First midterm FYS4480 – Quantum mechanics for many-particle systems, deadline October 22. Total score 100 points.

FYS4480 – Quantum mechanics for many-particle systems

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Introduction

We have already encountered in various weekly exercises a schematic model called the Lipkin model, see Nucl. Phys. **62** (1965) 188). We repeat here some of the basic properties for the interaction among 4 fermions that can occupy two different energy levels. Each levels has degeneration $d = 4$. The two levels have quantum numbers $\sigma = \pm 1$, with the upper level having $\sigma = +1$ and energy $\varepsilon_1 = \varepsilon/2$. The lower level has $\sigma = -1$ and energy $\varepsilon_2 = -\varepsilon/2$. In addition, the substates of each level are characterized by the quantum numbers $p = 1, 2, 3, 4$.

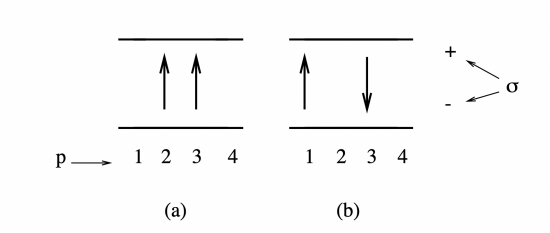
We define the single-particle states

$$|u_{\sigma=-1,p}\rangle = a^\dagger_{-p}|0\rangle \qquad |u_{\sigma=1,p}\rangle = a^\dagger_{+p}|0\rangle\,.$$

The single-particle states span an orthonormal basis. The Hamiltonian of the system is given by

$$\begin{aligned}
\hat{H} = &\quad \hat{H}_0 + \hat{H}_1 + \hat{H}_2 \\
\hat{H}_0 = &\quad \tfrac{1}{2}\varepsilon \textstyle\sum_{\sigma,p} \sigma a^\dagger_{\sigma,p} a_{\sigma,p} \\
\hat{H}_1 = &\quad \tfrac{1}{2}V \textstyle\sum_{\sigma,p,p'} a^\dagger_{\sigma,p} a^\dagger_{\sigma,p'} a_{-\sigma,p'} a_{-\sigma,p} \\
\hat{H}_2 = &\quad \tfrac{1}{2}W \textstyle\sum_{\sigma,p,p'} a^\dagger_{\sigma,p} a^\dagger_{-\sigma,p'} a_{\sigma,p'} a_{-\sigma,p}
\end{aligned}$$

where V and W are constants. The operator H_1 can move pairs of fermions as shown in the left part of the fugure (a). while H_2 is a spin-exchange term. As shown in (b), H_2 moves a pair of fermions from a state $(p\sigma, p' - \sigma)$ to a state $(p - \sigma, p'\sigma)$.



It is a model which has been used widely in many-body physics and recently also in quantum computing, see for example https://journals.aps.org/prc/abstract/10.1103/PhysRevC.104.024305. In the weekly exercises we showed that the quasispin operators

$$\begin{aligned}\hat{J}_+ &= \sum_p a^\dagger_{p+} a_{p-} \\ \hat{J}_- &= \sum_p a^\dagger_{p-} a_{p+} \\ \hat{J}_z &= \tfrac{1}{2}\sum_{p\sigma} \sigma a^\dagger_{p\sigma} a_{p\sigma} \\ \hat{J}^2 &= J_+ J_- + J_z^2 - J_z\end{aligned}$$

obey the commutation relations for angular momentum and that we could express $\hat{H}$ in terms of the above quasispin operators and the number operator

$$\hat{N} = \sum_{p\sigma} a^\dagger_{p\sigma} a_{p\sigma}.$$

Commutation relations (10pts) Show that $\hat{H}$ commutes with J^2, viz., J is a good quantum number. Does it commute with J_z?

Wick's theorem Consider thereafter a state with all four fermions in the lowest level (see the above figure). We can write this state as

$$|\Phi_0\rangle = |\Phi_{J_z=-2}\rangle = a^\dagger_{1-} a^\dagger_{2-} a^\dagger_{3-} a^\dagger_{4-} |0\rangle .$$

This state has $J_z = -2$ (convince yourself about this) and belongs to the set of possible projections of $J = 2$. We introduce the shorthand notation $|J, J_z\rangle$ for states with different values of spin J and its projection J_z. We can think of this as our computational basis for $J = 2$ and all five projections J_z. We will also assume that the state Φ_0 can be considered as an ansatz for the ground state of the system.

Use Wick's theorem to calculate the expectation values of

$$\langle\Phi_0| \hat{N} |\Phi_0\rangle ,$$

and

$$\langle\Phi_0| \hat{H} |\Phi_0\rangle .$$

Using quasispin operators (10pts) Show that you can obtain the same result for

$$\langle\Phi_0|\,\hat{H}\,|\Phi_0\rangle\,.$$

using the quasispin representation of the Hamiltonian (plus the number operator). Comment your results.

Setting up all basis states for $J = 2$ (10pts) We will now use the quasispin operators to construct all possible states with spin $J = 2$ using as starting point a state with all fermions in the lowest single-particle state

$$|\Phi_{J_z=-2}\rangle = a^\dagger_{1-}a^\dagger_{2-}a^\dagger_{3-}a^\dagger_{4-}\,|0\rangle\,.$$

This state has $J_z = -2$ and belongs to the set of projections for $J = 2$. We will use the shorthand notation $|J, J_z\rangle$ for states with different spon J and spin projection J_z. The other possible states have $J_z = -1$, $J_z = 0$, $J_z = 1$ and $J_z = 2$.

Use the raising or lowering operators J_+ and J_- in order to construct the states for spin $J_z = -1$ $J_z = 0$, $J_z = 1$ and $J_z = 2$. The action of these two operators on a given state with spin J and projection J_z is given by ($\hbar = 1$) by $J_+\,|J, J_z\rangle = \sqrt{J(J+1) - J_z(J_z+1)}\,|J, J_z+1\rangle$ and $J_-\,|J, J_z\rangle = \sqrt{J(J+1) - J_z(J_z-1)}\,|J, J_z-1\rangle$.

Finding the eigenvalues using Full Configuration Interaction Theory (10pts) Use the quasispin operators to construct the Hamiltonian matrix H for the five-dimensional space that has total spin $J = 2$ and spin projections $J_z = -2, -1, 0, 1, 2$. Find thereafter the eigenvalues for the following parameter sets:

$$\begin{array}{lll} (1) & \varepsilon = 2, & V = -1/3, \quad W = -1/4 \\ (2) & \varepsilon = 2, & V = -4/3, \quad W = -1 \end{array}$$

Which state is the ground state? Comment your results in terms of the coefficients of the various eigenfunctions.

Hartree-Fock theory, general part (15pts) The standard way to perform a Hartree-Fock calculation is to expand the single-particle functions in a known basis and vary the coefficients, that is, the new function single-particle wave function $|p\rangle$ is written as a linear expansion in terms of a fixed basis ϕ

$$\psi_p = \sum_\lambda C_{p\lambda}\phi_\lambda,$$

This lead to a new Slater determinant which is related to the previous via a unitary transformation. We consider a Slater determinant built up of single-particle orbitals ϕ_λ where the indices λ refer to specific single-particle states.

The unitary transformation

$$\psi_p = \sum_\lambda C_{p\lambda}\phi_\lambda,$$

brings us into the new basis ψ. The new basis is orthonormal and C is a unitary matrix.

Minimizing with respect to $C^*_{p\alpha}$, remembering that $C^*_{p\alpha}$ and $C_{p\alpha}$ (and that the indices contain all single-particle quantum numbers including spin) are independent and defining

$$h^{HF}_{\alpha\gamma} = \langle\alpha|h|\gamma\rangle + \sum_p \sum_{\beta\delta} C^*_{p\beta}C_{p\delta}\langle\alpha\beta|V|\gamma\delta\rangle_{AS},$$

show that you can write the Hartree-Fock equations as

$$\sum_\gamma h^{HF}_{\alpha\gamma}C_{p\gamma} = \epsilon^{\rm HF}_p C_{p\alpha}.$$

Explain the meaning of the different terms and define the Hartree-Fock operator in second quantization. Write down its diagrammatic representation as well. The greek letters refer to the wave functions in the original basis while roman letters refer to the new basis.

Hartree-Fock theory for the Lipkin model (15pts) The single-particle states for the Lipkin model

$$|u_{\sigma=-1,p}\rangle = a^\dagger_{-p}|0\rangle \qquad |u_{\sigma=1,p}\rangle = a^\dagger_{+p}|0\rangle$$

can now be used as basis for a new single-particle state $|\phi_{\alpha,p}\rangle$ via a unitary transformation

$$|\phi_{\alpha,p}\rangle = \sum_{\sigma=\pm1} C_{\alpha\sigma}|u_{\sigma,p}\rangle$$

with $\alpha = \pm1$ and $p = 1,2,3,4$. Why is p the same in $|\phi\rangle$ as in $|u\rangle$? Show that the new basis is orthonormal.

Hartree-Fock energy (15pts) With the new basis we can construct a new Slater determinant given by $|\Psi\rangle$

$$|\Psi\rangle = \prod_{p=1}^{4} b^\dagger_{\alpha,p}|0\rangle$$

with $b^\dagger_{\alpha,p}|0\rangle = |\phi_{\alpha,p}\rangle$. h) Use the Slater determinanten from the previous exercise to calculate

$$E = \langle\Psi|H|\Psi\rangle,$$

as a function of the coefficients $C_{\sigma\alpha}$. We assume the coefficients to be real.

Stability of the Hartree-Fock equations (15pts) Using our Hartree-Fock results for the energy, show that

$$\frac{\epsilon}{3} > V + W,$$

has to be fulfilled in order to find a minimum in the energy. Comment your results.

Hint: calculate the functional derivative of the energy with respect to the coefficients $C_{\sigma\alpha}$.