Midterm Exam - "Statistical Field Theory"

November 5, 2013

1. *Use a separate sheet for every exercise.*
2. *Write your name and initials in 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

The Nobel Prize in Physics for 2010 was awarded to A. Geim and K. Novoselov for their experimental realization of graphene. Graphene consists of a single layer of carbon atoms arranged on a honeycomb lattice (see Fig. 1).

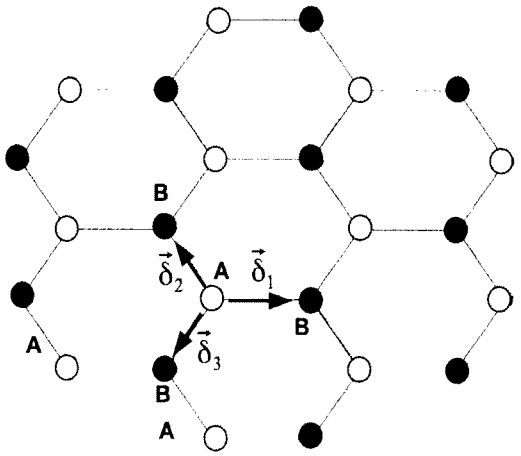

Figure 1: Honeycomb lattice of carbon atoms forming graphene. The empty and filled sites represent the atoms on the two (triangular) sublattices A and B of the honeycomb lattice, while the vectors $\vec{\delta}_i$, with $i = 1, 2, 3$, connect the nearest neighboring sites.

The effective Hamiltonian of graphene is described in terms of two species (flavors) of *electrons*, a, b, living on two different sublattices, A and B. We will consider the usual non-interacting term for the nearest-neighbors hopping (note that nearest neighboring sites reside on different sublattices; see Fig. 1)

$$H_t = -t \sum_{\sigma=\pm 1} \sum_{\langle ij \rangle} a^\dagger_{i,\sigma} b_{j,\sigma} + \text{h.c.}, \tag{1}$$

where $\sigma = \pm 1$ corresponds to spin up $(+1)$ and spin down (-1). Now, we introduce a term describing local attractive density-density interaction,

$$H_I = \frac{g}{2} \sum_{i,\sigma=\pm 1} \left(a^\dagger_{i,\sigma} a_{i,\sigma} a^\dagger_{i,-\sigma} a_{i,-\sigma} + b^\dagger_{i,\sigma} b_{i,\sigma} b^\dagger_{i,-\sigma} b_{i,-\sigma} \right), \tag{2}$$

with $g < 0$. In order to study superconductivity in graphene, we introduce an order parameter,

$$\Delta = \langle a_{i,\downarrow} a_{i,\uparrow} \rangle = \langle b_{i,\downarrow} b_{i,\uparrow} \rangle. \tag{3}$$

(1.0)**(1)** Perform a mean-field approximation to show that H_I becomes the effective mean-field pairing Hamiltonian

$$H_P = \frac{g}{2} \sum_{i\sigma} \sigma \Delta \left(a^\dagger_{i,\sigma} a^\dagger_{i,-\sigma} + b^\dagger_{i,\sigma} b^\dagger_{i,-\sigma} \right) + h.c. - 2gN|\Delta|^2. \tag{4}$$

Here N is the total number of sites in each sublattice. Expand the fields as their mean field value plus fluctuations and keep only linear terms in the fluctuations. Don't forget that you have to re-express the fluctuations in terms of the fields.

(0.5)**(2)** Show that the full Hamiltonian in the grand-canonical ensemble in momentum space is

$$\begin{aligned} H &= H_t + H_\mu + H_P \\ &= -t \sum_{\mathbf{k}\sigma} \left(\gamma_{\mathbf{k}} a^\dagger_{\mathbf{k},\sigma} b_{\mathbf{k},\sigma} + h.c. \right) - \mu \sum_{\mathbf{k}\sigma} \left(a^\dagger_{\mathbf{k},\sigma} a_{\mathbf{k},\sigma} + b^\dagger_{\mathbf{k},\sigma} b_{\mathbf{k},\sigma} \right) \\ &\quad + \frac{g}{2} \sum_{\mathbf{k}\sigma} \sigma \Delta \left(a^\dagger_{\mathbf{k},\sigma} a^\dagger_{-\mathbf{k},-\sigma} + b^\dagger_{\mathbf{k},\sigma} b^\dagger_{-\mathbf{k},-\sigma} \right) + h.c. - 2gN|\Delta|^2. \end{aligned} \tag{5}$$

Write $\mathbf{r}_j = \mathbf{r}_i + \vec{\delta}$ and use that $\gamma_{\mathbf{k}} \equiv \sum_{\vec{\delta}_i} e^{i\mathbf{k}\cdot\vec{\delta}_i}$, where $\vec{\delta}_i$, $i = 1, 2, 3$, are the vectors connecting nearest neighboring sites in the lattice (see Fig. 1).

(0.5)**(3)** Introducing the spinor representation,

$$\Psi_{\mathbf{k}} \equiv \begin{pmatrix} a_{\mathbf{k},\uparrow} \\ b_{\mathbf{k},\uparrow} \\ a^\dagger_{-\mathbf{k},\downarrow} \\ b^\dagger_{-\mathbf{k},\downarrow} \end{pmatrix} \tag{6}$$

the Hamiltonian can be written as

$$H = \sum_{\mathbf{k}} \Psi^\dagger_{\mathbf{k}} \hat{\omega}_{\mathbf{k}} \Psi_{\mathbf{k}} + E_0, \tag{7}$$

where $\hat{\omega}_{\mathbf{k}}$ is a 4×4 matrix and $E_0 = -2gN|\Delta|^2 - 2\mu N$. Determine $\hat{\omega}_{\mathbf{k}}$.

(1.0)**(4)** Consider the case $g = 0$ in Eq. (7), when the matrix $\hat{\omega}_{\mathbf{k}}$ reads

$$\hat{\omega}_{\mathbf{k}} = \begin{pmatrix} -\mu & -t\gamma_{\mathbf{k}} & 0 & 0 \\ -t\gamma_{\mathbf{k}}^{*} & -\mu & 0 & 0 \\ 0 & 0 & \mu & t\gamma_{\mathbf{k}} \\ 0 & 0 & t\gamma_{\mathbf{k}}^{*} & \mu \end{pmatrix} \tag{8}$$

Diagonalize this matrix to find the eigenvalues for $g = 0$. You can check your results, knowing that the result for general g and t (that you **do not** have to derive) reads

$$\omega_{\mathbf{k},\sigma}^{2} = (t|\gamma_{\mathbf{k}}| + \sigma\mu)^{2} + g^{2}|\Delta|^{2}. \tag{9}$$

What is the physical meaning of this diagonalization?

(1.0)**(5)** Starting from the partition function

$$Z = e^{-\beta\Omega} = \mathrm{Tr}e^{-\beta H}, \tag{10}$$

determine the thermodynamical potential Ω. You will find that

$$\Omega = -\frac{1}{\beta}\sum_{\mathbf{k},\sigma,\sigma'} \ln\left(1 + e^{-\beta\omega_{\mathbf{k},\sigma,\sigma'}}\right) + E_{0}, \tag{11}$$

where we have rewritten the roots of Eq. (9) using $\sigma' \equiv \pm 1$ in the form

$$\omega_{\mathbf{k},\sigma,\sigma'} = \sigma'\sqrt{(t|\gamma_{\mathbf{k}}| + \sigma\mu)^{2} + g^{2}|\Delta|^{2}}. \tag{12}$$

(1.0)**(6)** Show that the gap equation becomes

$$g\sum_{\mathbf{k},\sigma,\sigma'} \frac{N_{FD}(\omega_{\mathbf{k},\sigma,\sigma'})}{\omega_{\mathbf{k},\sigma,\sigma'}} = 4N, \tag{13}$$

where $N_{FD}(\omega_{\mathbf{k},\sigma,\sigma'})$ is the Fermi-Dirac distribution function.

(1.0)**(7)** Now consider pairing between the electrons living on the nearest-neighboring sites. Write down the order parameters characterizing possible pairings in this case. What is the main physical difference now as compared with the onsite pairing discussed above.

Su-Schrieffer-Heeger model of a polyacetylene chain

Polyacetylene consists of bonded CH groups forming an isomeric long-chain polymer. According to molecular orbital theory, the carbon atoms are expected to be sp^2-hybridized (as in graphene) suggesting a planar configuration of the molecule. An unpaired electron is expected to occupy a single π-orbital which is oriented perpendicular to the plane. The weak overlap of the π-orbitals delocalizes the electrons into a narrow conduction band. According to the nearly free electron theory, one might expect the half-filled conduction band of a polyacetylene chain to be metallic. However, the energy of a half-filled band of a one-dimensional system can always be lowered by imposing a periodic lattice distortion known as a Peierls instability (see Figure 2). The aim of this problem is to explore this instability.

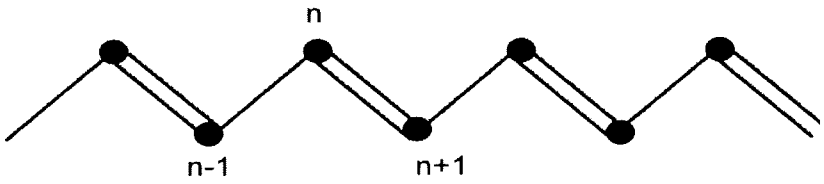

Figure 2: Schematic representation of the polyacetylene chain with the Peierls distorsion. The double bonds correspond to short links on the lattice.

(1.5)(8) At its simplest level, the conduction band of polyacetylene can be modeled by a simple (arguably over-simplified) microscopic Hamiltonian, due to Su, Shrieffer, and Heeger, in which the hopping matrix elements of the electrons are modulated by the lattice distortion of the atoms. By taking the displacement of an atomic site, labelled by n, to be u_n, and treating their dynamics as classical, the effective Hamiltonian can be cast in the form

$$H = -t\sum_{n=1}^{N}\sum_{\sigma}(1+u_n)(c^{\dagger}_{n,\sigma}c_{n+1,\sigma} + \text{h.c.}) + \sum_{n=1}^{N}\frac{k_s}{2}(u_{n+1}-u_n)^2 \qquad (14)$$

where, for simplicity, the boundary conditions are taken to be periodic, summation over the spins σ is assumed, and the lattice constant of the undistorted lattice is set to unity. The first term describes the hopping of electrons between neighboring sites with a matrix element modulated by the periodic distortion of the bond-length, while the last term represents the associated increase in the elastic energy. Taking the lattice distortion to be periodic, $u_n = (-1)^n\alpha$, with $\alpha \ll 1$ as a real parameter describing the lattice distortion, and the number of sites N to be even, show that the first term of the Hamiltonian in Fourier space can be written as

$$H_t = -t\sum_{k,\sigma}\{[\,(1+\alpha)e^{2ik} + (1-\alpha)]a^{\dagger}_{k,\sigma}b_{k,\sigma} + \text{h.c.}\}. \qquad (15)$$

Hint: Note that the lattice distortion lowers the symmetry of the lattice. The Hamiltonian is most easily diagonalized by distinguishing the two sublattices defined by taking sites labelled by even and odd integers, respectively, i.e., by doubling the size of the elementary unit cell. Use here that the Fourier transform of the electron annihilation operators on the two sublattices is

$$a_{m,\sigma} \equiv c_{2m,\sigma} = \sqrt{\frac{2}{N}} \sum_{k=-\pi/2}^{\pi/2} a_{k,\sigma}\, e^{2imk} \tag{16}$$

$$b_{m.\sigma} \equiv c_{2m-1,\sigma} = \sqrt{\frac{2}{N}} \sum_{k=-\pi/2}^{\pi/2} b_{k,\sigma}\, e^{2imk}, \tag{17}$$

with $1 \leq m \leq N/2$ as an integer. The doubling of the unit cell implies that the Brillouin zone is now defined for the momenta $-\pi/2 \leq k \leq \pi/2$.

(1.0)**(9)** Show that the spectrum of the electronic (tight-binding) Hamiltonian consists of two bands ($\pm$) with energies $\epsilon_{\pm}(k) = \pm 2t\sqrt{1 + (\alpha^2 - 1)\sin^2 k}$.

(0.5)**(10)** Show that the Peierls distortion of the lattice opens up a gap in the spectrum at the Fermi level of the half-filled system (one electron per lattice site in average).

(0.5)**(11)** Now, take also into consideration the elastic energy of the lattice due to the Peierls distortion. Show that the total electronic and elastic energy of the half-filled system in the ground state is

$$E_{\rm tot} = 2Nk_s\alpha^2 + \int_{-\pi/2}^{\pi/2} dk\ \epsilon_-(k). \tag{18}$$

(0.5)**(12)** Show then that the one-dimensional system is always unstable towards the Peierls distortion. To complete this calculation, you will need the approximate formula for the (elliptic) integral,

$$\int_{-\pi/2}^{\pi/2} dk\ \sqrt{1 - (1 - \alpha^2)\sin^2 k} \simeq 2 + \alpha^2[a_1 - b_1 \ln(\alpha^2)] + \mathcal{O}[\alpha^2 \ln(\alpha^2)], \tag{19}$$

where a_1 and b_1 are (unspecified) numerical constants.