Theory of Condensed Matter

Exercises on second quantization

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1 Starters

1. For $\alpha \neq \beta$, compute the matrix element $\langle 0|c_\alpha c_\beta c_\alpha^\dagger c_\beta^\dagger|0\rangle$ for fermions and for bosons.
2. Consider free fermions with spin 1/2 in a box of volume V. Write the hamiltonian $\hat{H}_0$ in second quantization in the Fourier momentum representation.
   (a) Write the expression of the ground state $|\mathrm{FS}\rangle$.
   (b) Compute the following quantities
   $$\langle \hat{n}_{k\sigma}\rangle = \langle \mathrm{FS}|c_{k\sigma}^\dagger c_{k\sigma}|\mathrm{FS}\rangle, \qquad E_0 = \langle \mathrm{FS}|\hat{H}_0|\mathrm{FS}\rangle, \qquad N_0 = \langle \mathrm{FS}|\hat{N}|\mathrm{FS}\rangle,$$
   in the thermodynamic limit $V \to +\infty$.
3. In the case of fermions, prove that
   $$c_\alpha^\dagger|\{n_\beta\}\rangle = \begin{cases} (-1)^{\sum_{\beta<\alpha} n_\beta}\,|n_1\, n_2 \ldots \overset{\alpha}{1}\; n_{\alpha+1}\ldots n_N\rangle & \text{if } n_\alpha = 0 \\ 0 & \text{if } n_\alpha = 1 \end{cases} \tag{1}$$
   and
   $$c_\alpha|\{n_\beta\}\rangle = \begin{cases} 0 & \text{if } n_\alpha = 0 \\ (-1)^{\sum_{\beta<\alpha} n_\beta}\,|n_1\, n_2 \ldots \overset{\alpha}{0}\; n_{\alpha+1}\ldots n_N\rangle & \text{if } n_\alpha = 1 \end{cases} \tag{2}$$
4. Show that the change of basis
   $$c_\beta^\dagger = \sum_\alpha U_{\beta\alpha} c_\alpha^\dagger,$$
   preserves the canonical commutation relations iff U is a unitary matrix. Is $U_{\beta\alpha} = \langle\beta|\alpha\rangle$ a unitary matrix ? Show that the expression of the number operator $\hat{N} = \sum_\alpha c_\alpha^\dagger c_\alpha$ is not modified by the above transformation.
5. For bosons, show that
   $$|n_1\, n_2 \ldots\rangle = \prod_i \frac{(b_i^\dagger)^{n_i}}{\sqrt{n_i!}}|0\rangle.$$
6. Compute the commutator $[\hat{H}_0, \hat{N}]$ for free fermions. What is the meaning of the result ? Is it modified when interactions are taken into account ?
7. Consider spinless free fermions or free bosons.
   (a) Derive the expression $\hat{H}_0 = \sum_k \varepsilon_k c_k^\dagger c_k$ from $\hat{H}_0 = -(\hbar^2/2m)\int dr\, \psi^\dagger(r)\nabla^2\psi(r)$.
   (b) Derive the expression of the Coulomb pair potential in the momentum representation starting from $\hat{V}_{\mathrm{Coulomb}} = \frac{1}{2}\sum_{\sigma_1,\sigma_2}\int dr_1\, dr_2\, V(r_1 - r_2)\, \Psi_{\sigma_1}^\dagger(r_1)\Psi_{\sigma_2}^\dagger(r_2)\Psi_{\sigma_2}(r_2)\Psi_{\sigma_1}(r_1)$.
8. Consider the one-dimensional tight-binding model ($t > 0$)
   $$\hat{H} = -t\sum_i \left(c_i^\dagger\, c_{i+1} + \mathrm{h.c.}\right), \tag{3}$$
   with periodic boundary conditions $c_{N_s+1} = c_1$, describing the hopping of electrons on a lattice of N_s sites with lattice spacing a. Diagonalize the hamiltonian by going to the Fourier space and show that the eigenenergies are given by
   $$\varepsilon_k = -2t\cos(ka).$$
   What are the admissible values for the wavevector k ?

9. The local density operator is given for a single particle by $\hat{\rho}(\mathbf{r}) = |\mathbf{r}\rangle\langle\mathbf{r}|$. Give the expression of $\hat{\rho}(\mathbf{r})$ in second quantization in a given basis $|\varphi_\lambda\rangle$ of one-particle states. Give $\hat{\rho}(\mathbf{r})$ in the basis of position states $|\mathbf{r}\rangle$. In the basis of momentum states $|\mathbf{k}\rangle$, give $\hat{\rho}(\mathbf{r})$ and then its Fourier transform
$$\hat{\rho}(\mathbf{q}) = \int d\mathbf{r}\, \hat{\rho}(\mathbf{r}) e^{-i\mathbf{q}\cdot\mathbf{r}}$$

2 Spin operator

We consider fermions with spin 1/2. We denote by $\alpha =\uparrow,\downarrow$ the spin component. The spin operator of the many-body system assumes the form

$$\hat{\mathbf{S}} = \sum_\lambda c^\dagger_{\lambda\alpha'} \frac{\sigma_{\alpha'\alpha}}{2} c_{\lambda\alpha} \tag{4}$$

where $\sigma = (\sigma_x, \sigma_y, \sigma_z)$ is a vector composed by the standard Pauli matrices [1], and λ denotes the set of additional quantum numbers (wavevector, lattice site index, etc).

1. Forget about spin for one moment and consider a finite Hilbert space with N one-particle states. We use the notation $c^\dagger = (c^\dagger_1, c^\dagger_2, \ldots, c^\dagger_N)$ as a vector with N entries. Prove the following identity
$$[c^\dagger\, A\, c, c^\dagger\, B\, c] = c^\dagger\, [A, B]\, c$$
where A and B are $N \times N$ matrices.
2. Use the previous result to show that the spin operator in Eq. (4) satisfies the commutation relations of the Lie group SU(2).
3. Can we say something specific about $\hat{\mathbf{S}}^2$?
4. Give the spin raising and lowering operators $\hat{S}^\pm = \hat{S}_x \pm i\hat{S}_y$ in terms of creation and annihilation operators.

We take the Hubbard model in the atomic limit : a single site governed by the hamiltonian

$$\hat{H} = \varepsilon_d(\hat{n}_\uparrow + \hat{n}_\downarrow) + U\, \hat{n}_\uparrow \hat{n}_\downarrow$$

where $\hat{n}_\sigma = d^\dagger_\sigma d_\sigma$.

5. Give the size of the corresponding Hilbert space.
6. Diagonalize the hamiltonian.
7. Precise the spin for each eigenstate.

3 Hartree-Fock

We consider a gas of N electrons with spin 1/2. The hamiltonian includes kinetic and Coulomb energies, $\hat{H} = \hat{T} + \hat{V}$ or

$$\hat{H} = \sum_{\sigma,\mathbf{k}} \varepsilon_k\, c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \frac{1}{2V} \sum_{\sigma_1,\sigma_2} \sum_{\mathbf{q},\mathbf{k}_1,\mathbf{k}_2} \frac{e^2}{\varepsilon_0\, q^2}\, c^\dagger_{\mathbf{k}_1+\mathbf{q},\sigma_1} c^\dagger_{\mathbf{k}_2-\mathbf{q},\sigma_2} c_{\mathbf{k}_2,\sigma_2} c_{\mathbf{k}_1,\sigma_1}. \tag{5}$$

This hamiltonian can not be diagonalized. We shall therefore treat the Coulomb interaction $\hat{V}$ in perturbation theory.

1. What is the ground state of the system in the absence of $\hat{V}$?

1.
$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

2. Show that the correction to the ground state energy, to leading order in $\hat{V}$, has two contributions : a direct Hartree term, which in this case is infinite, and an exchange Fock term.
3. Compute the Fock term using the identity

$$\mathcal{V}_q = \sum_{\mathbf{k}} \theta[\varepsilon_F - \varepsilon_{\mathbf{k}}]\theta[\varepsilon_F - \varepsilon_{\mathbf{k+q}}] = \frac{4\pi k_F^3}{3}\left[1 - \frac{3}{4}\frac{q}{k_F} + \frac{1}{16}\left(\frac{q}{k_F}\right)^3\right] \qquad \text{for} \quad |\mathbf{q}| < 2k_F$$

and zero for $|\mathbf{q}| \geq 2k_F$. Find the result

$$\frac{\delta E}{V} = -\frac{k_F^4}{4\pi^3}\frac{e^2}{4\pi\varepsilon_0}.$$

4 Finite temperature and thermodynamics

We recall that the partition function Z in the grand canonical ensemble is given by

$$Z = \mathrm{Tr} e^{-\beta(\hat{H} - \mu\hat{N})}$$

where the trace is taken over all states of the many-body Hilbert space. μ denotes here the chemical potential. The mean value of an operator $\hat{O}$ acting in the many-body Hilbert space is then given by

$$\langle\hat{O}\rangle = \frac{1}{Z}\,\mathrm{Tr}\left[\hat{O}\, e^{-\beta(\hat{H} - \mu\hat{N})}\right].$$

1. Suppose that the hamiltonian is diagonal in the occupation number for some particular one-particle basis,

$$\hat{H} = \sum_{\lambda} \varepsilon_\lambda \hat{n}_\lambda.$$

This implies in passing that particles are independent, *i.e.* not interacting. Show that the partition function factorizes as $Z = \prod_\lambda Z_\lambda$.
2. Give the expression of Z_λ for fermions and for bosons.
3. Compute $\langle\hat{n}_\lambda\rangle$ for fermions and for bosons. Which distributions do we find ?