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Advanced Statistical Physics - Problem Set 4

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Due Date: Tuesday, May 8, 09:15 a.m., mailbox inside ITP

Internet: Advanced Statistical Physics exercises

5. The Néel state

4 + 4 + 4 + 4 Points

In this problem set, you will learn about antiferromagnetism in a half filled lattice model with

$$\langle \hat{n}(\boldsymbol{r}_j) \rangle = \sum_\sigma \langle \hat{\psi}^\dagger_\sigma(\boldsymbol{r}_j) \hat{\psi}_\sigma(\boldsymbol{r}_j) \rangle = 1$$

for every lattice site $\boldsymbol{r}_j$. In the following, we consider a 2D square lattice with lattice constant $a = 1$.

(a) Before taking interactions into account, let us consider the kinetic energy of electrons hopping between nearest neighbouring sites only. The Hamiltonian is

$$H_0 = -t \sum_\sigma \sum_{\langle \boldsymbol{r}_i, \boldsymbol{r}_j \rangle} \hat{\psi}^\dagger_\sigma(\boldsymbol{r}_i) \hat{\psi}_\sigma(\boldsymbol{r}_j) \ ,$$

with t being the nearest neighbour hopping amplitude, and $\langle \boldsymbol{r}_i, \boldsymbol{r}_j \rangle$ denoting that $\boldsymbol{r}_i$ and $\boldsymbol{r}_j$ are nearest neighbour lattice sites.

Using the Fourier decomposition of the field operators, show that H_0 is diagonal in momentum space and can be expressed as

$$H_0 = \sum_\sigma \sum_{\boldsymbol{k}} \varepsilon(\boldsymbol{k}) \hat{c}^\dagger_{\boldsymbol{k},\sigma} \hat{c}_{\boldsymbol{k},\sigma} \ ,$$

with $\varepsilon(\boldsymbol{k}) = -2t \left[\cos k_x + \cos k_y\right]$. What are the allowed values for $\boldsymbol{k}$ and what is the range of the $\boldsymbol{k}$-summation if we consider a $N \times N$ lattice with periodic boundary conditions? In order to understand the following tasks, sketch the Fermi surface of the 2D square lattice in the first Brillouin zone.

Hint: The Fermi surface Ω is defined as $\Omega = \{\boldsymbol{k}, \varepsilon(\boldsymbol{k}) = \varepsilon_F\}$, with ε_F being the Fermi energy. You might use that $\varepsilon_F = 0$ and

$$\cos x + \cos y = 2 \cos\left(\frac{x+y}{2}\right) \cos\left(\frac{x-y}{2}\right) \ .$$

(b) If the on-site contribution of the Coulomb interaction is dominant, the Hamiltonian is of Hubbard type. Using the identity $\sum_i \sigma^i_{\alpha\beta} \sigma^i_{\gamma\delta} = 2\delta_{\alpha\delta}\delta_{\beta\gamma} - \delta_{\alpha\beta}\delta_{\gamma\delta}$ and neglecting terms renormalizing the chemical potential, the interaction Hamiltonian is given by

$$H_{\text{int}} = -\frac{2U}{3} \sum_{\boldsymbol{r}_j} \left(\hat{\boldsymbol{S}}(\boldsymbol{r}_j) \right)^2 \ .$$

Here, $\hat{S}_i(\boldsymbol{r}) = \frac{1}{2}\sum_{\alpha,\beta}\hat{\psi}^\dagger_\alpha(\boldsymbol{r})\sigma^i_{\alpha\beta}\hat{\psi}_\beta(\boldsymbol{r})$, with σ^i denoting the i-th Pauli matrix is the spin operator in a second quantized notation, and U is the on-site interaction strength. In the following, we want to perform a mean field analysis for the Hubbard Hamiltonian. The mean field decoupling of H_{int} yields

$$H^{\text{MF}}_{\text{int}} = \frac{3}{8U}\sum_{\boldsymbol{r}_j}\Big(\boldsymbol{M}(\boldsymbol{r}_j)\Big)^2 - \sum_{\boldsymbol{r}_j}\boldsymbol{M}(\boldsymbol{r}_j)\cdot\hat{\boldsymbol{S}}(\boldsymbol{r}_j) \ ,$$

with the magnetization $\boldsymbol{M}(\boldsymbol{r}_j)$ given by $\boldsymbol{M}(\boldsymbol{r}_j) = -(4U/3)\langle\hat{\boldsymbol{S}}(\boldsymbol{r}_j)\rangle$.

Show that in momentum space the mean field Hubbard Hamiltonian is given by

$$H^{\text{MF}}_{\text{int}} = \sum_{\boldsymbol{k}}\left[\frac{3}{8U}|\boldsymbol{M}(\boldsymbol{k})|^2 + \boldsymbol{M}^*(\boldsymbol{k})\cdot\hat{\boldsymbol{S}}(\boldsymbol{k})\right] \ ,$$

with $\hat{S}_i(\boldsymbol{q}) = \frac{1}{2}\sum_{\boldsymbol{k}}\sum_{\alpha\beta}\hat{c}^\dagger_{\boldsymbol{k}-\boldsymbol{q},\alpha}\sigma^i_{\alpha\beta}\hat{c}_{\boldsymbol{k},\beta}$ being the spin operator in momentum space.

An antiferromagnetic state is characterized by a magnetization $\boldsymbol{M}(\boldsymbol{r}_j) = \boldsymbol{M}_0\cos(\boldsymbol{Q}\cdot\boldsymbol{r}_j)$, with order parameter momentum $\boldsymbol{Q} = (\pi,\pi)$. Describe the meaning of the vector $\boldsymbol{Q}$ by using your sketch of the Fermi surface from task (a). The vector $\boldsymbol{Q}$ is called the nesting vector. Is there another nesting vector $\boldsymbol{Q}'$ for the 2D square lattice at half filling?

(c) Show that the total mean field Hamiltonian in momentum space is given by

$$\begin{aligned} H^{\text{MF}} &= \frac{3}{8U}M_0^2N^2 + \sum_\sigma\sum_{\boldsymbol{k}}\varepsilon(\boldsymbol{k})\hat{c}^\dagger_{\boldsymbol{k},\sigma}\hat{c}_{\boldsymbol{k},\sigma} \\ &\quad + \frac{1}{4}\sum_{\alpha\beta}\boldsymbol{\sigma}_{\alpha\beta}\cdot\boldsymbol{M}_0\sum_{\boldsymbol{k}}\hat{c}^\dagger_{\boldsymbol{k},\alpha}\hat{c}_{\boldsymbol{k}+\boldsymbol{Q},\beta} + \frac{1}{4}\sum_{\alpha\beta}\boldsymbol{\sigma}_{\alpha\beta}\cdot\boldsymbol{M}_0\sum_{\boldsymbol{k}}\hat{c}^\dagger_{\boldsymbol{k},\alpha}\hat{c}_{\boldsymbol{k}-\boldsymbol{Q},\beta} \ . \end{aligned}$$

In order to find the eigenvalues, we introduce the spinor

$$\hat{\Psi}_\sigma(\boldsymbol{k}) = \begin{pmatrix}\hat{c}_{\boldsymbol{k},\sigma} \\ \hat{c}_{\boldsymbol{k}+\boldsymbol{Q},\sigma}\end{pmatrix} \ .$$

Due to the doubling of degrees of freedom and by using the parity symmetry $\varepsilon(\boldsymbol{k}) = \varepsilon(-\boldsymbol{k})$ of the dispersion relation, we can restrict the range of the $\boldsymbol{k}$-summation to the upper half of the BZ denoted by $I = \{\boldsymbol{k}, -\pi \le k_x \le \pi, 0 \le k_y \le \pi\}$. Show that the Hamiltonian can be recast in the form

$$H^{\text{MF}} = \frac{3}{8U}M_0^2N^2 + \sum_{\sigma\sigma'}\sum_{\boldsymbol{k}\in I}\hat{\Psi}^\dagger_\sigma(\boldsymbol{k})\mathcal{H}_{\sigma\sigma'}(\boldsymbol{k})\hat{\Psi}_{\sigma'}(\boldsymbol{k}) \ ,$$

with

$$\mathcal{H}(\boldsymbol{k}) = \begin{pmatrix}\sigma^0\cdot\varepsilon(\boldsymbol{k}) & \frac{1}{2}\boldsymbol{\sigma}\cdot\boldsymbol{M}_0 \\ \frac{1}{2}\boldsymbol{\sigma}\cdot\boldsymbol{M}_0 & -\sigma^0\cdot\varepsilon(\boldsymbol{k})\end{pmatrix} = \tau^z\otimes\sigma^0\cdot\varepsilon(\boldsymbol{k}) + \tau^x\otimes\boldsymbol{\sigma}\cdot\frac{\boldsymbol{M}_0}{2} \ ,$$

with $\sigma^0 = \mathbb{I}_2$ being the identiy matrix, and τ^x and τ^z being Pauli matrices.

Diagonalize $\mathcal{H}$ and determine its eigenvalues in order to find the spectrum of the Hamiltonian. Show that the system aquires a band gap given by

$$\Delta = |\boldsymbol{M}_0| \equiv M_0 \ .$$

Hint: You may use that $\varepsilon(\boldsymbol{k}+\boldsymbol{Q}) = -\varepsilon(\boldsymbol{k})$. Further, you may want to calculate $\mathcal{H}^2$ first and next determine its eigenvalues. Then, argue how to relate the eigenvalues of $\mathcal{H}$ and $\mathcal{H}^2$. You will come up with the result that there are two eigenvalues $E_\pm(\boldsymbol{k}) = \pm E(\boldsymbol{k})$, which are both doubly degenerate.

(d) For the remainder of this task, we apply the limit $N \to \infty$ and consider the energy per lattice site $\mathcal{E} = E/N^2$, with E being the total energy of the system. Using your result from the previous task, show that $\mathcal{E}$ is given by

$$\mathcal{E} = \frac{3}{8U} M_0^2 - 2 \int\limits_{\substack{0 \le k_i \le \pi \\ k_x + k_y \le \pi}} \frac{d\boldsymbol{k}}{(2\pi)^2}\, E(\boldsymbol{k}) \ .$$

Show that energy minimization leads to the condition

$$\frac{3}{2U} M_0 = \int\limits_{\substack{0 \le k_i \le \pi \\ k_x + k_y \le \pi}} \frac{d\boldsymbol{k}}{(2\pi)^2} \frac{M_0}{\sqrt{\varepsilon(\boldsymbol{k})^2 + \frac{1}{4} M_0^2}} \ .$$

Identify the two possible solutions and find an expression for the gap parameter $\Delta = M_0$ as a function of the interaction strength U and the hopping parameter t in the limit of small Δ.

Hint: The integral is logarithmically divergent in the limit $M_0 \to 0$. In fact, the integral is dominated by contributions with momenta around $k_x + k_y = \pi$. Thus, we make the approximation that

$$\cos\left(\frac{k_x + k_y}{2}\right) \approx \frac{\pi - k_x - k_y}{2} \qquad \text{and} \qquad \cos\left(\frac{k_x - k_y}{2}\right) \approx 1 \ .$$

This allows to compute the integral over occupied momenta by neglecting the actual dependence on $k_x - k_y$. Your result should be

$$\frac{3}{2U} \simeq \frac{1}{2\pi} \frac{1}{2t} \sinh^{-1}\left(\frac{2t\pi}{M_0}\right) .$$

Use this to find an expression for M_0 in the weak coupling limit $U/2t \to 0$.