SUMMARY TEXT FILE

This folder contains a number of computer programs to be used in conjunction with the book:

Series Expansion Methods for Strongly Interacting Lattice Models
Jaan Oitmaa, Chris Hamer and Weihong Zheng
Cambridge University Press 2006
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Each program file contains the following:

- a program listing
- a sample input file
- a sample output file, or part thereof
- general notes of explanation

The user will need to edit each file appropriately to create a compilable FORTRAN program and to provide their own input file(s) in the correct format.

The following files are included, each identified with a number, a name, a filename, together with a brief description.

1. **Summary** (readme.pdf)
This summary file.

2. **Graph symmetry number** (symm)
A simple program to read in graphs from a file and compute their symmetry numbers. The input graphs are described in pair format. A subroutine symm computes the symmetry number using the 'pegs in holes' algorithm (Appendix B).

3. **Graph generation** (gen)
This program generates connected graphs without constraints, up to a maximum number of vertices and bonds, as described in Section 2.2. A subroutine symred checks for canonical labelling. The output is a list of graphs and a distribution table (cf. Table A.1)

4. **Graph sorter** (sort)
A simple program to take the output graph list from gen.f (or elsewhere) and sort in order of increasing number of bonds and number of vertices. For large lists this program in inefficient and it is better to use successive filtering.

5. **Graph counter** (count)
This program obtains weak, strong, or free lattice constants of connected graphs on an arbitrary lattice. Input consists of lattice data, a code for type of embedding, and a graph list in pair format. The output is a modified graph list with lattice constants included.

6. **Generator for disconnected graphs** (disc)
This program generates a list of disconnected graphs of any number of components, up to some specified number of bonds and/or veertices, from a list of connected graphs.

7. **Graph generator for SC lattice** (gensc)
A modified version of the graph generating program, with constraints for the simple cubic lattice (in fact any bipartite lattice with q.le.6). The constraints are described in Section 2.3 of the book.

8. **Graph counter for tree graphs** (treecnt)
This program computes weak (high T) lattice constants of tree graphs using an efficient indirect method, as explained in Section 2.2 of the book.

9. **Graph counter for disconnected (separated) graphs** (sepcnt)
This program computes weak (high T) lattice constants of separated graphs by embedding into graphs with fewer vertices and components.

10. **G graph generator** (ggrafs)
This program generates G graphs for Free Graph Expansion, by decorating bare graphs, as described in Section 3.3 of the book.

11. **X graph generator** (xgrafs)
This program generates X graphs for Free Graph Expansion, by decorating bare graphs, as described in Section 3.3 of the book.

12. **Free Graph Expansion** (free2)
This is the main program for the Free Graph Expansion for N = 2, referred to in Section 3.3 of the book. A word of caution: this program was developed specifically for the book, and has not been tested or optimized to the extent of the other programs.

13. **Computation of Subgraph Data** (subgr)
This program computes subgraphs and their embedding factors for a list of input graphs, for used in linked-cluster perturbation expansions. The formulation given here is for strong ('low T') embeddings.

14. **Cluster Perturbation Theory** (tim1)
This program carries out pertubation theory for finite clusters, for the transverse field Ising model in the ordered phase, as described in Section 4.3 and Appendix 4. It can also be used as a model for writing analogous programs for other Hamiltonians.

15. **Bulk Perturbation Series** (tim2)
This program is a simple extension of tim1, and combines cluster series with subcluster subtraction. The reduced quantities are then combined to give series for the bulk lattice. It can again be used as a model for other cases.

16. **One-particle Excitation Series** (tim3)
The 2-block orthogonal transformation (TBOT) method is used to compute the effective Hamiltonian and transition amplitudes for finite clusters, for the transverse field Ising model in the disordered phase, as described in Section 4.5 of the book.

17. **Thermodynamic Perturbation Theory** (tpert)
This program carries out a finite T perturbation expansion for the free energy of individual clusters, as discussed in Section 7.5. The particular implementation is for a dimer expansion for the alternating Heisenberg chain, described in Section 7.5.1. It can be modified for other systems and extended to compute reduced quantities and to obtain series for the bulk system.

The program is inefficient and should be modified, as explained in the Notes, for high order calculations.

We welcome feedback from readers on any of the computer codes.

Readers may also be interested in the following web sites:
http://www.ms.unimelb.edu.au/~tonyg/: This provides codes for series analysis, written by A.J. Guttmann (see Guttmann (1989) for listings). These codes can be freely downloaded.

http://brahms.th.physik.uni-bonn.de/ClusterExpansion/DOC/Intro.html: This site provides information, from the University of Bonn group, on various aspects of cluster expansions. Program listings are not provided but can, as we understand, be obtained from the authors.

http://www.thp.uni-koeln.de/~gu/:This site provides information, from the University of Cologne group, on various aspects of series expansions via the continuous unitary transformation method.

http://www.phys.unsw.edu.au/~zwh/: This site provides additional information on linked cluster series expansions from our group.