Ruward

Midterm Exam - "Statistical Field Theory"

November 4, 2014

1. *Each exercise is worth 1 point.*
2. *Write your name and initials on all sheets, 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.*

Superconductivity in Graphene

Graphene consists of a single layer of carbon atoms arranged on a honeycomb lattice (see Fig. 1). The effective Hamiltonian of graphene is described in terms of two species (flavors) of *electrons*, a, b that live on two different sublattices, A and B. The operators $a^\dagger_{i\sigma}$ create an electron on lattice site i with spin σ on sublattice A, while $b^\dagger_{j\sigma}$ does the same on sublattice B. The Hamiltonian of the system consists of non-interacting and interacting parts,

$$\hat{H} = \hat{H}_t + \hat{H}_I.$$

The non-interacting part of the Hamiltonian is described by the usual nearest-neighbor hopping term (note that nearest-neighboring sites reside on different sublattices; see Fig. 1),

$$\hat{H}_t = -t\sum_\sigma \sum_{\langle ij\rangle} \hat{a}^\dagger_{i\sigma}\hat{b}_{j\sigma} + \text{h.c.}, \tag{1}$$

where $\sigma = \pm 1$ corresponds to spin up ($\uparrow$) and spin down ($\downarrow$). $\langle i, j\rangle$ denotes nearest neighbor sites at $\vec{x}_i$ and $\vec{x}_j$, and h.c. is a shorthand notation for Hermitean conjugate.

The interaction consists of two parts,

$$\hat{H}_I = \hat{H}_I^0 + \hat{H}_I^1.$$

The term $\hat{H}_I^0$ describes the on-site interactions among electrons,

$$\hat{H}_I^0 = \frac{g_0}{2}\sum_\sigma\sum_i \left(\hat{a}^\dagger_{i\sigma}\hat{a}_{i\sigma}\hat{a}^\dagger_{i-\sigma}\hat{a}_{i-\sigma} + \hat{b}^\dagger_{i\sigma}\hat{b}_{i\sigma}\hat{b}^\dagger_{i-\sigma}\hat{b}_{i-\sigma}\right), \tag{2}$$

while $\hat{H}_I^1$ accounts for the nearest-neighbor interaction,

$$\hat{H}_I^1 = g_1\sum_{\sigma\sigma'}\sum_{\langle i,j\rangle} \hat{a}^\dagger_{i\sigma}\hat{a}_{i\sigma}\hat{b}^\dagger_{j\sigma'}\hat{b}_{j\sigma'}. \tag{3}$$

We will perform a mean-field approximation in this problem, considering $g_0 < 0$ and $g_1 < 0$.

Let us first define one of the order parameters (this is the familiar superconductivity order parameter that describes on-site Cooper pairs),

$$\Delta_0 = \langle \hat{a}_{i\downarrow}\hat{a}_{i\uparrow}\rangle = \langle \hat{b}_{i\downarrow}\hat{b}_{i\uparrow}\rangle.$$

- (1) Perform a mean-field approximation on the on-site interaction term $\hat{H}_I^0$ to obtain

$$\hat{H}_I^0 = g_0 \sum_i \Delta_0 \hat{a}^\dagger_{i\uparrow}\hat{a}^\dagger_{i\downarrow} + \text{more terms},$$

where you have to determine all the terms.

- (2) It was discussed in class that having more order parameters in addition to Δ_0 was possible. Prove the following identity,

$$\sum_{\sigma\sigma'} \hat{a}^\dagger_{i\sigma}\hat{a}_{i\sigma}\hat{b}^\dagger_{j\sigma'}\hat{b}_{j\sigma'} = c_1 \hat{\mathcal{B}}_{ij}\hat{\mathcal{B}}^\dagger_{ij} + c_2 \hat{\mathcal{D}}^\dagger_{ij}\hat{\mathcal{D}}_{ij} + \sum_\sigma \hat{a}^\dagger_{i\sigma}\hat{a}_{i\sigma}, \tag{4}$$

where

$$\hat{\mathcal{B}}_{ij} = \hat{a}^\dagger_{i\uparrow}\hat{b}_{j\uparrow} + \hat{a}^\dagger_{i\downarrow}\hat{b}_{j\downarrow} \tag{5}$$

and

$$\hat{\mathcal{D}}_{ij} = \hat{a}_{i\downarrow}\hat{b}_{j\uparrow} - \hat{a}_{i\uparrow}\hat{b}_{j\downarrow} \tag{6}$$

(you have to find the numbers c_1 and c_2).

It turns out that in graphene we may safely put the first and third term in Eq. (4) to zero (it means that we do not consider the order parameter $\langle\hat{\mathcal{B}}_{ij}\rangle$ that corresponds to a so-called spin-liquid phase). Plugging the remaining identity into Eq. (3) we obtain (4)

$$\hat{H}_I^1 = g_1 c_2 \sum_{\langle i,j\rangle} \hat{\mathcal{D}}^\dagger_{ij}\hat{\mathcal{D}}_{ij}. \tag{7}$$

- (3) Perform a mean-field approximation to $\hat{H}_I^1$ in Eq. (7) in terms of the mean-field parameter

$$\Delta_{ij} = \langle\hat{\mathcal{D}}_{ij}\rangle. \tag{8}$$

Argue that the translational and rotational symmetry of the honeycomb lattice force the order parameter $\Delta_{ij} = \Delta_1$ to be a constant for i and j nearest neighbors. Write down the total Hamiltonian for the system in the grand-canonical ensemble, which is now expressed entirely in terms of one-body operators and constants.

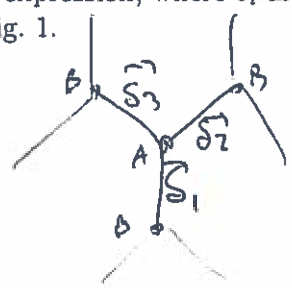
↳ because we did a mean field $(H - \mu N)$

- (4) Apply Fourier transformation on the Hamiltonian that you wrote down in the exercise (3) using

$$\hat{a}^\dagger_{i\sigma} = \sqrt{\frac{2}{N}} \sum_{\mathbf{k}} \hat{a}^\dagger_{\mathbf{k}\sigma} e^{\imath \mathbf{k}\,\mathbf{x}_i}$$

just Fourier transform

and similar expressions for the other operators to write down the Hamiltonian in the grand-canonical ensemble in **k**-space. Here, N is the total number of sites. Recognize $\gamma_{\mathbf{k}} = \sum_{i=1}^{3} e^{-\imath \mathbf{k}\cdot\vec{\delta}_i}$ in your expression, where $\vec{\delta}_i$ are the vectors that connect the nearest neighbors, see Fig. 1.



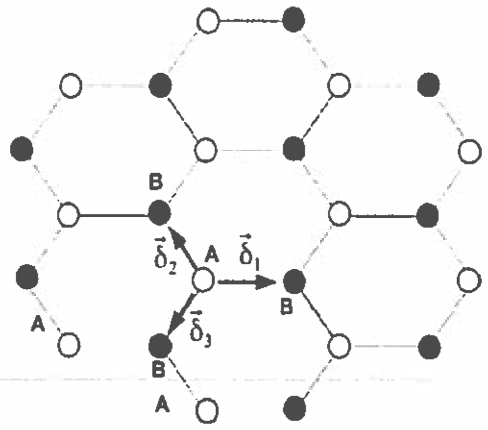


Figure 1: Honeycomb lattice of carbon atoms forming graphene. The empty and filled sites represent the atoms on the two (triangular) sublattices A and B of the honeycomb lattice, while the vectors $\vec{\delta}_i$, with $i = 1, 2, 3$, connect the nearest neighboring sites.

- (5) Introducing the spinor representation,

$$\hat{\Psi}_{\mathbf{k}} \equiv \begin{pmatrix} \hat{a}_{\mathbf{k},\uparrow} \\ \hat{b}_{\mathbf{k},\uparrow} \\ \hat{a}^{\dagger}_{-\mathbf{k},\downarrow} \\ \hat{b}^{\dagger}_{-\mathbf{k},\downarrow} \end{pmatrix}, \tag{9}$$

the Hamiltonian can be written as

$$\hat{H} = \sum_{\mathbf{k}} \hat{\Psi}^{\dagger}_{\mathbf{k}} \overline{\omega}_{\mathbf{k}} \hat{\Psi}_{\mathbf{k}} + E_0, \tag{10}$$

where $\overline{\omega}_{\mathbf{k}}$ is a 4×4 matrix and E_0 is a constant. Determine $\overline{\omega}_{\mathbf{k}}$ and E_0.

Δ_{ii} if it's not real you can redefine it's imaginary part to Δ_0

- (6) In principle Δ_{ij} and Δ_0 may both be complex. However, upon appropriately rescaling the operators $\hat{a}_{\mathbf{k}\sigma}$, $\hat{b}_{\mathbf{k}\sigma}$ and order parameter Δ_0 by complex numbers of unit modulus while keeping t, μ and the interaction constants real, one may take Δ_{ij} to be real. Show this. Show also that the commutation relations of operators $\hat{a}_{\mathbf{k}\sigma}$ and $\hat{b}_{\mathbf{k}\sigma}$ are unaffected. Determine the spectrum of this Hamiltonian for $g_1 = g_0 = 0$ by determining the eigenvalues of $\overline{\omega}_{\mathbf{k}}$. easy case.

gauge trans.

- (7) For g_1 and g_0 finite, the matrix $\overline{\omega}_{\mathbf{k}}$ has 4 distinct eigenvalues,

don't prove this.

$$\omega_{\mathbf{k}\sigma\sigma'} = \underset{\pm}{\sigma} \sqrt{t^2 |\gamma_{\mathbf{k}}|^2 + \mu^2 + g_0^2\Delta_0^2 + g_1^2\Delta_1^2 |\gamma_{\mathbf{k}}|^2 + 2\underset{\pm}{\sigma'} |\gamma_{\mathbf{k}}| \, |t\mu - g_0 g_1 \Delta_0 \Delta_1|},$$

where σ, σ' do not mean spin labels, but independent $\pm$ signs for the possible four values of $\omega_{\mathbf{k}}$. Starting from the partition function

$$Z = e^{-\beta\Omega} = \mathrm{Tr} e^{-\beta H}, \tag{11}$$

$$\sigma\sigma' = \begin{cases} 1 & 1 \\ 1 & -1 \\ -1 & 1 \\ -1 & -1 \end{cases}$$

No crazy calculations! use your → express things in the right basis

and from the Hamiltonian (10), explain carefully how to obtain the thermodynamical potential Ω and show that the result is

$$\Omega = -\frac{1}{\beta} \sum_{\mathbf{k},\sigma,\sigma'} \ln\left(1 + e^{-\beta\omega_{\mathbf{k},\sigma,\sigma'}}\right) + E_0. \tag{12}$$

- (8) Obtain the self-consistent equations for the order parameters Δ_0 and Δ_1. Show that in the limit $\beta \to \infty$ ($T \downarrow 0$) one of the equations reduces to

$$\Delta_0 N = \frac{1}{2} \sum_{\mathbf{k}\sigma'} \frac{1}{\omega_{\mathbf{k}\sigma'}} [g_0\Delta_0 - \sigma' s|\gamma_{\mathbf{k}}|g_1\Delta_1], \tag{13}$$

where s is $s = \mathrm{sgn}(t\mu - g_0 g_1 \Delta_0 \Delta_1)$ and $\omega_{\mathbf{k}\sigma'} \equiv \omega_{\mathbf{k},\sigma=-,\sigma'}$. ($\sigma = -\sigma'$ in eqn (11))

- (9)To get some insight into superconductivity in graphene, we will now study the self-consistent equation (13). From here on, we will only consider the case $\Delta_0 \neq 0$ and will set $\Delta_1 = 0$. We are still at zero temperature and we consider the half-filling case ($\mu = 0$). This means that all important excitations are around the Dirac cone, around which

$T \to 0$ $\mu = 0$ $\Delta_0 N = \frac{1}{2} \sum_{k\sigma'} \frac{1}{\omega_{k\sigma'}} [g_0 \Delta_0]$

$$|\gamma_{\mathbf{k}}| \approx \frac{3}{2}k.$$

[[problems here

Starting from equation (13), calculate the order parameter dependence on the coupling constant and plot the function $\Delta_0 = \Delta_0(g_0)$. For which values of g_0 does the phase transition occur? How is this situation different from ordinary superconductivity? **Hint:** when performing the $\mathbf{k}$ integral, introduce the momentum cutoff Λ, which is large but not infinite. ↳ do the integral yourself with a trick.

high mom. cutoff

- (10) Instead of assuming a constant Δ_{ij}, one can also make the following ansatz for the order parameters,

Δ_σ can just a constant. or $\Delta \cos$

$$\Delta_{\sigma\sigma}(\vec{x}, \vec{y}) = \Delta_\sigma \cos\left(\vec{Q} \cdot (\vec{x} + \vec{y}) + \alpha\right),$$

$$\frac{1}{2}\left(\Delta_{\downarrow\uparrow}(\vec{x}, \vec{y}) + \Delta_{\uparrow\downarrow}(\vec{x}, \vec{y})\right) = \Delta \cos(\vec{Q} \cdot (\vec{x} + \vec{y}) + \alpha),$$

$$\frac{1}{2}\left(\Delta_{\downarrow\uparrow}(\vec{x}, \vec{y}) - \Delta_{\uparrow\downarrow}(\vec{x}, \vec{y})\right) = \Delta'.$$

go to (9)

If we assume this

What is the physical interpretation of this type of order parameters? What can you say about the Cooper pairs in this case?

triplet !