

INTRODUCTION TO MANY BODY PHYSICS: 620. Fall 2011

Answers to Questions 4. (Mon, Nov 7th)

1. (a) We begin by noting that the matrix elements for the tight-binding Hamiltonian are

$$\langle i|H|j\rangle = \begin{cases} \epsilon & (i = j) \\ -t & (i, j, \text{ nearest neighbors}) \\ 0 & (\text{otherwise}) \end{cases} \quad (1)$$

where ϵ is the energy of an isolated orbital and $-t$ is the hopping matrix element. Now the orbital at site A , position \mathbf{r}_i is connected to orbitals at sites B which are located in the unit cells at positions \mathbf{r}_j , $\mathbf{r}_j - \mathbf{b}$ and $\mathbf{r}_j - \mathbf{a}$. (Note the minus signs). Consequently, the tight-binding Hamiltonian takes the form

$$H = \overbrace{-t \sum_j \left\{ \left[\psi_B^\dagger(\mathbf{r}_i) + \psi_B^\dagger(\mathbf{r}_i - \mathbf{a}) + \psi_B^\dagger(\mathbf{r}_i - \mathbf{b}) \right] \psi_A(\mathbf{r}_i) + \text{H.c} \right\}}^{\text{hopping between nearest neighbors}} + (\epsilon - \mu) \sum_i (n_A(i) + n_B(i)). \quad (2)$$

Here $\psi_{A,B}^\dagger(\mathbf{r}_j)$ creates an electron at site A or B respectively in the unit cell located at position \mathbf{r}_j .

- (b) If we Fourier transform, writing

$$\psi_\lambda^\dagger(\mathbf{r}_j) = \frac{1}{\sqrt{N_s}} \sum_{\mathbf{k}} c_{\mathbf{k}\lambda}^\dagger e^{-i\mathbf{k}\cdot\mathbf{r}_j} \quad (\lambda = A, B) \quad (3)$$

then substituting into the Hamiltonian, we obtain

$$\begin{aligned} H &= -\frac{t}{N_s} \sum_{j, \mathbf{k}, \mathbf{k}'} \left[c_{\mathbf{k}B}^\dagger (1 + e^{i\mathbf{k}\cdot\mathbf{a}} + e^{i\mathbf{k}\cdot\mathbf{b}}) c_{\mathbf{k}A} e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}_j} + \text{H.c} \right] + (\epsilon - \mu) \sum_{\mathbf{k}\lambda} c_{\mathbf{k}\lambda}^\dagger c_{\mathbf{k}\lambda} \\ &= \sum_{\mathbf{k}} \left(c_{\mathbf{k}B}^\dagger, c_{\mathbf{k}A}^\dagger \right) \begin{bmatrix} \epsilon - \mu & \Delta(\mathbf{k}) \\ \Delta^*(\mathbf{k}) & \epsilon - \mu \end{bmatrix} \begin{pmatrix} c_{\mathbf{k}B} \\ c_{\mathbf{k}A} \end{pmatrix} \end{aligned} \quad (4)$$

where

$$\Delta(\mathbf{k}) = -t(1 + e^{i\mathbf{k}\cdot\mathbf{a}} + e^{i\mathbf{k}\cdot\mathbf{b}})$$

The eigenvalues of the matrix

$$\begin{bmatrix} \epsilon - \mu & \Delta^*(\mathbf{k}) \\ \Delta(\mathbf{k}) & \epsilon - \mu \end{bmatrix}$$

are

$$\begin{aligned} \epsilon_{\mathbf{k}\pm} &= \pm |\Delta(\mathbf{k})| + (\epsilon - \mu) \\ &= \pm t \sqrt{(3 + 2 \cos(\mathbf{k}\cdot\mathbf{a}) + 2 \cos(\mathbf{k}\cdot\mathbf{b}) + 2 \cos(\mathbf{k}\cdot(\mathbf{a} - \mathbf{b})))} + (\epsilon - \mu) \end{aligned} \quad (5)$$

(see Fig. 1)

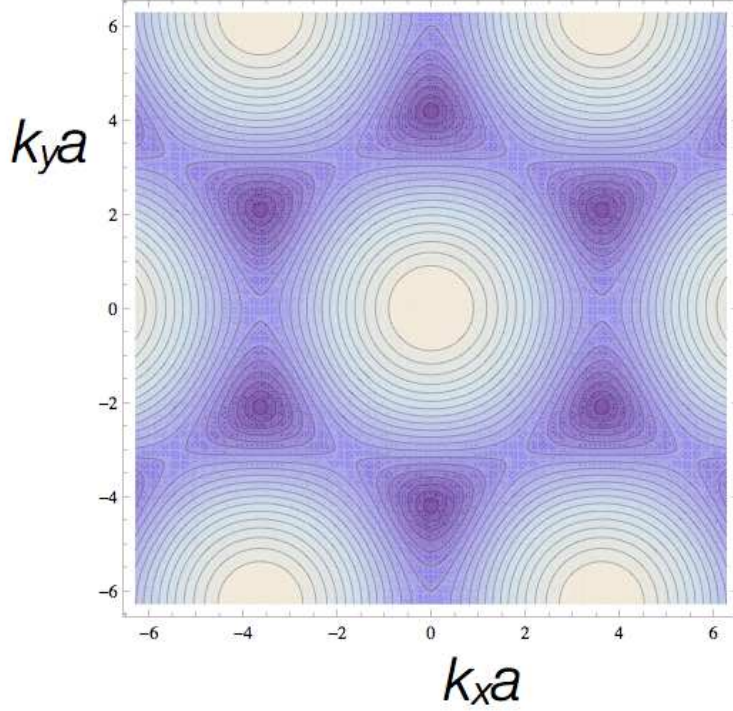


Figure 1: Contour plot of dispersion $\epsilon_{\mathbf{k}+}$ given by equation (5).

(c) If $e^{i\mathbf{K}\cdot\mathbf{a}} = e^{i\frac{2\pi}{3}}$, $e^{i\mathbf{K}\cdot\mathbf{b}} = e^{-i\frac{2\pi}{3}}$, then clearly,

$$\Delta(\mathbf{K}) \propto (1 + e^{i\mathbf{K}\cdot\mathbf{a}} + e^{i\mathbf{K}\cdot\mathbf{b}}) = (1 + e^{i\frac{2\pi}{3}} + e^{-i\frac{2\pi}{3}}) = 0$$

To satisfy the conditions

$$\begin{aligned} \mathbf{K}\cdot\mathbf{a} &= \frac{\sqrt{3}}{2}(K_x a) + \frac{1}{2}K_y a = \frac{2\pi}{3} \\ \mathbf{K}\cdot\mathbf{b} &= \frac{\sqrt{3}}{2}(K_x a) - \frac{1}{2}K_y a = -\frac{2\pi}{3} \end{aligned} \quad (6)$$

we require $K_x = 0$, $K_y = \frac{4\pi}{3a}$, or $\mathbf{K} = \frac{4\pi}{3a}\mathbf{j}$. When $\mathbf{k} = \pm\mathbf{K}$, $\Delta(\mathbf{k}) = \Delta(\pm\mathbf{K}) = 0$.

(d) If we expand $\Delta(\mathbf{p} + \mathbf{K})$ for small \mathbf{p} , we obtain

$$\begin{aligned} \Delta(\mathbf{k}) &= -t[1 + e^{i\frac{2\pi}{3}}(1 + i\mathbf{p}\cdot\mathbf{a}) + e^{-i\frac{2\pi}{3}}(1 + i\mathbf{p}\cdot\mathbf{b})] \\ &= -it[e^{i\frac{2\pi}{3}}\mathbf{p}\cdot\mathbf{a} + e^{-i\frac{2\pi}{3}}\mathbf{p}\cdot\mathbf{b}] \\ &= -it\left[\left(-\frac{1}{2} + i\frac{\sqrt{3}}{2}\right)\mathbf{p}\cdot\mathbf{a} + \left(-\frac{1}{2} - i\frac{\sqrt{3}}{2}\right)\mathbf{p}\cdot\mathbf{b}\right] \end{aligned}$$

$$= it \left[\frac{\sqrt{3}}{2} p_x a - i \frac{\sqrt{3}}{2} p_y a \right] = \overbrace{\left(\frac{\sqrt{3} t a}{2} \right)}^{\tilde{c}} [p_y + i p_x] \quad (7)$$

so that we can write

$$\begin{aligned} \begin{bmatrix} \epsilon - \mu & \Delta(\mathbf{p} + \mathbf{K}) \\ \Delta^*(\mathbf{p} + \mathbf{K}) & \epsilon - \mu \end{bmatrix} &\approx \begin{bmatrix} \epsilon - \mu & \tilde{c}(p_y + i p_x) \\ \tilde{c}(p_y - i p_x) & \epsilon - \mu \end{bmatrix} = (\epsilon - \mu) \mathbb{1} + \tilde{c} (p_y \sigma_x - p_x \sigma_y) \\ &= (\epsilon - \mu) \mathbb{1} + \tilde{c} (\vec{\sigma} \times \mathbf{p}) \end{aligned} \quad (8)$$

In the vicinity of $\mathbf{k} \sim \mathbf{K}$, we thus have

$$\begin{aligned} \sum_{\mathbf{p} \sim 0} \left(c_{\mathbf{p}+\mathbf{K}B}^\dagger, c_{\mathbf{p}+\mathbf{K}A}^\dagger \right) \begin{bmatrix} \epsilon - \mu & \Delta(\mathbf{p} + \mathbf{K}) \\ \Delta^*(\mathbf{p} + \mathbf{K}) & \epsilon - \mu \end{bmatrix} \begin{pmatrix} c_{\mathbf{p}+\mathbf{K}B} \\ c_{\mathbf{p}+\mathbf{K}A} \end{pmatrix} \\ = \sum_{\mathbf{p} \sim 0} \psi_{\mathbf{p}+}^\dagger \left((\epsilon - \mu) \mathbb{1} + \tilde{c} \vec{\sigma} \times \mathbf{p} \right) \psi_{\mathbf{p}+} \end{aligned} \quad (9)$$

where

$$\psi_{\mathbf{p}+} = \begin{pmatrix} c_{\mathbf{p}+\mathbf{K}B} \\ c_{\mathbf{p}+\mathbf{K}A} \end{pmatrix}, \quad (10)$$

Similarly, for $\mathbf{k} = \mathbf{p} - \mathbf{K}$, where \mathbf{p} is small, we have

$$\begin{bmatrix} \epsilon - \mu & \Delta(\mathbf{p} - \mathbf{K}) \\ \Delta^*(\mathbf{p} - \mathbf{K}) & \epsilon - \mu \end{bmatrix} \approx \begin{bmatrix} \epsilon - \mu & -\tilde{c}(p_y - i p_x) \\ -\tilde{c}(p_y + i p_x) & \epsilon - \mu \end{bmatrix} = (\epsilon - \mu) \mathbb{1} + \tilde{c} (\mathbf{p} \times \vec{\sigma}^T) \quad (11)$$

so that

$$\sum_{\mathbf{p} \sim 0} \left(c_{\mathbf{p}-\mathbf{K}B}^\dagger, c_{\mathbf{p}-\mathbf{K}A}^\dagger \right) \begin{bmatrix} \epsilon - \mu & \Delta(\mathbf{p} - \mathbf{K}) \\ \Delta^*(\mathbf{p} - \mathbf{K}) & \epsilon - \mu \end{bmatrix} \begin{pmatrix} c_{\mathbf{p}-\mathbf{K}B} \\ c_{\mathbf{p}-\mathbf{K}A} \end{pmatrix} = \sum_{\mathbf{p} \sim 0} \psi_{\mathbf{p}-}^\dagger \left((\epsilon - \mu) \mathbb{1} + \tilde{c} (\vec{\sigma} \times \mathbf{p}) \right) \psi_{\mathbf{p}-} \quad (12)$$

where

$$\psi_{\mathbf{p}-} = \begin{pmatrix} c_{\mathbf{p}-\mathbf{K}A} \\ -c_{\mathbf{p}-\mathbf{K}B} \end{pmatrix}, \quad (13)$$

Combining the two contributions (9) and (12), the low energy Hamiltonian thus has the form

$$H = \sum_{\mathbf{p}\lambda} \psi_{\mathbf{p}\lambda}^\dagger \left(\tilde{c} (\vec{\sigma} \times \mathbf{p}) + (\epsilon - \mu) \mathbb{1} \right) \psi_{\mathbf{p}\lambda} \quad (14)$$

2. (a) If we take the expression for the Free energy

$$F(\lambda) = -T \ln Z(\lambda) = -T \ln \text{Tr} [e^{-\beta[H_0 + \lambda V]}] \quad (15)$$

and differentiate it, we obtain

$$\frac{\partial F}{\partial \lambda} = -\frac{T}{Z} \frac{\partial Z}{\partial \lambda}. \quad (16)$$

Now

$$\frac{\partial Z}{\partial \lambda} = \text{Tr}\left[\frac{\partial e^{-\beta[H_o+\lambda V]}}{\partial \lambda}\right] = -\beta \text{Tr}[V e^{-\beta[H_o+\lambda V]}] \quad (17)$$

so that

$$\frac{\partial F}{\partial \lambda} = \frac{\text{Tr}[V e^{-\beta[H_o+\lambda V]}]}{Z} = \langle V \rangle = \langle V_{int} \rangle / \lambda. \quad (18)$$

(b) By integrating the result of part (a) over λ , we obtain

$$\Delta F = \int_0^1 d\lambda \frac{\partial F}{\partial \lambda} = \int_0^1 \frac{d\lambda}{\lambda} \langle V_{int}(\lambda) \rangle \quad (19)$$

(c) If the interaction energy has an expansion $\langle V_{int}(\lambda) \rangle = \lambda V_1 + \lambda^2 V_2 + \lambda^3 V_3 + \dots$, then

$$\Delta E = \int_0^1 \frac{d\lambda}{\lambda} \langle \phi | V_{int}(\lambda) | \phi \rangle = V_1 + \frac{1}{2} V_2 + \frac{1}{3} V_3 + \dots \quad (20)$$

(d) When we turn on the interaction, the change in the ground-state energy involves the contributions from both the change in the Hamiltonian and the change in the ground-state. The factors of $\frac{1}{n}$ appearing in front of the n-th order terms reflect the fact that the ground-state relaxes in response to the change in hamiltonian, so that the change in the ground-state energy from each term is less than the corresponding change in the expectation value of the interaction.

3. (a) The crosses represent the scattering amplitude $V_{k,k'}$ and the lines represent the propagators.

(b) Diagrammatically, we have:

$$\begin{aligned} \Rightarrow \Rightarrow &= \rightarrow \rightarrow + \rightarrow \times \rightarrow + \rightarrow \times \rightarrow \times \rightarrow + \dots \\ &= \rightarrow \rightarrow + \rightarrow \bullet \rightarrow \end{aligned}$$

or

$$G_{\mathbf{k},\mathbf{k}'}(E) = G_{\mathbf{k}}^{(0)}(E) \delta_{\mathbf{k},\mathbf{k}'} + G_{\mathbf{k}}^{(0)}(E) t_{\mathbf{k},\mathbf{k}'}(E) G_{\mathbf{k}'}^{(0)}(E) \quad (21)$$

where the “blob” is the t-matrix, represented by the following sum of diagrams

$$\begin{aligned} \bullet &= \times + \times \rightarrow \times + \times \rightarrow \times \rightarrow \times + \dots \\ &= \times + \times \rightarrow \bullet \end{aligned}$$

Written algebraically, this becomes

$$t_{\mathbf{k},\mathbf{k}'}(E) = U(\mathbf{k} - \mathbf{k}') + \int \frac{d^d q}{2\pi} \frac{U(\mathbf{k} - \mathbf{q})}{E - E(q) + i\delta} t_{\mathbf{q},\mathbf{k}'}(E) \quad (22)$$

where we assume that the Fermi surface is empty (i.e $\mu = 0$, so that $\delta_{\mathbf{k}} = \delta$ for all states.)

- (c) If $U(x) = U\delta^{(d)}(x)$, then $U(q) = U$ and the t-matrix is now momentum independent. We may immediately solve (22) to obtain

$$t(\omega) = \frac{U}{1 - UF(\omega)} \quad (23)$$

where

$$F(\omega) = \int \frac{d^d k}{(2\pi)^d} G^{(0)}(k, \omega)$$

- (d) Let us examine how the integral in the denominator of the t-matrix scales with energy at low energies. We take the case of a “drained Fermi sea”, in which the chemical potential $\mu = 0$, so that for $\omega < 0$,

$$\begin{aligned} F(\omega) &= \int \frac{d^d k}{(2\pi)^d} G^{(0)}(k, \omega) \propto \int d\epsilon \epsilon^{(\frac{d}{2}-1)} \frac{1}{\omega - \epsilon + i\delta} \\ &\propto -(-\omega)^{(\frac{d}{2}-1)} \\ &\propto -\ln\left(\frac{\Lambda}{-\omega}\right), \quad (d = 2). \end{aligned} \quad (24)$$

Thus in dimensions $d \leq 2$, if $U < 0$, the denominator of the t-matrix

$$1 - UF(\omega) = 1 + |U|F(\omega) \sim 1 - \frac{|U|}{(-\omega)^{(2-d)/2}}$$

will pass through zero at some small $\omega = -\omega^* \propto |U|^{2/(2-d)}$, for arbitrarily small $|U|$, giving rise to a pole in the t-matrix. To see that this means the development of a bound-state, consider the density of one-particle states

$$\rho(\omega) = \sum_{\lambda} \delta(\omega - E_{\lambda}) \quad (25)$$

where E_{λ} is the energy of the eigenstate $|\lambda\rangle$. We may rewrite this in the form

$$\begin{aligned} \rho(\omega) &= -\frac{1}{\pi} \text{Im} \sum_{\lambda} \frac{1}{(\omega - E_{\lambda} + i\delta)} \\ &= -\frac{1}{\pi} \text{Im} \sum_{\lambda} \langle \lambda | \hat{G}(\omega) | \lambda \rangle \\ &= -\frac{1}{\pi} \text{Im} \text{Tr} \left[\hat{G}(\omega) \right], \end{aligned} \quad (26)$$

where $\hat{G}(\omega) = (\omega - H + i\delta)^{-1}$. We may also take the trace by summing over the momentum eigenstates, rather than energy eigenstates, so that

$$\begin{aligned} \rho(\omega) &= -\frac{1}{\pi} \sum_{\mathbf{k}} \text{Im} \langle \mathbf{k} | \hat{G}(\omega) | \mathbf{k} \rangle \\ &= -\frac{1}{\pi} \sum_{\mathbf{k}} \text{Im} G_{\mathbf{k},\mathbf{k}}(\omega) \end{aligned} \quad (27)$$

Writing the Green-function in terms of the t-matrix, the change in the density of states due to scattering is then

$$\Delta\rho(\omega) = -\frac{1}{\pi}\text{Im} \left[\left(\int \frac{d^d k}{(2\pi)^d} G^{(0)}(k, \omega) \right)^2 t(\omega) \right] \quad (28)$$

Near the pole at negative energies, we may write this in the form

$$\Delta\rho(\omega) = -\frac{1}{\pi}\text{Im}[F(\omega)^2 t(\omega)] = -\frac{1}{\pi}\text{Im} \left[\left(\frac{1}{U} - \frac{1}{t(\omega)} \right)^2 t(\omega) \right] \approx -\frac{1}{U^2\pi}\text{Im} [t(\omega)] \quad (29)$$

Thus a pole in $t(\omega)$ implies a pole at negative energies in the density of states, indicating a bound-state.