TFY4210/FY8302 Quantum Theory of Solids

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This problem set constitutes the final exam for TFY4210/FY8302 Quantum Theory of Solids. Together with this document, you should have received an EXAMINATION PAPER via the INSPERA digital system. Please read that carefully before proceeding as it explains the rules and expectations for this examination.

Problem 1: Tight-binding model (Points: 10+10+5+10+5 = 40)

Consider a two-dimensional square lattice with dimensions $L \times L$. We take the lattice constant to be $a = 1$, so there are in total $N = L^2$ lattice sites. There is one atomic orbital at each lattice site, where each orbital can contain up to two electrons with opposite spins. To describe the spin-σ electron state at lattice site i, we use the usual creation operator $c_{i\sigma}^\dagger$ and annihilation operator $c_{i\sigma}$. In terms of these second-quantized operators, we consider the tight-binding Hamiltonian

$$\mathcal{H} = -\mu \sum_{i\sigma} c_{i\sigma}^\dagger c_{i\sigma} - t \sum_{\langle ij\rangle\sigma} c_{i\sigma}^\dagger c_{j\sigma} - h \sum_i (c_{i\uparrow}^\dagger c_{i\uparrow} - c_{i\downarrow}^\dagger c_{i\downarrow}), \tag{1}$$

where t is the nearest-neighbor hopping amplitude, μ is the chemical potential, and h is an exchange splitting.

(a) We will now introduce the Fourier-transformed operators

$$c_{\boldsymbol{k}\sigma}^\dagger = \frac{1}{\sqrt{N}} \sum_i c_{i\sigma}^\dagger \exp(-i\boldsymbol{k}\cdot\boldsymbol{r}_i), \quad c_{\boldsymbol{k}\sigma} = \frac{1}{\sqrt{N}} \sum_i c_{i\sigma} \exp(+i\boldsymbol{k}\cdot\boldsymbol{r}_i), \tag{2}$$

where $\boldsymbol{r}_i$ is the location of lattice site i. Show that the provided Hamiltonian can then be written purely in terms of the number operators $n_{\boldsymbol{k}\sigma} = c_{\boldsymbol{k}\sigma}^\dagger c_{\boldsymbol{k}\sigma}$,

$$\mathcal{H} = \sum_{\boldsymbol{k}\sigma} E_{\boldsymbol{k}\sigma} n_{\boldsymbol{k}\sigma}, \tag{3}$$

and derive a closed analytical expression for the excitation energy $E_{\boldsymbol{k}\sigma}$.

(b) Show that to order $\mathcal{O}(\boldsymbol{k}^2)$, the dispersion relation can be approximated as free electrons with an effective mass m^*. Sketch the two curves $E_{\boldsymbol{k}\uparrow}$ and $E_{\boldsymbol{k}\downarrow}$ as functions of $|\boldsymbol{k}|$, and comment on the physical interpretation of h.

(c) Write an expression for the expectation value $\langle n_{\boldsymbol{k}\sigma}\rangle$ for the number of electrons with quantum numbers $(\boldsymbol{k}, \sigma)$. Express your answer in terms of $E_{\boldsymbol{k}\sigma}$.

(d) If we collect the annihilation operators $c_{i\sigma}$ at every lattice site into a single vector $\boldsymbol{c} = (c_{1\uparrow}, c_{1\downarrow}, \ldots, c_{N\uparrow}, c_{N\downarrow})$, we can rewrite eq. (1) in matrix form:

$$\mathcal{H} = \boldsymbol{c}^\dagger \boldsymbol{H} \boldsymbol{c}. \tag{4}$$

Write an explicit expression for the elements $H_{i\sigma,j\sigma'}$ of the resulting matrix. [Hint: You may want to first express i in terms of 2D coordinates (x_i, y_i), and then express $H_{i\sigma,j\sigma'}$ in terms of these coordinates.]

(e) Let us now consider the density of states of the system, which we define as

$$D(E) = \frac{1}{N} \sum_n \delta(E - E_n), \tag{5}$$

where $\{E_n\}$ are the excitation energies of the system. Explain (briefly!) how one can numerically calculate the density of states. This includes (i) how to determine $\{E_n\}$ and (ii) how to evaluate $\sum_n \delta(E - E_n)$ afterwards.

Problem 2: Heisenberg model (Points: 5+10+10+5 = 30)

Consider a system of localized spins on a two-dimensional square lattice with lattice constant $a = 1$. The spin at lattice site i is denoted $\boldsymbol{S}_i$, and the magnitude of each spin is given by $\boldsymbol{S}_i^2 = S^2$. This system can be described via the model

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} \boldsymbol{S}_i \cdot \boldsymbol{S}_j, \tag{6}$$

where the exchange parameter J is a non-zero real number.

(a) Sketch the classical ground state of the system for (i) $J > 0$ and (ii) $J < 0$. How do the ground states change in a quantum-mechanical treatment?

(b) We now focus on the case $J > 0$. Use a leading-order Holstein–Primakoff transformation to express $\mathcal{H}$ in terms of the bosonic operators a_i and $a_i^\dagger$.

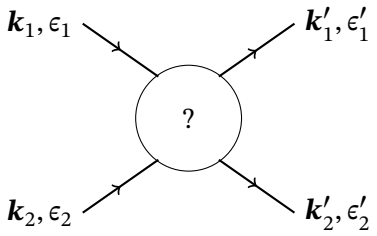
(c) Fourier-transform the bosonic operators a_i and $a_i^\dagger$, and show that this diagonalizes the Hamiltonian in the form $\mathcal{H} = E_0 + \sum_{\boldsymbol{q}} E_{\boldsymbol{q}} n_{\boldsymbol{q}}$ where $n_{\boldsymbol{q}} = a_{\boldsymbol{q}}^\dagger a_{\boldsymbol{q}}$.

(d) Write an expression for the expectation value $\langle n_{\boldsymbol{q}} \rangle$ for the number of magnons with wave vector $\boldsymbol{q}$ at any given time. Express your answer in terms of $E_{\boldsymbol{q}}$.

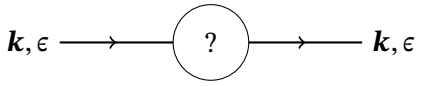
Problem 3: Feynman diagrams (Points: 5+5+5+10+5 = 30)

In this problem, we will consider the Feyman diagram method of performing perturbative calculations for systems with weak electron–phonon interactions. For this exercise, you might want to consult the attached list of Feynman rules.

(a) Sketch all diagrams up to order $\mathcal{O}(g^4)$ that contribute to electron–electron scattering. Draw each relevant diagram with the external legs.



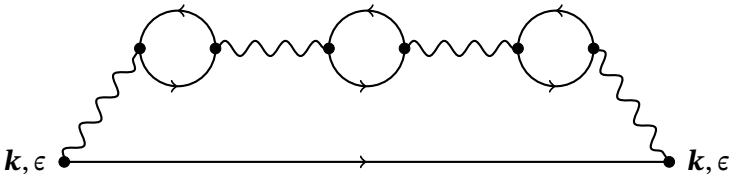
(b) Sketch all diagrams up to order $\mathcal{O}(g^4)$ that contribute to the interacting electron propagator $G(\boldsymbol{k}, \epsilon)$. Include all diagrams, not just the ones that contribute to the electron self-energy. Draw them with the external legs.



(c) Explain using diagrams why we only have to include amputated one-particle irreducible diagrams in the electron self-energy $\Sigma(\epsilon, \boldsymbol{k})$. [Hint: Expand the Dyson equation $G = G_0(1 - \Sigma G_0)^{-1}$ to $\mathcal{O}(\Sigma^2)$ and sketch relevant terms.]

(d) We now focus on the lowest-order contribution to the electron self-energy Σ: the $\mathcal{O}(g^2)$ contribution. Write down the integral representation of this Feynman diagram, perform the energy integration explicitly, and show that the result can be written $\Sigma(\boldsymbol{k}, \epsilon) = \sum_{\boldsymbol{q}} |g_{\boldsymbol{q}}|^2 \, I(\epsilon, \boldsymbol{k}, \boldsymbol{q})$ for some function I.

(e) Consider now the following higher-order contribution to $\Sigma(\boldsymbol{k}, \epsilon)$. Write down the integral representation of this diagram. (Note: You do not have to perform any integration in this task. Moreover, you can express the results in terms of G_0 and D_0; there is no need to insert their definitions here.)



Equations

The meaning and validity of each symbol and equation is assumed to be known. The equations are in natural units $\hbar = k_B = 1$, which you can use throughout this exam.

- Bosons:

$$[a_\lambda, a_{\lambda'}] = 0, \qquad [a_\lambda, a_{\lambda'}^\dagger] = \delta_{\lambda,\lambda'}, \qquad [a_\lambda^\dagger, a_{\lambda'}^\dagger] = 0.$$

- Fermions:

$$\{c_\lambda, c_{\lambda'}\} = 0, \qquad \{c_\lambda, c_{\lambda'}^\dagger\} = \delta_{\lambda,\lambda'}, \qquad \{c_\lambda^\dagger, c_{\lambda'}^\dagger\} = 0.$$

- Spins:

$$[S_n, S_m] = \sum_\ell i\epsilon_{nm\ell} S_\ell, \qquad [S_z, S_\pm] = \pm S_\pm, \qquad S_\pm = S_x \pm iS_y.$$

- Pauli matrices:

$$\boldsymbol{\sigma} = \sigma_1 \boldsymbol{e}_x + \sigma_2 \boldsymbol{e}_y + \sigma_3 \boldsymbol{e}_z, \qquad (\boldsymbol{a}\cdot\boldsymbol{\sigma})(\boldsymbol{b}\cdot\boldsymbol{\sigma}) = (\boldsymbol{a}\cdot\boldsymbol{b})\sigma_0 + i(\boldsymbol{a}\times\boldsymbol{b})\cdot\boldsymbol{\sigma};$$

$$\sigma_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ +i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} +1 & 0 \\ 0 & -1 \end{pmatrix}.$$

- Dirac delta function:

$$\int \mathrm{d}x\, f(x)\,\delta(x - x') = f(x'), \qquad \lim_{\eta\to 0^+} \frac{\eta}{\eta^2 + x^2} = \pi\delta(x).$$

- Kronecker deltas:

$$\sum_{n=1}^{N} f_n \delta_{n,m} = f_m, \qquad \sum_{n=1}^{N} \exp[i(\boldsymbol{k} - \boldsymbol{k}')\cdot\boldsymbol{r}_n] = N\delta_{\boldsymbol{k},\boldsymbol{k}'}.$$

- Holstein–Primakoff transformation:

$$S_{i+} = \sqrt{2S - a_i^\dagger a_i}\; a_i, \qquad S_{i-} = a_i^\dagger \sqrt{2S - a_i^\dagger a_i}, \qquad S_{iz} = S - a_i^\dagger a_i.$$

- Fermi–Dirac and Bose–Einstein statistics:

$$f_{\mathrm{FD}}(E) = \frac{1}{\exp(E/T) + 1}, \qquad f_{\mathrm{BE}}(E) = \frac{1}{\exp(E/T) - 1}.$$

- Residue integration:

$$\lim_{r\to\infty} \oint_{\Gamma(r)} \mathrm{d}z \left(\frac{1}{z - \alpha + i0^+} \cdot \frac{1}{z - \beta + i0^+} \right) = 0,$$

$$\lim_{r\to\infty} \oint_{\Gamma(r)} \mathrm{d}z \left(\frac{1}{z - \alpha + i0^+} \cdot \frac{1}{z - \beta - i0^+} \right) = \frac{2\pi i}{\beta - \alpha},$$

$$\lim_{r\to\infty} \oint_{\Gamma(r)} \mathrm{d}z \left(\frac{1}{z - \alpha - i0^+} \cdot \frac{1}{z - \beta + i0^+} \right) = \frac{2\pi i}{\alpha - \beta},$$

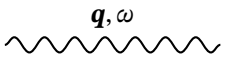
$$\lim_{r\to\infty} \oint_{\Gamma(r)} \mathrm{d}z \left(\frac{1}{z - \alpha - i0^+} \cdot \frac{1}{z - \beta - i0^+} \right) = 0.$$

  The contour $\Gamma(r)$ goes from $z = -r$ to $z = +r$ along the real line, and then follows the path $z = re^{i\theta}$ in the complex plane from $\theta = 0$ to $\theta = \pi$.

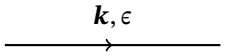
Feynman rules

To order $\mathcal{O}(g^{2n})$ in the electron–phonon interaction $g_{\boldsymbol{q}}$, the Feynman rules are:

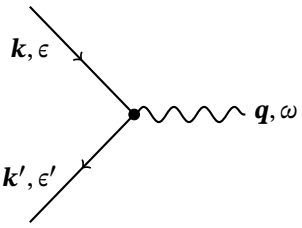
- Draw all topologically distinct diagrams with at most $2n$ vertices. Remember that only amputated one-particle irreducible diagrams contribute to self-energies.
- For each line and vertex that appears in a diagram, assign the following factors:



$$D_0(\boldsymbol{q},\omega) = \frac{1}{\omega - \omega_{\boldsymbol{q}} + i0^+} - \frac{1}{\omega + \omega_{\boldsymbol{q}} - i0^+}$$



$$G_0(\boldsymbol{k},\epsilon) = \frac{\theta(\epsilon_{\boldsymbol{k}} - \epsilon_F)}{\epsilon - \epsilon_{\boldsymbol{k}} + i0^+} + \frac{\theta(\epsilon_F - \epsilon_{\boldsymbol{k}})}{\epsilon - \epsilon_{\boldsymbol{k}} - i0^+}$$



$g_{\boldsymbol{q}}$

- Ensure that momentum and energy is conserved at each vertex. In some cases, the results can afterwards be further simplified using $g_{-\boldsymbol{q}} = g^*_{+\boldsymbol{q}}$.
- Give each diagram a prefactor $i^n(-2)^\ell$, where n comes from the order $\mathcal{O}(g^{2n})$ of the diagram and ℓ is the number of closed electron loops in the diagram.
- Integrate or sum over all internal energy and momentum variables. Each energy integral that is introduced in this process comes with a prefactor $1/2\pi$.

When evaluating Feynman integrals, you are allowed to assume without proof that the entire integrand vanishes at complex infinity.