Final Exam - Statistical Field Theory

January 29, 2018, 13:30 - 16:30

1. For every exercise, it is indicated how many points it is worth. The total exam consists of 10 points.
2. Write your name and initials on every sheet, on the first sheet also your address and your student ID number.
3. Write clearly, unreadable work cannot be corrected.
4. You are NOT allowed to use any kind of books or lecture notes.

Spin-density waves in graphene

1 The model (0.5 pts)

In this exercise, we are going to consider the formation of spin-density waves in graphene doped near the so-called van-Hove singularity, which is characterized by a large peak in the density of states. In undoped graphene, the electrons interact via a long-range Coulomb force. However, if graphene is doped such that the Fermi-energy is near the van-Hove singularity, this interaction is screened and the material can be described by a tight-binding model with a Hubbard term. Above a critical interaction strength U_{crit}, a spin-density-wave phase arises.

Here, we are going to investigate this phase transition in more detail. We will perform a Hubbard-Stratonovitch transformation to derive an effective action in terms of an eight-component matrix, which accounts for charge and spin degrees of freedom in each of the A and B graphene sublattices.

The tight-binding model describing spinful electrons in graphene, including the onsite Hubbard term U is given by

$$\hat{H} = -t \sum_{\langle i,j\rangle,s} \left(a^\dagger_{i,s} b_{j,s} + b^\dagger_{i,s} a_{j,s} \right) + U \sum_{j\in\{A,B\}} c^\dagger_{j,\uparrow} c^\dagger_{j,\downarrow} c_{j,\downarrow} c_{j,\uparrow}, \tag{1}$$

where the operators $c^{(\dagger)}_{j,s}$ represent annihilation (creation) operators for a given spin s ($\uparrow$ or $\downarrow$) and can be either $a^{(\dagger)}_{j,s}$ or $b^{(\dagger)}_{j,s}$, depending on the sublattice label A or B, respectively (see Fig. 1). Furthermore, the first sum involving the hopping parameter t only runs over the nearest neighbors i and j, which is represented by $\langle i,j\rangle$. The lattice constant $a_0 = 1$.

1. (0.5) Write down the corresponding Euclidean action for the a, b (and c) operators in the grand-canonical ensemble for this Hamiltonian. Specify the non-interacting (S_0) and interacting (S_{int}) parts explicitly.

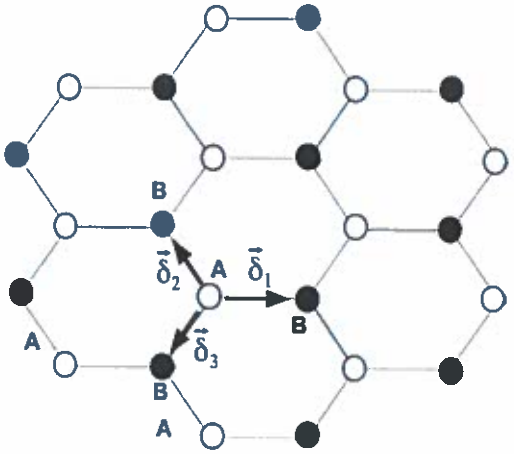

Figure 1: Honeycomb lattice of carbon atoms forming graphene. The empty and filled sites represent the atoms on the two (triangular) sublattices A and B of the honeycomb lattice, while the vectors $\vec{\delta}_i$, with $i = 1, 2, 3$, connect the nearest-neighboring sites.

2 The non-interacting part (3.0 pts)

We first focus on the non-interacting part of the model. Note the specific structure of graphene in Fig. 1.

2. (1.0) Expand the a and b fields in Fourier space,

$$c_{i,s}(\tau) = \frac{1}{\sqrt{N\hbar\beta}} \sum_{\mathbf{k},n} c_{\mathbf{k},n,s} e^{-i\mathbf{k}\cdot\mathbf{r}_i - i\omega_n \tau}, \tag{2}$$

where, again, c can be either an a or b operator, N denotes the number of sites per sublattice, $\omega_n = \pi(2n+1)/\hbar\beta$ are the fermionic Matsubara frequencies, and $\beta = 1/(k_B T)$, and write down the non-interacting action. You might want to use $\gamma_{\mathbf{k}} = \sum_{i=1}^{i=3} \exp[-i\mathbf{k}\vec{\delta}_i]$. In the end, you should obtain an action of the form

$$S_0 = -\sum_{\mathbf{k},n,s} \begin{pmatrix} a^\dagger_{\mathbf{k},n,s} & b^\dagger_{\mathbf{k},n,s} \end{pmatrix} \begin{pmatrix} \mu + i\hbar\omega_n & t\gamma_{\mathbf{k}} \\ t\gamma^*_{\mathbf{k}} & \mu + i\hbar\omega_n \end{pmatrix} \begin{pmatrix} a_{\mathbf{k},n,s} \\ b_{\mathbf{k},n,s} \end{pmatrix} \tag{3}$$

3. (0.5) Determine first the inverse non-interacting Green's function $G^{-1}_{0,\mathbf{k},n,s;\mathbf{k}',n',s'}$ and invert the (2×2) matrix to obtain the non-interacting Green's function $G_{0,\mathbf{k},n,s;\mathbf{k}',n',s'}$.

4. (1.5) If we focus on the (1,2) off-diagonal component of the Green's function, we find

$$G^{(1,2)}_{0,\mathbf{k},n,s;\mathbf{k}',n',s'} = \frac{-\hbar t\gamma_{\mathbf{k}}}{((\mu + i\hbar\omega_n)^2 - t^2|\gamma_{\mathbf{k}}|^2)} \delta_{\mathbf{k},\mathbf{k}'}\delta_{n,n'}\delta_{s,s'}. \tag{4}$$

Perform the Matsubara sum for this component to find an expression for $G^{(1,2)}_{0,\mathbf{k},s;\mathbf{k}',s'}$ in terms of the Fermi-Dirac distribution.

3 Treating the interactions (4.5 pts)

Now, we consider the interacting part. The idea is to rewrite the Hubbard term into electronic- and spin-degrees of freedom and later to integrate out the fermionic a and b operators. We define $c_j^\dagger = (c_{j\uparrow}^\dagger, c_{j\downarrow}^\dagger)$

5. (1.0) Show that the Hubbard term can be rewritten as

$$c_{j,\uparrow}^\dagger c_{j,\downarrow}^\dagger c_{j,\downarrow} c_{j,\uparrow} = \frac{1}{8} n_j^2 - \frac{1}{2} \mathbf{S}_j \cdot \mathbf{S}_j + \frac{1}{4}(c_{j,\uparrow}^\dagger c_{j,\uparrow} + c_{j,\downarrow}^\dagger c_{j,\downarrow}), \tag{5}$$

where $n_j = c_j^\dagger c_j$ is the on-site number operator and $\mathbf{S}_j = (1/2)\sum_{k=x,y,z} c_j^\dagger \sigma_k \hat{e}_k c_j$ describes the spin on the lattice site j, where $\hat{e}_k$ denotes the unit vector and σ_k are the Pauli matrices

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \text{and} \qquad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{6}$$

We absorb the term $\frac{1}{4}(c_{j,\uparrow}^\dagger c_{j,\uparrow} + c_{j,\downarrow}^\dagger c_{j,\downarrow})$ as a shift in the chemical potential and ignore it for the remainder of the exercises.

6. (1.0) Perform a Hubbard-Stratonovich transformation that eliminates these quartic terms in the action. Therefore, we insert an identity

$$I = \mathcal{N}_\rho \int \mathcal{D}[\rho^\alpha] e^{-\frac{1}{2}\sum_j \rho_j^\alpha U^{-1} \rho_j^\alpha}, \tag{7}$$

and

$$I = \mathcal{N}_\mathbf{M} \int \mathcal{D}[\mathbf{M}^\alpha] e^{-\frac{1}{2}\sum_j \mathbf{M}_j^\alpha U^{-1} \mathbf{M}_j^\alpha} \tag{8}$$

for the auxiliary bosonic fields ρ^α and $\mathbf{M}^\alpha$, where α represents the sublattices A and B. Note that $\mathbf{M}^\alpha$ has three components $(M_x^\alpha, M_y^\alpha, M_z^\alpha)$, such that we introduced *eight* auxiliary bosonic fields in this step (one corresponding to the electronic and three to the magnetic degrees of freedom in each sublattice A and B). For the remainder, you may absorb the measures $\mathcal{N}_\rho$ and $\mathcal{N}_\mathbf{M}$ in the measure of the path integral.

Next, apply something like the following transformation (you should still add some additional factor(s)) $\rho_j^\alpha \to \rho_j^\alpha - i n_j^\alpha U$ and $\mathbf{M}_j^\alpha \to \mathbf{M}_j^\alpha - \mathbf{S}_j^\alpha U$ and eliminate the quartic term in S_{int}.

7. (1.5) Find the right Fourier transformation for ρ^α and $\mathbf{M}^\alpha$, such that the action acquires the form below. You might want to use at some point the short-hand notation $k = (\omega_n, \mathbf{k})$ and $r = (\tau, \mathbf{r})$.

$$S_0 + S_{int} = -\hbar \sum_{k,k'} \begin{pmatrix} a_{k,\uparrow}^\dagger & a_{k,\downarrow}^\dagger & b_{k,\uparrow}^\dagger & b_{k,\downarrow}^\dagger \end{pmatrix} \cdot \mathbf{G}_{k,k'}^{-1} \cdot \begin{pmatrix} a_{k',\uparrow} \\ a_{k',\downarrow} \\ b_{k',\uparrow} \\ b_{k',\downarrow} \end{pmatrix}$$
$$+ \frac{U^{-1}}{2} \sum_{k,\alpha} \left[|\mathbf{M}_k^\alpha|^2 + |\rho_k^\alpha|^2 \right]. \tag{9}$$

8. (0.5) Identify the self-energy and explain its physical meaning.

9. (0.5) Integrate out the fermionic fields (perform the path integral in the fermionic fields) and write down the effective action S_{eff}.

4 The phase transition (2.0 pts)

By integrating out the fermionic fields, you obtained a partition function of the form

$$Z = \int d[\mathrm{M}]d[\rho]e^{-S_{\text{eff}}/\hbar}. \tag{10}$$

Now, we introduce the eight-component vector $\mathcal{M}_k = (\rho_k^a, \mathrm{M}_k^a, \rho_k^b, \mathrm{M}_k^b)^{\mathrm{T}}$ for convenience. In order to study the phase transition, we want to determine the spin susceptibility. Therefore, we expand the fields around their mean-field value $\mathcal{M}_k = \langle \mathcal{M}_k \rangle + \delta\mathcal{M}_k$ and demand the linear terms in $\delta\mathcal{M}_k$ to vanish, thus obtaining a self-consistency equation for the mean-field expectation values. This procedure allows us to determine the spin susceptibility χ.

10. (0.5) Why do we need the linear terms to vanish in a mean-field approximation?

A phase change to a spin-density wave occurs when the susceptibility χ diverges, and this happens at a critical value where $0 = \det(\eta\chi^{-1} - U_c)$, where η is some matrix.

11. (0.5) At a critical $U = U_c$, we have a phase transition. Name the difference between a classical and a quantum phase transition and explain which one occurs in graphene near the van-Hove singularity.

12. (1.0) Knowing that this is a 2^{nd}-order phase transition, write the Landau free energy in terms of the order parameter $\mathcal{M}_k$ and discuss the sign of the coefficients in the expansion. Can you relate any of these coefficients to the susceptibility?