Applied Quantum Mechanics

Chapter 6 problems

LAST NAME FIRST NAME

Problem 6.1

(a) Write down the Hamiltonian for a particle of mass m in a one-dimensional harmonic oscillator potential in terms of momentum $\hat{p}_x$ and position $\hat{x}$.

(b) If one defines new operators

$$\hat{b} = \left(\frac{m\omega}{2\hbar}\right)^{1/2}\left(\hat{x} + \frac{i\hat{p}_x}{m\omega}\right)$$

$$\hat{b}^\dagger = \left(\frac{m\omega}{2\hbar}\right)^{1/2}\left(\hat{x} - \frac{i\hat{p}_x}{m\omega}\right)$$

show that the Hamiltonian can be expressed as

$$\hat{H} = \frac{\hbar\omega}{2}(\hat{b}\hat{b}^\dagger + \hat{b}^\dagger\hat{b})$$

(c) Derive the commutation relation $[\hat{b}, \hat{b}^\dagger]$ by writing out the differential form of $\hat{b}$ and $\hat{b}^\dagger$ and operating on a dummy wave function.

(d) Using your result from (c) show that the Hamiltonian is

$$\hat{H} = \hbar\omega\left(\hat{b}^\dagger\hat{b} + \frac{1}{2}\right)$$

Problem 6.2

(a) Find the expectation value of position and momentum for the first excited state for a particle of mass m in a one-dimensional harmonic oscillator potential.

(b) Find the value of the product in uncertainty in position Δx and momentum Δp_x for the first excited state of a particle of mass m in a one-dimensional harmonic oscillator potential.

Problem 6.3

Often an operator $\hat{A}$ is time-independent but the corresponding numerical value of the observable A has a spread in values ΔA about an average value $\langle A(t)\rangle$ and varies with time because the system is described by a wave function $\psi(x, t)$ which is not an eigenstate. The change in $\langle A(t)\rangle$ in time interval Δt is the slope $\frac{\mathrm{d}}{\mathrm{d}t}\langle A(t)\rangle$ multiplied by Δt. Hence, the exact time t at which the numerical value of the observable A passes through a specific value will actually have a spread in values Δt such that

$$\Delta t = \Delta A / \left|\frac{\mathrm{d}}{\mathrm{d}t}\langle A\rangle\right|$$

(a) Use the generalized uncertainty relation $\Delta A \Delta B \geq \left|\frac{1}{2}\langle[\hat{A}, \hat{B}]\rangle\right|$ for time independent operators $\hat{A}$ and $\hat{B}$ to show that $\Delta E \Delta t \geq \frac{\hbar}{2}$.

(b) Show that the spread in photon number Δn and phase $\Delta\phi$ for light of frequency ω is

$$\Delta n \Delta\phi \geq \frac{1}{2}$$

and that for a Poisson distribution of such photons

$$\Delta\phi \geq \frac{1}{2\sqrt{\langle n\rangle}}$$

(c) Apply the results in (b) and determine Δn and $\Delta\phi$ for a 100 ps pulse of λ = 1500 nm wavelength light from a 10 μW source.

Problem 6.4

A particle of charge *e*, mass *m*, and momentum *p* oscillates in a one-dimensional harmonic potential $V(x) = m\omega_0^2 x^2/2$ and is subject to an oscillating electric field $|\mathbf{E}|\cos(\omega t)$.

(a) Write down the Hamiltonian of the system.

(b) Find $\frac{\mathrm{d}}{\mathrm{d}t}\langle x\rangle$.

(c) Find $\frac{\mathrm{d}}{\mathrm{d}t}\langle p\rangle$ and show that $\frac{\mathrm{d}}{\mathrm{d}t}\langle p\rangle = -\langle\frac{\mathrm{d}}{\mathrm{d}x}V(x)\rangle$. Under what conditions is the quantum mechanical result $m\frac{\mathrm{d}^2}{\mathrm{d}t^2}\langle x\rangle = -\langle\frac{\mathrm{d}}{\mathrm{d}x}V(x)\rangle$ the same Newton's second law in which force on a particle is $F = m\frac{\mathrm{d}^2x}{\mathrm{d}t^2} = -\frac{\mathrm{d}}{\mathrm{d}x}V(x)$?

(d) Find $\frac{\mathrm{d}}{\mathrm{d}t}\langle H\rangle$.

(e) Use your results in (b) and (c) to find the time dependence of the expectation value of position $\langle x\rangle(t)$. What happens to the maximum value of $\langle x\rangle$ as a function of time when $\omega_0 = \omega$ and when ω is close in value to ω_0?

Problem 6.5

Express the total ground state energy of a one dimensional harmonic oscillator as the sum of potential and kinetic energy terms involving displacement Δx and momentum Δp_x. Assume the minimum uncertainty relation $\Delta x \Delta p_x = \hbar/2$ and find the ground state energy of the system.

Problem 6.6

(a) What is the minimum energy E_0 stored in a resonant *LC* circuit?

(b) Find an expression for the value of capacitance *C* if the charging energy associated with the coulomb blockade for the capacitor is the same as E_0.

(c) If the inductor has value $L = 10^{-8}$ H, what is the resonant oscillation frequency of the circuit and what is the value of the capacitance *C*?

(d) If the current in the circuit can be measured to an accuracy of one electron per oscillation, how accurately can the voltage of the circuit be determined?

Problem 6.7

An electron is confined by a one-dimensional harmonic potential created by a uniform static positive charge distribution.

(a) What is the value of the mean electric-field dipole moment of the elastically bound electron when it is in eigenstate $|\phi_n\rangle$?

(b) What is the value of the mean electric-field dipole moment in the presence of a uniform static electric field **E** in the x direction?

(c) What is the static electric susceptibility and permittivity of the system?

(d) Estimate the frequency dependent electric susceptibility of the system.

Problem 6.8

For the one dimensional harmonic oscillator we have

$$\hat{b} = \left(\frac{m\omega}{2\hbar}\right)^{1/2}\left(\hat{x} + \frac{i\hat{p}_x}{m\omega}\right)$$

(a) Show that $\langle n|\hat{b}^\dagger|m\rangle = \langle m|\hat{b}|n\rangle^*$ and $\langle\hat{b}^\dagger n|\hat{b}^\dagger n\rangle = \langle n|\hat{b}\hat{b}^\dagger n\rangle$.

(b) Is $\hat{b}^\dagger$ a Hermitian operator?

(c) Is $\hat{n} = \hat{b}^\dagger\hat{b}$ a Hermitian operator?

Problem 6.9

(a) Numerically evaluate and plot the time evolution of expectation value of position $\langle x(t)\rangle$, probability $|\psi(x, t)|^2$, and current density $J(x, t)$, for a superposition of the ground-state, ψ_0, and first excited state, ψ_1, of an electron confined to motion in a one-dimensional rectangular potential well of width L and infinite potential elsewhere. The superposition state is

$$\psi = \frac{1}{\sqrt{N+1}}\sum_{n=0}^{N}\psi_n$$

where $N = 1$. Repeat the calculation but now for a superposition state in which $N = 9$ and explain the differences in the results of the two calculations.

You may find it convenient to use the movie function in MATLAB.

(b) Numerically evaluate the time evolution of $\langle x(t)\rangle$ and $|\psi(x, t)|^2$ for a superposition of the ground-state and first excited state of the harmonic oscillator as illustrated in Fig. 6.6.

(c) Numerically evaluate the time evolution of $\langle x(t)\rangle$ and $|\psi(x, t)|^2$ for $N = 18$ and $\Delta N = 2$ in Example 6.4 in which the superposition state is

$$\psi = \frac{1}{\sqrt{2\Delta N}}\sum_{n=N-\Delta N}^{n=N+\Delta N}\psi_n$$

(d) The coherent quantum superposition that best describes the classical harmonic oscillator is

$$\psi_\alpha = \sum_{n=0}^{\infty} a_{\alpha,n}|n\rangle e^{-i\omega_n t}$$

where $a_{\alpha,n} = \dfrac{\alpha^n e^{\frac{-|\alpha|^2}{2}}}{\sqrt{n!}}$, $\omega_n = \omega\left(n + \dfrac{1}{2}\right)$, and α is a positive integer. Numerically evaluate the time evolution of $\langle x(t)\rangle$ and $|\psi(x, t)|^2$ for $\alpha = 1$, $\alpha = 2$ and $\alpha = 9$. Comment on anything you learn.

Problem 6.10

Pure exponential decay $e^{-t/\tau}$ starting from a constant value at time $t = 0$ is forbidden in a closed unitary system evolving due to a Hermitian time-independent Hamiltonian $\hat{H}$.

(a) The probability amplitude that an initial sate $|\alpha\rangle$ is observed in state $|\beta\rangle$ at time t is $a_{\alpha\beta}(t) = \langle\beta|\hat{U}(t)|\alpha\rangle$, where $\hat{U}(t)$ is the unitary time evolution operator. Analytically show that the probability of measuring and observing state $|\alpha\rangle$ is symmetric in time.

(b) Show analytically that any measurable state of the system cannot evolve as a simple exponential, $e^{-t/\tau}$, for either short times ($t \ll \tau$) or long times ($t \gg \tau$), thereby proving that exponential decay is incompatible with unitary evolution.

(c) Show numerically that the initial change in expectation value of position for the closed unitary system described in Problem 6.9(a) with $N \gg 2$ does not evolve as a simple exponential.

Problem 6.11

(a) Consider the wave function in problem 6.9(a) with $N = 4$. Calculate numerically the real part of ψ as a function of time at position $x_0 = L/5$ and find the value of the revival time (the minimum time it takes for the wave function to return to its original state). Show that peaks in the FFT spectrum are energy eigenvalues of the system. Show that this result generalizes to states of an arbitrary potential, $V(x)$, so long as x_0 is not an eigenfunction node.

(b) Demonstrate how to use the information in (a) to find the eigenfunctions ψ_n. Show that the numerical approach generalizes and so may be used to find the eigenstates of an arbitrary potential, $V(x)$.

(c) Consider the wave function in problem 6.9(d) with $\alpha = 2$. Calculate numerically the real part of ψ as a function of time at position $x_0 = 0$. Show that peaks in the FFT spectrum are energy eigenvalues of the system.

Comment on anything you learn.

Problem 6.12

Find the eigenenergies, eigenfunctions, and degeneracy of an isotropic two-dimensional harmonic oscillator by separation into Cartesian coordinates.

Problem 6.13

The canonical coherent state of Problem 6.9(d) is found by considering eigenstates $|\alpha\rangle$ of the harmonic oscillator operator $\hat{b}$ such that

$$\hat{b}|\alpha\rangle = \alpha|\alpha\rangle \tag{1}$$

where

$$|\alpha\rangle = \sum_{n=0}^{\infty} a_n|n\rangle \tag{2}$$

and a_n are coefficients of the known harmonic oscillator states $|n\rangle$.

(a) Substitute (2) into (1), keep the sum from $n = 0$, multiply from the left by state $\langle m|$ and show that

$$|\alpha\rangle = a_0 \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |n\rangle$$

(b) Use the normalization condition $\langle\alpha|\alpha\rangle = 1$ to find a_0 and show that

$$|\alpha\rangle = e^{-|\alpha|^2/2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |n\rangle$$

(c) Show that the probability $P_n = |\langle n|\alpha\rangle|^2$ that state $|n\rangle$ occurs in $|\alpha\rangle$ is a Poisson distribution

$$P_n = \frac{e^{-\bar{n}}\bar{n}^n}{n!}$$

where average $\bar{n} = \langle\alpha|\hat{b}^\dagger\hat{b}|\alpha\rangle = |\alpha|^2$.

(d) What is the average energy in coherent state $|\alpha\rangle$ and what is its classical turning point?

Problem 6.14

Numerical methods exist to solve dynamics of a classical particle of mass m with position x and momentum p described by Hamiltonian of the form $H = T(p) + V(x)$. For the simple harmonic oscillator with spring constant κ the kinetic energy $T = p^2/2m$ and potential energy $V = m\omega^2 x^2/2$, where angular frequency $\omega = \sqrt{\kappa/m}$.

(a) Defining canonical relations $-\frac{\mathrm{d}H}{\mathrm{d}x} = \frac{\mathrm{d}p}{\mathrm{d}t}$ and $\frac{\mathrm{d}H}{\mathrm{d}p} = \frac{\mathrm{d}x}{\mathrm{d}t}$, show that

$$\dot{x} = \upsilon \equiv \frac{\mathrm{d}x}{\mathrm{d}t}$$

$$\dot{\upsilon} = -\omega^2 x$$

and that the analytic solution for position is $x(t) = x(0)\cos(\omega t) + (\upsilon(0)/\omega)\sin(\omega t)$.

(b) A phase-space plot of p as a function of x is an ellipse whose area is constant because energy is conserved. Rewrite equations for $\dot{x}$ and $\dot{\upsilon}$ in (a) using discretization of space and time where $dx = \Delta x$ and $dt = \Delta t$, such that $x_n = n\Delta x$ and $t_n = n\Delta t$, to obtain a set of equations for x_{n+1} and υ_{n+1} in terms of x_n, υ_n, Δt, and ω. Write the set of linear equations in matrix form $z_{n+1} = \mathbf{A}z_n$, such that $z_n = \mathbf{A}z_{n-1} = \ldots\mathbf{A}^n z_0$.

(c) Numerical stability implies that the phase-space vector norm $\|z_n\|$ remains bounded for all n. For any consistent matrix norm

$$\rho(\mathbf{A}) = \max_i(|\lambda_i|) = \lim_{n\to\infty} \|\mathbf{A}^n\|^{1/n}$$

where λ_i are the eigenvalues of $\mathbf{A}$. The spectral radius theorem states that given a matrix $\mathbf{A}$ over the complex numbers, the iterations $z_n = \mathbf{A}^n z_0$ are bounded if $\rho(\mathbf{A}) \le 1$. Show under Euler discretization in part (b), energy is not conserved by explicitly demonstrating that $\rho(\mathbf{A}) > 1$. Thus the phase-space area is not conserved over time.

(d) In addition to the utility of the Baker-Campbell-Hausdorff formula in quantum mechanics (see Problem 5.14(b)), the identity can be exploited to integrate Hamiltonians of the form $H = T(p) + V(x)$. By constructing explicit and time-reversible symplectic integrators of higher order, it is possible to suppress numerical error stemming from the energy non-conserving discretization of sets of coupled equations. If $e^{\hat{A}+\hat{B}} = e^{-\frac{1}{2}[\hat{A},\hat{B}]}e^{\hat{A}}e^{\hat{B}}$ is true, show that $e^{2\hat{A}+\hat{B}} = e^{\hat{A}}e^{\hat{B}}e^{\hat{A}}$.

(e) For Hamiltonians of the form $H = T(p) + V(x) = p^2/2m + V(x)$, show that $e^{t\frac{\mathrm{d}}{\mathrm{d}t}} = e^{t(P+X)}$, where $P = -\dfrac{\mathrm{d}V}{\mathrm{d}x}\dfrac{\mathrm{d}}{\mathrm{d}p}$ and $X = \dfrac{\mathrm{d}T}{\mathrm{d}p}\dfrac{\mathrm{d}}{\mathrm{d}x}$.

(f) Since $[\hat{A},[\hat{A},\hat{B}]] \neq 0$ in general, show that to order $O(\Delta t^2)$, the symmetric symplectic integrator can be written as $U(\Delta t)^{t/\Delta t} = e^{t(P+X)} + O(\Delta t^2)$, where $U(\Delta t)^{t/\Delta t} = (e^{\Delta tP/2}e^{\Delta tX}e^{\Delta tP/2})^{t/\Delta t}$. What does this result indicate about the energy conserving properties of a symplectic integrator?