_p b^+_{p\sigma} b_{p\sigma} - W_0 \sum_{kp} \left(b^+_{p\uparrow} b^+_{-p\downarrow} c_{-k\downarrow} c_{k\uparrow} + c^+_{k\uparrow} c^+_{-k\downarrow} b_{-p\downarrow} b_{p\uparrow} \right)$$

It is understood that k and p are vectors.

It is straightforward to set up the equations of motion for g_s and g_π and then obtain the required expressions by Fourier transforming.

Here we will get the result using diagrams. Dyson equation for g_s is



$$g_s(k\uparrow,\omega_n) = g_s^0(k\uparrow,\omega_n) - \frac{1}{\hbar} g_s^0(k\uparrow,\omega_n)\,\Delta_\pi\, F_s^+(k,\omega_n)$$

$$F_s^+(k,\omega_n) = \frac{1}{\hbar} g_s^0(-k\downarrow,-\omega_n)\,\Delta_\pi^*\, g_s(k\uparrow,\omega_n)$$

Thus

$$g_s(k\uparrow,\omega_n) = g_s^0(k\uparrow,\omega_n) - \frac{1}{\hbar^2} g_s^0(k\uparrow,\omega_n)\,|\Delta_\pi|^2\, g_s^0(-k\downarrow,-\omega_n)\, g_s(k\uparrow,\omega_n)$$

$$\Rightarrow g_s(k\uparrow,\omega_n) = \frac{g_s^0(k\uparrow,\omega_n)}{1 + g_s^0(k\uparrow,\omega_n)\, g_s^0(-k\downarrow,-\omega_n)\,|\Delta_\pi|^2/\hbar^2}$$

$$= \frac{1}{g_s^{0^{-1}}(k\uparrow,\omega_n) + g_s^0(-k\downarrow,-\omega_n)\,|\Delta_\pi|^2/\hbar^2}$$

$$= \frac{1}{i\omega_n - \bar{\epsilon}_k/\hbar + \frac{1}{-i\omega_n - \bar{\epsilon}_k/\hbar}\frac{|\Delta_\pi|^2}{\hbar^2}}$$

$$= \frac{-(i\omega_n + \bar{\epsilon}_k/\hbar)}{\omega_n^2 + \epsilon_k^2/\hbar^2 + |\Delta_\pi|^2/\hbar^2}$$

$$= \frac{-\hbar(i\hbar\omega_n + \bar{\epsilon}_k)}{(\hbar\omega_n)^2 + \epsilon_k^2 + |\Delta_\pi|^2}$$

Similar equation holds for g_π with $\Delta_\pi \to \Delta_s$.

b) $$\Delta_s^* = W_0 \sum_k F_s^+(k, \tau = 0^-) = \frac{U_0}{\beta\hbar} \sum_{kn} F_s^+(k, \omega_n) e^{i\omega_n 0^+}$$

$$F_s^+(k, \omega_n) = g_s^0(-k\downarrow, -\omega_n)\, \Delta_\pi^*\, g_s(k\uparrow, \omega_n)/\hbar$$

Thus

$$\Delta_s^* = \frac{W_0}{\beta\hbar} \sum_{kn} \frac{1}{-i\omega_n - \bar{\epsilon}_k/\hbar} \left(\frac{\Delta_\pi^*}{\hbar}\right) \frac{-\hbar(i\hbar\omega_n + \bar{\epsilon}_k)}{(\hbar\omega_n)^2 + \bar{\epsilon}_k^2 + |\Delta_\pi|^2}$$

$$= \frac{W_0}{\beta} \sum_{kn} \frac{\Delta_\pi^*}{(\hbar\omega_n)^2 + \bar{\epsilon}_k^2 + |\Delta_\pi|^2}$$

$$= W_0 k_B T \sum_{kn} \frac{\Delta_\pi^*}{(\hbar\omega_n)^2 + \bar{\epsilon}_k^2 + |\Delta_\pi|^2}$$

Similarly

$$\Delta_\pi^* = W_0 k_B T \sum_{pn} \frac{\Delta_s^*}{(\hbar\omega_n)^2 + \bar{\xi}_p^2 + |\Delta_s|^2}$$

c) From the above equations for Δ_s^* and Δ_π^*, we obtain

$$\Delta_s^* = (w_0 k_B T)^2 \sum_{kn} \frac{1}{\hbar^2\omega_n^2 + \bar{\epsilon}_k^2 + |\Delta_\pi|^2} \sum_{pm} \frac{\Delta_\pi^*}{\hbar^2\omega_m^2 + \bar{\xi}_p^2 + |\Delta_s|^2}$$

Now we follow the procedure leading from Eq. (12.90) to Eq. (12.94). At $T = T_c$, $\Delta_s = \Delta_\pi = 0$. We evaluate the sums over n and m and replace the sums over wave vectors with integrals. We get

$$\frac{1}{w_0^2 D_{\sigma s}(0) D_{\sigma\pi}(0)} = \left[\ln\left(\frac{2\hbar\omega_D}{\pi k_B T_c}\right) + \gamma\right]^2$$

$$\Rightarrow T_c \simeq 1.14\, \hbar\omega_D \exp\left[\frac{-1}{w_0\sqrt{D_{\sigma s}(0) D_{\sigma\pi}(0)}}\right]$$

d) This follows directly from the solution of the preceeding problem. Here

$$\Delta_s^* = \frac{v_0}{\beta\hbar} \sum_n F_s^+(\vec{r},\vec{r},\omega_n)$$

$$= \frac{w_0}{\beta\hbar^2} \int d^3\ell\, \tilde{g}^0(\vec{\ell},\vec{r},-\omega_n)\, g(\vec{\ell},\vec{r},\omega_n)\, \Delta_\pi^*(\vec{\ell})$$

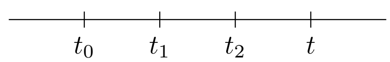
Proceeding exactly as in problem 12.9c, we obtain the desired result.

Chapter 13

Problem 1.

$$W(t,t_0) = 1 - \frac{i}{\hbar}\int_{t_0}^{t} dt_1 H(t_1) + (-\frac{i}{\hbar})^2 \int_0^t dt_1 \int_{t_0}^{t_1} dt_2 H(t_1)H(t_2) + \cdots$$

Here $t < t_0$. Let us consider the term with two integrals. The times are now arranged as in the following figure:



with time increasing from left to right.

$$A \equiv \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 H(t_1)H(t_2)$$

$$= \frac{1}{2}[\int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 H(t_1)H(t_2) + \int_{t_0}^{t} dt_2 \int_0^{t_1} dt_1 H(t_2)H(t_1)]$$

The second term on the RHS is equal to the first term; it is obtained from the first term by relabelling the indices. In the first term on the RHS, $t_2 > t_1$, and so we can introduce $\theta(t_2 - t_1)$ and extend the limits of integration over t_2 from t_0 to t. For the second term on the RHS, we can introduce $\theta(t_1 - t_2)$:

$$A = \frac{1}{2}\int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 [\theta(t_2 - t_1)H(t_1)H(t_2) + \theta(t_1 - t_2)H(t_2)H(t_1)]$$

$$= \frac{1}{2}\int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2\, \tilde{T}[H(t_1)H(t_2)]$$

We can generalize this to all terms in the expansion for $W(t,t_0)$, and thus obtain Eq.(13.7).

Problem 2.

The properties of $W(t,t')$ can be obtained directly from the defining equation,

$$|\Psi_s(t)\rangle = W(t,t_0)\,|\Psi_s(t_0)\rangle$$

setting $t_0 = t$,

$$|\Psi_s(t)\rangle = W(t,t)\,|\Psi_s(t)\rangle \implies W(t,t) = 1$$

Next

$$|\Psi_s(t)\rangle = W(t,t'')\,|\Psi_s(t'')\rangle$$

$$= W(t,t'')W(t'',t')\,|\Psi_s(t')\rangle$$

But,

$$|\Psi_s(t)\rangle = W(t,t')\,|\Psi_s(t')\rangle \quad \implies \quad W(t,t') = W(t,t'')W(t'',t')$$

Next,

$$1 = \langle \Psi_s(t) \,|\, \Psi_s(t) \rangle = \left\langle \Psi_s(t_0) \,\middle|\, W^\dagger(t,t_0)W(t,t_0) \,\middle|\, \Psi_s(t_0) \right\rangle = \langle \Psi_s(t_0) \,|\, \Psi_s(t_0) \rangle$$

$$\implies W^\dagger(t,t_0)W(t,t_0) = 1 \quad \implies W^\dagger(t,t_0) = W^{-1}(t,t_0)$$

Finally,

$$1 = W(t,t) = W(t,t_0)W(t_0,t)$$

$$\implies W(t_0,t) = W^{-1}(t,t_0)$$

Problem 3.

$$\varrho_s(t) = \sum_n P_n\,|\Psi_{n_s}(t)\rangle\,\langle\Psi_{n_s}(t)|$$

$$Tr[\varrho_s(t)A_s] = \sum_m \langle\Psi_{m_s}(t)|\,\varrho_s(t)A_s\,|\Psi_{m_s}(t)\rangle$$

$$= \sum_{m,n} P_n\,\langle\Psi_{m_s}(t)\,|\,\Psi_{n_s}(t)\rangle\,\langle\Psi_{n_s}(t)|\,A_s\,|\Psi_{m_s}(t)\rangle$$

$$= \sum_{m,n} P_n\delta_{m,n}\,\langle\Psi_{n_s}(t)|\,A_s\,|\Psi_{m_s}(t)\rangle$$

$$= \sum_n P_n\,\langle\Psi_{n_s}(t)|\,A_s\,|\Psi_{n_s}(t)\rangle$$

$$= \langle A\rangle\,(t)$$

Problem 4.

The relation

$$|\Psi_I(t)\rangle = S(t,t_0)\,|\Psi_I(t_0)\rangle$$

is similar to the corresponding relation

$$|\Psi_s(t)\rangle = W(t,t_0)\,|\Psi_s(t_0)\rangle$$

This relation in the Schrödinger picture was used in Problem 2. to derive the properties of $W(t,t_0)$. The $S(t,t_0)$ satisfies the same properties satisfied by $W(t,t_0)$. The proof of Eq. (13.26) is obtained by following the same steps used to derive Eq. (13.8): simply $|\Psi_s\rangle \longrightarrow |\Psi_I\rangle$, $W \longrightarrow S$.

Problem 5.

$$G^T(1,1') = -i\theta(t-t')\left\langle \Psi_H(1)\Psi_H^\dagger(1')\right\rangle \mp i\theta(t'-t)\left\langle \Psi_H^\dagger(1')\Psi_H(1)\right\rangle$$

We add and subtract the term $-i\theta(t'-t)\left\langle \Psi_H(1)\Psi_H^\dagger(1')\right\rangle$,

$$\begin{aligned}
G^T(1,1') &= -i\theta(t-t')\left\langle \Psi_H(1)\Psi_H^\dagger(1')\right\rangle \mp i\theta(t'-t)\left\langle \Psi_H^\dagger(1')\Psi_H(1)\right\rangle \\
&\quad -i\theta(t'-t)\left\langle \Psi_H(1)\Psi_H^\dagger(1')\right\rangle + i\theta(t'-t)\left\langle \Psi_H(1)\Psi_H^\dagger(1')\right\rangle \\
&= -i[\theta(t-t') + \theta(t'-t)]\left\langle \Psi_H(1)\Psi_H^\dagger(1')\right\rangle \\
&\quad +i\theta(t'-t)\left\langle \Psi_H(1)\Psi_H^\dagger(1') \mp \Psi_H^\dagger(1')\Psi_H(1)\right\rangle \\
&= -i\left\langle \Psi_H(1)\Psi_H^\dagger(1')\right\rangle + i\theta(t'-t)\left\langle [\Psi_H(1), \Psi_H^\dagger(1')]_\mp\right\rangle \\
&= G^>(1,1') + G^A(1,1')
\end{aligned}$$

If, instead, we add and subtract $-i\theta(t-t')\left\langle \Psi_H^\dagger(1')\Psi_H(1)\right\rangle$**, we obtain**

$$G^T(1,1') = -i\theta(t-t')\left\langle \Psi_H(1)\Psi_H^\dagger(1')\right\rangle \mp i\theta(t'-t)\left\langle \Psi_H^\dagger(1')\Psi_H(1)\right\rangle$$

$$-i\theta(t-t')\left\langle \Psi_H^\dagger(1')\Psi_H(1)\right\rangle + i\theta(t-t')\left\langle \Psi_H^\dagger(1')\Psi_H(1)\right\rangle$$

For Fermions, combine the first and third terms.

$$G^T = -i\theta(t-t')\left\langle [\Psi_H(1), \Psi_H^\dagger(1')]_+\right\rangle + i[\theta(t'-t)+\theta(t-t')]\left\langle \Psi_H^\dagger(1')\Psi_H(1)\right\rangle$$

$$= G^R + i\left\langle \Psi_H^\dagger(1')\Psi_H(1)\right\rangle$$

$$= G^R + G^<$$

For Bosons,

$$G^T(1,1') = -i\theta(t-t')\left\langle \Psi_H(1)\Psi_H^\dagger(1') - \Psi_H^\dagger(1')\Psi_H(1)\right\rangle$$

$$-i[\theta(t'-t)+\theta(t-t')]\left\langle \Psi_H^\dagger(1')\Psi_H(1)\right\rangle$$

$$= G^R(1,1') - i\left\langle \Psi_H^\dagger(1')\Psi_H(1)\right\rangle$$

$$= G^R(1,1') + G^<(1,1')$$

In both cases (fermions and bosons), we have

$$G^T = G^R + G^<$$

To obtain the corresponding expression for $G^{\tilde{T}}$**, we us Eq. (13.44),**

$$G^T + G^{\tilde{T}} = G^> + G^<$$

Thus

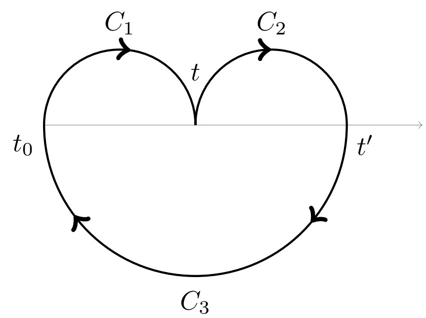
$$G^{\tilde{T}} = G^> + G^< - G^T$$

Since $G^T = G^R + G^<$**, we obtain** $G^{\tilde{T}} = G^> - G^R$

Using $G^T = G^> + G^A$, we obtain $G^{\tilde{T}} = G^< - G^A$

Problem 6.

Now the contour looks like



$$iG(1,1') = \pm \left\langle \Psi_H^\dagger(1')\Psi_H(1) \right\rangle$$

$$= \pm \left\langle S(t_0,t')\hat{\Psi}^\dagger(1')S(t',t)\hat{\Psi}(1)S(t,t_0) \right\rangle$$

Where the $-(+)$ sign refers to fermions (bosons).

We can rewrite Eq.(13.49) as

$$iG_C(1,1') = \left\langle T_C[e^{-\frac{i}{\hbar}\int_C \hat{H}'(\tau_1)d\tau_1}\hat{\Psi}(1)\hat{\Psi}^\dagger(1')] \right\rangle$$

$$= \pm \left\langle T_C[e^{-\frac{i}{\hbar}\int_C \hat{H}'(\tau_1)d\tau_1}\hat{\Psi}^\dagger(1')\hat{\Psi}(1)] \right\rangle \equiv \pm \langle D \rangle$$

D is identical to B introduced in deriving Eq. (13.49) for the case $\tau \overset{c}{>} \tau'$ except for the interchange of $\Psi(1)$ and $\Psi^\dagger(1')$.

Thus $\qquad D = P\hat{\Psi}^\dagger(1')Q\hat{\Psi}(1)P$

Now C_1 extends from t_0 to t, C_2 from t to t', and C_3 from t' to t_0; hence

$$D = S(t_0, t')\hat{\Psi}^\dagger(1')S(t', t)\hat{\Psi}(1)S(t, t_0)$$

This proves the validity of Eq. (13.49) for the case $\tau \overset{c}{<} \tau'$.