Project 3, FYS-KJM4480, Fall 2009

Project 3, deadline 12pm Friday November 20

This is the last project. We present a simplified Hamiltonian (which has many common traits with the Lipkin model of project 1) consisting of an unperturbed Hamiltonian and a so-called pairing interaction term. It is a model which to a large extent mimicks some central features of atomic nuclei, certain atoms and systems which exhibit superfluiditity or superconductivity. To study this system, we will use a mix of many-body perturbation theory, Hartree-Fock theory and the configuration interaction method. The latter will also provide us with the exact answer. When setting up the Hamiltonian matrix you will need to solve an eigenvalue problem (as you did for the Lipkin model). This can easily be done with either octave or Matlab.

We define first the Hamiltonian, with a definition of the model space and the single-particle basis. Thereafter, we present the various exercises.

Introduction and Hamiltonian

The Hamiltonian acting in the complete Hilbert space (usually infinite dimensional) consists of an unperturbed one-body part, $\hat{H}_0$, and a perturbation $\hat{V}$.

We limit ourselves to at most two-body interactions, our Hamiltonian is then represented by the following operators

$$\hat{H} = \sum_{\alpha\beta} \langle \alpha | h_0 | \beta \rangle a_\alpha^\dagger a_\beta + \frac{1}{4} \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | V | \gamma\delta \rangle a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma,$$

where $a_\alpha^\dagger$ and a_α etc. are standard fermion creation and annihilation operators, respectively, and $\alpha\beta\gamma\delta$ represent all possible single-particle quantum numbers. The full single-particle space is defined by the completeness relation $\hat{\mathbf{1}} = \sum_{\alpha=1}^{\infty} |\alpha\rangle\langle\alpha|$. In our calculations we will let the single-particle states $|\alpha\rangle$ be eigenfunctions of the one-particle operator $\hat{h}_0$.

The above Hamiltonian acts in turn on various many-body Slater determinants constructed from the single-basis defined by the one-body operator $\hat{h}_0$. As an example, the two-particle model space $\mathcal{P}$ is defined by an operator

$$\hat{P} = \sum_{\alpha\beta=1}^{m} |\alpha\beta\rangle\langle\alpha\beta|,$$

where we assume that $m = \dim(\mathcal{P})$ and the full space is defined by

$$\hat{P} + \hat{Q} = \hat{\mathbf{1}},$$

with the projection operator

$$\hat{Q} = \sum_{\alpha\beta=m+1}^{\infty} |\alpha\beta\rangle\langle\alpha\beta|,$$

being the complement of $\hat{P}$.

Our specific model consists of N doubly-degenerate and equally spaced single-particle levels labelled by $p = 1, 2, \ldots$ and spin $\sigma = \pm 1$. These states are schematically portrayed in Fig. 1. The first two single-particle levels define a possible model space, indicated by the label $\mathcal{P}$. The remaining states span the excluded space $\mathcal{Q}$.

We write the Hamiltonian as

$$\hat{H} = \hat{H}_0 + \hat{V},$$

where

$$\hat{H}_0 = \xi \sum_{p\sigma} (p-1) a_{p\sigma}^\dagger a_{p\sigma}$$

and

$$\hat{V} = -\frac{1}{2}g\sum_{pq} a^{\dagger}_{p+}a^{\dagger}_{p-}a_{q-}a_{q+}.$$

Here, H_0 is the unperturbed Hamiltonian with a spacing between successive single-particle states given by ξ, which we will set to a constant value $\xi = 1$ without loss of generality. The two-body operator $\hat{V}$ has one term only. It represents the pairing contribution and carries a constant strength g. The indices $\sigma = \pm$ represent the two possible spin values. The interaction can only couple pairs and excites therefore only two particles at the time, as indicated by the rightmost four-particle state in Fig. 1. There one of the pairs is excited to the state with $p = 9$ and the other to the state $p = 7$. The two middle possibilities are not possible with the present model. We label single-particle states within the model space as hole-states. The single-particle states outside the model space are then particle states. The model is not so different from the Lipkin model studied in project 1.

In our model we have kept both the interaction strength and the single-particle level as constants. In a realistic system like an atom or the atomic nucleus this is not the case.

Exercises

1. Show that the unperturbed Hamiltonian $\hat{H}_0$ and $\hat{V}$ commute with both the spin projection $\hat{S}_z$ and the total spin $\hat{S}^2$, given by

   $$\hat{S}_z := \frac{1}{2}\sum_{p\sigma} \sigma a^{\dagger}_{p\sigma}a_{p\sigma}$$

   and

   $$\hat{S}^2 := \hat{S}_z^2 + \frac{1}{2}(\hat{S}_+\hat{S}_- + \hat{S}_-\hat{S}_+),$$

   where

   $$\hat{S}_\pm := \sum_{p} a^{\dagger}_{p\pm}a_{p\mp}.$$

   This is an important feature of our system that allows us to block-diagonalize the full Hamiltonian. We will focus on total spin $S = 0$. In this case, it is convenient to define the so-called pair creation and pair annihilation operators

   $$\hat{P}^+_p = a^{\dagger}_{p+}a^{\dagger}_{p-},$$

   and

   $$\hat{P}^-_p = a_{p-}a_{p+},$$

   respectively.

   Show that you can rewrite the Hamiltonian (with $\xi = 1$) as

   $$\hat{H} = \sum_{p\sigma}(p-1)a^{\dagger}_{p\sigma}a_{p\sigma} - \frac{1}{2}g\sum_{pq}\hat{P}^+_p\hat{P}^-_q.$$

   Show also that Hamiltonian commutes with the product of the pair creation and annihilation operators. This model corresponds to a system with no broken pairs. This means that the Hamiltonian can only link two-particle states in so-called spin-reversed states.

2. Construct thereafter the Hamiltonian matrix for a system with no broken pairs and spin $S = 0$ for the case of the four lowest single-particle levels indicated in the Fig. 1. Our system consists of four particles only. Our single-particle space consists of only the four lowest levels $p = 1, 2, 3, 4$. You need to set up all possible Slater determinants. Find all eigenvalues by diagonalizing the Hamiltonian matrix. Vary your results for values of $g \in [-1, 1]$. We refer to this as the exact calculation. Comment the behavior of the ground state as function of g.

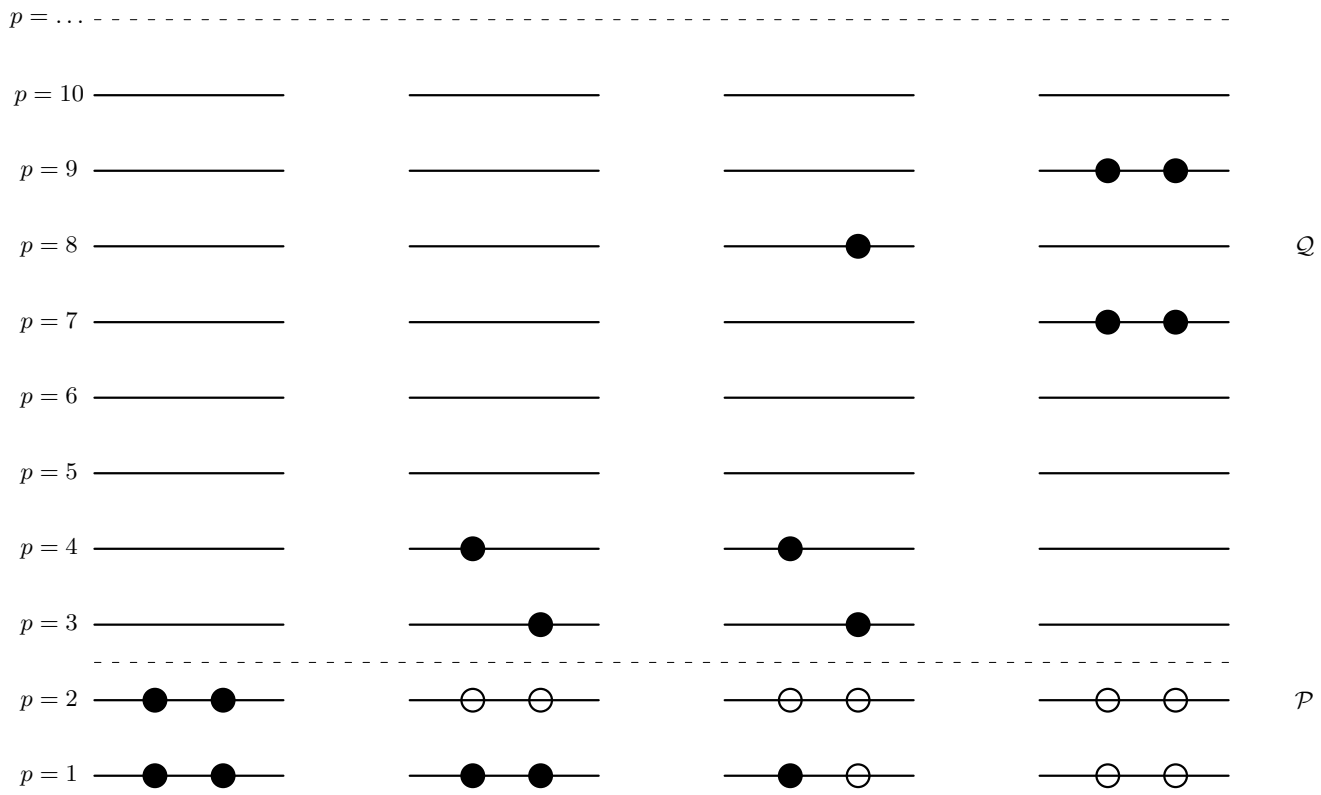

FIG. 1: Schematic plot of the possible single-particle levels with double degeneracy. The filled circles indicate occupied particle states while the empty circles represent vacant particle(hole) states. The spacing between each level p is constant in this picture. The first two single-particle levels define our possible model space, indicated by the label $\mathcal{P}$. The remaining states span the excluded space $\mathcal{Q}$. The first state to the left represents a possible ground state representation for a four-fermion system. In the second state to the left, one pair is broken. This possibility is however not included in our interaction.

3. Instead of setting up all possible Slater determinants, construct only an approximation to the ground state (where we assume that the four particles are in the two lowest single-particle orbits only) which includes at most two-particle-two-hole excitations. Diagonalize this matrix and compare with the exact calculation and comment your results. Can you set up which diagrams this approximation corresponds to?

4. Hereafter we will define our model space to consist of the single-particle levels $p = 1, 2$. The remaining levels $p = 3, 4$ define our excluded space. This means that our ground state Slater determinant consists of four particles which can be placed in the doubly degenerate orbits $p = 1$ and $p = 2$.

   We will now study the system using non-degenerate Rayleigh-Schrödinger perturbation theory to third order in the interaction. If we exclude the first order contribution, all possible diagrams (Hugenholz diagrams where the vertices have been opened) are shown in Fig. 2.

   Based on the form of the interaction, which diagrams contribute to the binding energy of the ground state? Write down the expressions for the diagrams that contribute and find the contribution to the ground state

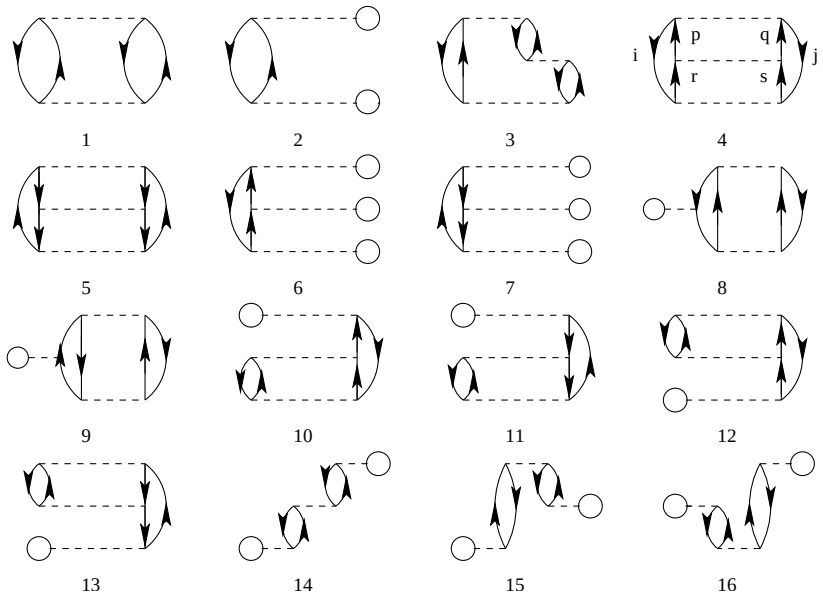

FIG. 2: Diagrams to third order in the interaction. The first order term is excluded.

energy as function $g \in [-1, 1]$. Comment your results. Compare these results with those you obtained in 2) and 3).

5. The diagrams with only two single particle states as intermediate states (for example diagrams 1 and 4 in Fig. 2) can be summed to infinite order since they can be expressed as a geometric series. Find this contribution and compare the final energy with the results from 2) and 3). Comment your results. You can also perform a resummation of diagrams like diagram 5 with hole lines as intermediate states only between various vertices. Can you find this result as well? Compare now the final results with the resummed two-particle and two-hole diagrams with the results from 2) and 3).

6. We will now set up the Hartree-Fock equations by varying the coefficients of the single-particle functions. The single-particle basis functions are defined as

$$\psi_p = \sum_{\lambda} C_{p\lambda}\psi_{\lambda}.$$

where in our case $p = 1, 2, 3, 4$ and $\lambda = 1, 2, 3, 4$, that is the first four lowest single-particle orbits of Fig. 1. Set up the Hartree-Fock equations for this system by varying the coefficients $C_{p\lambda}$ and solve them for values of $g \in [-1, 1]$. Comment your results and compare with the exact solution. Discuss also which diagrams in Fig. 2 that can be affected by a Hartree-Fock basis. Compute the total binding energy using a Hartree-Fock basis and comment your results.

7. To fourth order in perturbation theory we can produce diagrams with so-called four-particle-four-hole excitations. An example is given in Fig. 3. Find the contribution to the binding energy of the ground state from this type

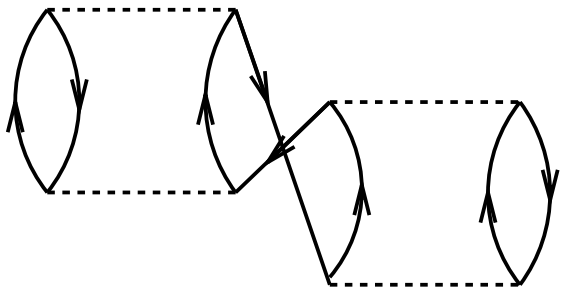

FIG. 3: An example of a fourth-order diagram with an intermediate state involving four-particle-four-hole excitations.

of contributions and compare with your previous results with and without a Hartree-Fock basis. Discuss in particular the connection with the results in exercise 2) with the full diagonalization where Slater determinants involving four-particle-four-hole excitations are involved.

8. When summing over all intermediate states in diagram 1 or 4 of Fig. 2, we have limited the sum over intermedate particle states to include the states $p = 3$ and $p = 4$ only. Compute this sum by taking the limit $p = \infty$. Comment your results.