

Midterm exam FYS-KJM4480, Fall 2011

Deadline 12pm Friday October 14. Use only your candidate number. It counts 30% of the final grade.

We present a simplified Hamiltonian 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 superfluidity or superconductivity. To study this system, we will use a mix of Hartree-Fock theory and exact diagonalization. The latter will also provide us with the exact answer. When setting up the Hamiltonian matrix you will need to solve an eigenvalue problem. This can easily be done with either octave or Matlab.

We define first the Hamiltonian, with a definition of 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 two-body interaction \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_α^\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-particle basis defined by the one-body operator \hat{h}_0 .

Our specific model consists of N doubly-degenerate and equally spaced single-particle levels labelled by $p = 1, 2, \dots$ and spin $\sigma = \pm 1$. These states are schematically portrayed in Fig. 1. The first two single-particle levels will define the states up to the Fermi level (our hole states), indicated by the label \mathcal{F} . The remaining states are particle (virtual) states.

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

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

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.

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.

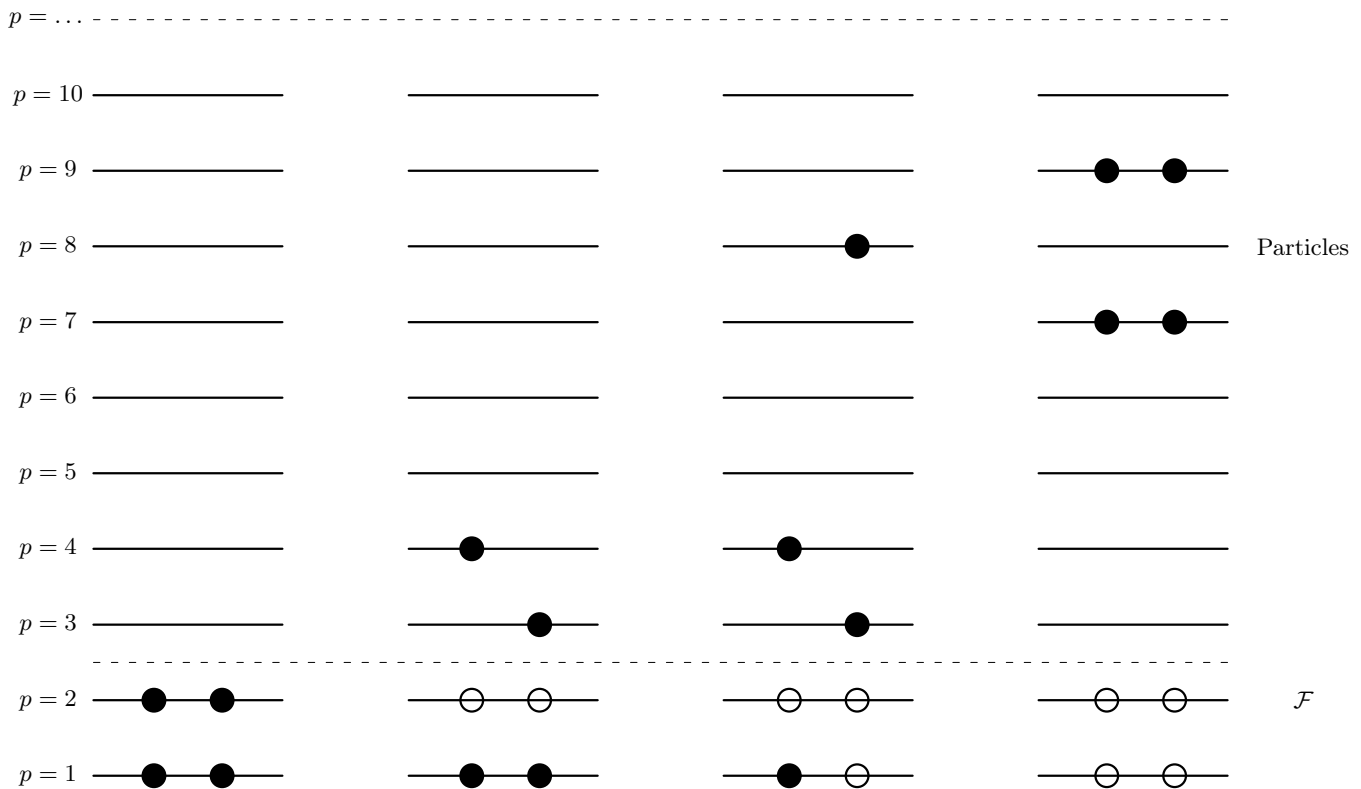


FIG. 1: Schematic plot of the possible single-particle levels with double degeneracy. The filled circles indicate occupied particle states while the empty circles represent vacant particle(hole) states. The spacing between each level p is constant in this picture. The first two single-particle levels define our hole states, indicated by the label \mathcal{F} . The remaining states are particle states. 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.

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

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

and

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

where

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

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

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

and

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

respectively.

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

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

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. Our system will now consist of four particles only and the single-particle space consists of only the four lowest levels $p = 1, 2, 3, 4$ in the Fig. 1. Define the Slater determinant ansatz for the ground state. Find the reference energy E_0 and write down the diagrams which contribute. Make sure that the two-body matrix elements are properly anti-symmetrized.
3. 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. Write down the diagrams which contribute. 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 .
4. 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 for $g \in [-1, 1]$ and comment your results. Can you set up which diagrams this approximation corresponds to? Do you get contributions of the type one-particle-two-hole?
5. Set up (the general expressions) the Hartree-Fock equations in second quantization. Write down the corresponding diagrams and find the expression for the Hartree-Fock operator. Discuss also the stability of the Hartree-Fock ground state energy. Insert then our model and find the expressions for the Hartree-Fock operator. Comment your results.
6. We will now set up the Hartree-Fock equations by varying the coefficients of the single-particle functions (one of the standard ways of solving these equations). 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, in particular in the light of the discussion in the previous exercise. Compare with the exact solution. Compute the total binding energy using a Hartree-Fock basis and comment your results.