Advanced Quantum Mechanics of Many-Body Systems
Homework 6

(6 Jan 2025)

Problem 1

Reconsider the problem analyzed in the lecture, concerning the mean-field treatment of the Hamiltonian $\sum_{i,j,\sigma} T_{ij} a^\dagger_{i\sigma} a_{j\sigma} + \frac{1}{2} U \sum_{i\sigma} n_{i\sigma} n_{i-\sigma}$. Assume however that the spatial dimensionality $d = 2$. When convenient, restrict to temperature $T = 0$ and approximate the dispersion by a form quadratic in k. Follow the reasoning from the lecture. Discuss the possibility of obtaining a ferromagnetic ground state. Where do the differences between $d = 2$ and $d = 3$ appear?

Problem 2

For a two-dimensional non-interacting gas of $N \gg 1$ electrons contained in a large square box of area A and at temperature $T > 0$:

(a) Write down the equation of motion for the one-electron retarded Green's function $G^{ret}_{\vec{k},\sigma}(E)$ and solve it. Obtain also $G^{ret}_{\vec{k},\sigma}(t - t')$.

(b) Write down an expression for the electronic spectral density $S_{\vec{k},\sigma}(E)$.

(c) Find an expression for the chemical potential $\mu(T, n)$, where $n = N/A$.

(d) Find an expression for the Fermi energy $\epsilon_F(n)$.

Hints: $\int_{-\infty}^{\infty} dx e^{-xt} \frac{1}{x+i0^+} = -2\pi i \theta(t)$, $-\frac{d}{dx}\left(\ln(1 + ze^{-x})\right) = \frac{1}{e^x z^{-1}+1}$.

Problem 3

Quantized vibrations of an ionic lattice are described in terms of a non-interacting phonon gas: $H = \sum_{\vec{q},\lambda} \hbar\omega_\lambda(\vec{q}) \left(a^\dagger_{\vec{q},\lambda} a_{\vec{q},\lambda} + \frac{1}{2} \right)$ with zero chemical potential μ. We define a one-phonon Green's function $G^\alpha_{\vec{q},\lambda}(t, t') = \langle\langle a_{\vec{q}\lambda}(t); a^\dagger_{\vec{q}\lambda}(t')\rangle\rangle^\alpha$, where $\alpha \in \{ret,\, adv\}$.

a) Find $G^\alpha_{\vec{q},\lambda}(E)$.

b) Find $G^\alpha_{\vec{q},\lambda}(t, t')$.

c) Find the internal energy U.

Problem 4

Consider a simple model of a hydrogen molecule defined by the Hamiltonian $H = \epsilon_0 \left(c^\dagger_1 c_1 + c^\dagger_2 c_2 \right) + t c^\dagger_2 c_1 + t^* c^\dagger_1 c_2$, where c_i $(i \in \{1, 2\})$ is an operator annihilating an electron at orbital $1s$ of the i-th atom, while ϵ_0 and t are constants.

We define the two retarded Green's functions:

$$G^{ret}_{11}(t) = -i\theta(t)\langle[c_1(t), c^\dagger_1]_+\rangle \quad \text{and} \quad G^{ret}_{21}(t) = -i\theta(t)\langle[c_2(t), c^\dagger_1]_+\rangle.$$

a) Derive the equations of motion for $G^{ret}_{11}(t)$ and $G^{ret}_{21}(t)$.

b) Fourier transform the obtained set of equations using $G(\omega + i\eta) = \int_{-\infty}^{\infty} dt e^{i(\omega+i\eta)t} G(t)$ $(\eta > 0)$ and find $G^{ret}_{11}(\omega + i\eta)$. Assuming the free retarded Green's function is given by $G^{ret}_{11,0}(\omega + i\eta) = (\omega + i\eta - \epsilon_0)^{-1}$ find the retarded self-energy $\Sigma_{11}(\omega + i\eta)$.

c) Using the obtained form of $G^{ret}_{11}(\omega + i\eta)$ find the corresponding spectral function $S(\omega + i\eta)$. Perform the limit $\eta \to 0^+$.