Problem set 3 - Many-body theory SFI7534

1. **Peierls instability.** Consider a model of one-dimensional array of coupled quantum Harmonic Oscillators given by

$$H_0 = \sum_{i=1}^{L} \frac{p_i^2}{2m} + \frac{k}{2}\left(Q_i - Q_{i+1}\right)^2 .$$

   (a) Compute the corresponding phonon spectrum.

   (b) Now let us consider the model in which electrons hop around that lattice. Consider also that the hopping constant depends on the distance between the ions. Therefore,

$$H = H_0 - t\sum_i \left[1 + \alpha\left(Q_i - Q_{i+1}\right)\right]\left(c_i^\dagger c_{i+1} + \text{h.c.}\right),$$

   where α is a small constant. For simplicity, disregard the spin degree of freedom [1], i.e., $c_i^\dagger$ (c_i) creates (annihilates) spinless fermions at the ith site. This is the Su-Schrieffer-Heeger (SSH) model for the Poly-acetylene. Obtain the electron-phonon coupling in terms of the creation and annihilation operators of fermions and phonons in the momentum Eigenstates. Notice that the scattering amplitude $g_{k,q}$ depend on the electron and on the phonon momenta.

   (c) In the case of half-filling (number of electrons $N = \frac{1}{2}L$), show that the ground state breaks the lattice translational symmetry, i.e.,

$$\langle Q_{j+1} - Q_j\rangle = q_0\left(-1\right)^j ,$$

   where q_0 is a constant. This is the so-called Peierls instability.

   (d) In the SSH model, replace the ions position by their ground-state average value and neglect their kinetic energy. Then compute the electronic dispersion of the resulting model (for $q_0 \neq 0$) and show it is an insulator for half-filling.

2. **Interacting bosons.** In the Bogoliubov theory for superfluidity, the order parameter is $\psi = \left\langle b_0 \right\rangle = \left\langle b_0^\dagger \right\rangle = \sqrt{N_0}$, where N_0 is the number of boson in the $k = 0$ state. This parameter has to be computed self-consistently.

   (a) Compute the parameter $\theta_{\mathbf{k}}$ of the Bogoliubov transformation that diagonalizes the corresponding mean-field Hamiltonian.

   (b) Use this result to compute the number of bosons out of the condensate

$$\Delta N = N - N_0 = \sum_{\mathbf{k}\neq 0}\left\langle \text{GS}\left| a_{\mathbf{k}}^\dagger a_{\mathbf{k}} \right| \text{GS}\right\rangle ,$$

   where $|\text{GS}\rangle$ is the ground state of the Bogoliubov bosons. Write your answer in the thermodynamic limit (where the sum is replaced by an integral) as an implicit equation for the condensate density N_0/V as a function of the density N/V, the particle mass m, the dispersion $\epsilon_k = \frac{k^2}{2m}$, and the interaction $\tilde{v}_{\mathbf{k}}$.

   (c) Assuming that $\tilde{v}_{k\to 0} = v_0 > 0$, show that ΔN diverges in one dimension. It means that no long-range superfluid order is possible even at $T = 0$ for finite repulsive interactions in $d = 1$.

   (d) Compute the integral in 2b numerically in the case of $d = 3$ and $\tilde{v}_k = g = \text{const}$ (meaning contact interactions). Make plots for N_0/V and N/V as a function of g.

3. **Fano model.** Consider the noninteracting Anderson impurity model

$$H = E_f \sum_\sigma f_\sigma^\dagger f_\sigma + \sum_{i,j,\sigma} t'_{i,j}\left(c_{i,\sigma}^\dagger c_{j,\sigma} + \text{h.c.}\right) + \sum_{i,\sigma} t_i\left(c_{i,\sigma}^\dagger f_\sigma + \text{h.c.}\right),$$

where $c_{i,\sigma}$ and f_σ are usual spin-1/2 fermionic operators.

(a) Give the physical meaning of each term in this Hamiltonian.

(b) In Fourier space, this Hamiltonian becomes

$$H = E_f \sum_{\sigma} f_{\sigma}^{\dagger} f_{\sigma} + \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} c_{\mathbf{k},\sigma}^{\dagger} c_{\mathbf{k},\sigma} + \sum_{\mathbf{k},\sigma} \left(t_{\mathbf{k}} c_{\mathbf{k},\sigma}^{\dagger} f_{\sigma} + \text{h.c.} \right), \tag{1}$$

which can be diagonalized in terms of the fermions

$$d_{n,\sigma}^{\dagger} = \sum_{\mathbf{k}} \alpha_{n,\mathbf{k}} c_{\mathbf{k},\sigma}^{\dagger} + \beta_n f_{\sigma}^{\dagger}, \tag{2}$$

where $\sum_{\mathbf{k}} |\alpha_{n,\mathbf{k}}|^2 + |\beta_n|^2 = 1$. The resulting Hamiltonian is thus

$$H = \sum_{n,\sigma} E_n d_{n,\sigma}^{\dagger} d_{n,\sigma} + \text{const.} \tag{3}$$

Compute the commutators of $c_{k,\sigma}$ and f_{σ} with the Hamiltonian in (1) and of $d_{n,\sigma}$ with the Hamiltonian in (3). Then use Eq. (2) to relate these commutators and find a set of linear equations for $\alpha_{n,\mathbf{k}}$ and β_n.

(c) Consider the operator

$$G(\omega - i\eta) = \frac{1}{\hbar(\omega - i\eta) - H}, \text{ with } \eta \to 0^+,$$

which is diagonal in the single-particle Eigenbasis of H: $\{|n,\sigma\rangle\} = \left\{ d_{n,\sigma}^{\dagger} |0\rangle \right\}$; i.e.,

$$G_{n,\sigma;m,\tau}(\omega - i\eta) = \langle n,\sigma| \frac{1}{\hbar(\omega - i\eta) - H} |m,\tau\rangle = \frac{\delta_{n,m}\delta_{\sigma,\tau}}{\hbar(\omega - i\eta) - E_n}.$$

Moreover, in any basis

$$\sum_{l} (\hbar(\omega - i\eta) - H)_{m,l} G_{l,n} = \delta_{m,n},$$

which is simply $(\hbar(\omega - i\eta) - H) G = \mathbb{I}$. Use the nondiagonal basis $\{|\mathbf{k},\sigma\rangle, |f,\sigma\rangle\}$ to show that

$$\begin{aligned}
(\Omega - E_f) G_{f,\sigma;f,\sigma} - \sum_{\mathbf{k}} t_{\mathbf{k}}^{*} G_{\mathbf{k},\sigma;f,\sigma} &= 1, \\
(\Omega - \epsilon_{\mathbf{k}}) G_{\mathbf{k},\sigma;f,\sigma} - t_{\mathbf{k}} G_{f,\sigma;f,\sigma} &= 0, \\
(\Omega - E_f) G_{f,\sigma;\mathbf{k},\sigma} - \sum_{\mathbf{q}} t_{\mathbf{q}}^{*} G_{\mathbf{q},\sigma;\mathbf{k},\sigma} &= 0, \\
(\Omega - \epsilon_{\mathbf{q}}) G_{\mathbf{q},\sigma;\mathbf{k},\sigma} - t_{\mathbf{q}} G_{f,\sigma;\mathbf{q},\sigma} &= \delta_{\mathbf{k},\mathbf{q}},
\end{aligned}$$

where $\Omega = \hbar(\omega - i\eta)$.

(d) Compute $G_{f,\sigma;f,\sigma}$.

(e) Show that the impurity spectral function (the hybridization of the f level with the system Eigenlevels with energy $\hbar\omega$) given by

$$A_f(\omega) \equiv \sum_{n} |\langle n,\sigma|f,\sigma\rangle|^2 \delta(E_n - \hbar\omega),$$

is related to G via

$$A_f(\omega) = \frac{1}{\pi} \lim_{\eta \to 0^+} \text{Im}\left(G_{f,\sigma;f,\sigma}(\omega - i\eta)\right).$$

(f) Assuming that $t_i = t\delta_{i,0}$ (i.e., $t_{\mathbf{k}} = t$), that the density of states is a constant, i.e.,

$$\rho(\omega) \equiv \sum_{\mathbf{k}} \delta(\epsilon_{\mathbf{k}} - \hbar\omega) = \rho_0 \theta(D - |\hbar\omega|),$$

with $\rho_0 = 1/(2D)$ (with D being the half bandwidth), and that $|t| \ll D$, show that the spectral function A_f is approximately a Lorentzian of width $\Gamma = \pi\rho_0 t^2$ peaked at E_f.

4. **1D Kondo effect.** Consider a spin-1/2 impurity interacting with a one-dimensional electron gas according to the following Hamiltonian

$$H = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} + \frac{J}{L}\mathbf{S} \cdot \sum_{\mathbf{k},\mathbf{q}} \sum_{\alpha,\beta} c^\dagger_{\mathbf{k},\alpha} \left(\frac{\boldsymbol{\sigma}_{\alpha,\beta}}{2}\right) c_{\mathbf{k},\beta},$$

where $c^\dagger_{\mathbf{k},\sigma}$ ($c_{\mathbf{k},\sigma}$) creates (annihilates) a plane-wave-like electron in a ring of length L with spin projection σ in the z-basis. The Kondo effect can be understood as the formation of a singlet between the magnetic impurity and a conduction electron in the limit of low energies. The energy scale for this bound state (which also controls the divergences of the perturbation theory) can be estimate via a variational method.

(a) Consider the variational state

$$|\Phi\rangle = \sum_{k>k_F} f(k) \left[c^\dagger_{\mathbf{k},\uparrow} |\text{FS}\rangle \otimes |\Downarrow\rangle - c^\dagger_{\mathbf{k},\downarrow} |\text{FS}\rangle \otimes |\Uparrow\rangle\right],$$

where $f(k)$ is the variational function to be determined, $|\text{FS}\rangle = \prod_{k\leq k_F} c^\dagger_{\mathbf{k},\uparrow} c^\dagger_{\mathbf{k},\downarrow} |0\rangle$ is the Fermi sea state, and $|\Uparrow\rangle$ and $|\Downarrow\rangle$ are the states of the impurity in the S^z basis. Provide a physical motivation of the variational state $|\Phi\rangle$.

(b) Minimizing $E = \langle \Phi |H| \Phi\rangle / \langle\Phi|\Phi\rangle$ as a functional of $f(k)$, show that

$$f(k) = \frac{3J}{4L} \times \frac{\sum_{q>k_F} f(q)}{E_{\text{FS}} + \epsilon_k - E}, \tag{4}$$

where $E_{\text{FS}} = 2\sum_{k<k_F} \epsilon_k$.

(c) Sum over $k > k_F$ in both sides of Eq. (4) and take the thermodynamic limit $L = \infty$. The resulting integral determines the variational energy E. In the limits of weak interaction and low energies, we can approximate $\epsilon_k \approx E_F + v_F (k - k_F)$ (where v_F is the Fermi velocity) and integrate only over the states such that $|\epsilon_k - E_F| < D$ (where D is an energy scale of the order of the bandwidth). Perform the integration and obtain the resulting expression for E.

(d) Using that $J \ll v_F$ (the weak interacting limit), show that $E = E_{\text{FS}} + E_F - E_b$ with the binding energy

$$E_b \approx E e^{-\frac{4}{3J\rho_F}},$$

with $\rho_F = (\pi v_F)^{-1}$ being the density of states at the Fermi energy. Why E_b is called a binding energy?

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[1] Actually, the Peierls instability depends on whether the fermions are spinful or spinless. See Fradkin and Hirsch, Phys. Rev. B 27, 1680 (1983).