Physics 502 - Solutions for assignment 4

(Dated: November 29, 2023)

1. Krönig-Penney model

a. The boundary conditions that lead to Bloch waves are:

$$\psi(x+a) = e^{ika}\psi(x) \qquad \text{and} \qquad \psi'(x+a) = e^{ika}\psi'(x)$$

and ψ, ψ' are continuous in the unit cell.

b. The Shödinger equation is:

$$-\frac{d^2}{dx^2}\psi(x) = \frac{2m}{\hbar^2}(E - V(x))\psi(x)$$

where V is U_0 or 0. In the region where $V = 0$ the solution can be written in terms of plane waves (or sine and cosine functions) with wave vector $K = \sqrt{\frac{2m}{\hbar^2}E}$. In the region where $V = U_0$ the form of the solution depends on the sign of $E - U_0$. Since we're interested in high barriers (at the end we take $U_0 \to \infty$) we can assume real exponents with coefficient $\lambda = \sqrt{\frac{2m}{\hbar^2}(U_0 - E)}$,

$$\psi(x) = \begin{cases} Ae^{iKx} + Be^{-iKx} & 0 < x < b \\ Ce^{\lambda x} + De^{-\lambda x} & b < x < a \end{cases}$$

Now we can use the boundary conditions to find the relation between K, λ and k. C and D can be expressed in terms of A and B using the conditions at a and 0 (the Bloch conditions).

$$A + B = Ce^{(\lambda+ik)a} + De^{-(\lambda-ik)a} \quad \text{and} \quad iK(A - B) = \lambda(Ce^{(\lambda+ik)a} - De^{-(\lambda-ik)a}).$$

Using the boundary condition at b we get two equations in A, B which can be represented as a matrix of coefficients. The two equations will have a non trivial solution if the determinant of the matrix is zero. This gives the relation:

$$\cos(ka) = -\frac{1}{2}(\frac{\lambda}{K} - \frac{K}{\lambda})\sinh(\lambda b)\sin(K(b-a)) + \cosh(\lambda b)\cos(K(b-a))$$

c. In the limit $b \to 0$, $U_0 \to \infty$ keeping $U_0 b$ at a constant value of $W_0\frac{\hbar^2}{ma}$ we can approximate $\cosh(\lambda b) \approx 1$, $\sinh(\lambda b) \approx \lambda b$, and $\lambda^2 \approx 2mU_0/\hbar^2$. The equation for k and K reduces to:

$$\cos(ka) = \frac{W_0}{Ka}\sin(Ka) + \cos(Ka).$$

d. The two first bands look similar to k^2 dispersion with a gap opening at the zone edge.

2. DOS in the Tight Binding model

The dispersion relation for d-dimensions is given by

$$\epsilon(\vec{k}) = -2t\sum_{i=1}^{d}\cos(k_i a).$$

The possible singularities are when the gradient $|\nabla\epsilon|$ is zero, i.e when $k_i = 0, \pm\frac{\pi}{a}$.

1D - The bottom and top of the band are at $k = 0$, $\epsilon = -2t$ and $k = \pm\frac{\pi}{a}$, $\epsilon = 2t$ respectively. The singularities at the edges are proportional to $|2t - |\epsilon||^{-\frac{1}{2}}$. There are no additional singularities inside the band.

2D - The bottom of the band is at $k = (0,0)$, $\epsilon = -4t$ and the top is at $k = (\pm\frac{\pi}{a}, \pm\frac{\pi}{a})$, $\epsilon = 4t$. The DOS is constant near these points and sharply drops to zero outside the band. There is an additional singularity inside the band. For $k = (\pm\frac{\pi}{a}, 0); (0, \pm\frac{\pi}{a})$ the energy is zero and so is the gradient of $\epsilon(\vec{k})$. For example, consider the point $k = (\pi, 0)$ ($a \equiv 1$). Near this point the energy is close to zero:

$$\epsilon(\vec{k}) = -2t(\cos(\pi - \delta k_x) + \cos(\delta k_y)) \approx -2t(-1 + \frac{1}{2}(\delta k_x)^2 + 1 - \frac{1}{2}(\delta k_y)^2) = t((\delta k_y)^2 - (\delta k_x)^2)$$

where δk_x is measured from π and δk_y is measured from 0. We can find the contribution of this point to the density of states near zero (let ϵ be positive for example) by integrating the approximate dispersion,

$$g(\epsilon) = 2\int \frac{d^2k}{(2\pi)^2 t}\delta(\epsilon - (k_y^2 - k_x^2)),$$

where we replaced the variables $(\delta k_x, \delta k_y)$ by $(k_x, k_y)/\sqrt{t}$. Writing the argument of the δ-function as $(\sqrt{\epsilon + k_x^2} + k_y)(\sqrt{\epsilon + k_x^2} - k_y)$ and focusing on positive values of k_y we have

$$g(\epsilon) = \frac{4}{t}\int \frac{d^2k}{(2\pi)^2}\frac{1}{2k_y}\delta(\sqrt{\epsilon + k_x^2} - k_y) = \frac{1}{2\pi^2 t}\int_{-\sqrt{(\pi t)^2 - \epsilon}}^{\sqrt{(\pi t)^2 - \epsilon}} dk_x \frac{1}{\sqrt{\epsilon + k_x^2}}.$$

The integration boundaries come from the fact that the delta function can only be satisfied if $\sqrt{\epsilon + k_x^2} < \pi t$ and, for small ϵ, can be approximated by $\pm\pi t$. The singularity is logarithmic since

$$\int_{-p}^{p}\frac{dx}{\sqrt{\epsilon + x^2}} = \log\left(\frac{\sqrt{p+\epsilon} + p}{\sqrt{p+\epsilon} - p}\right) \longrightarrow -\log(\epsilon)$$

for $|\epsilon| \ll |p|$.

3D - The bottom of the band is at $k = (0,0,0)$, $\epsilon = -6t$ and the top is at $k = (\pm\frac{\pi}{a}, \pm\frac{\pi}{a}, \pm\frac{\pi}{a})$, $\epsilon = 6t$. The DOS falls off as $\sqrt{||\epsilon| - 6t|}$, just as for free electrons in 3D. There are two additional singular points inside the band. For $k = (\pm\frac{\pi}{a}, 0, 0); (0, \pm\frac{\pi}{a}, 0); (0, 0, \pm\frac{\pi}{a})$ the energy is $-2t$ and for $k = (\pm\frac{\pi}{a}, \pm\frac{\pi}{a}, 0); (\pm\frac{\pi}{a}, 0, \pm\frac{\pi}{a}); (0, \pm\frac{\pi}{a}, \pm\frac{\pi}{a})$ the energy is $2t$. In both cases the gradient of $\epsilon(\vec{k})$

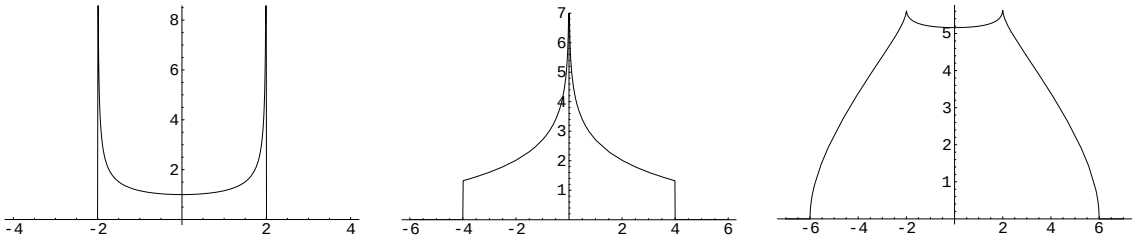

FIG. 1: Density of states for $d = 1, 2, 3$ in the tight binding model

is zero and the singularity is proportional to $\sqrt{||\epsilon| - 2t|}$ (saddle point singularity where only the derivative diverges).

3. Mean field analysis of the Hubbard model

a) Hartree-Fock decoupling of the interaction term

$$\begin{aligned} n_\uparrow n_\downarrow = c_\uparrow^\dagger c_\uparrow c_\downarrow^\dagger c_\downarrow \;\rightarrow\; & \langle c_\uparrow^\dagger c_\uparrow\rangle c_\downarrow^\dagger c_\downarrow + \langle c_\downarrow^\dagger c_\downarrow\rangle c_\uparrow^\dagger c_\uparrow \quad \text{(Hartree)} \\ + \; & \langle c_\uparrow^\dagger c_\downarrow\rangle c_\uparrow c_\downarrow^\dagger + \langle c_\uparrow c_\downarrow^\dagger\rangle c_\uparrow^\dagger c_\downarrow \quad \text{(Fock)}, \end{aligned} \tag{1}$$

where the site index i (the same on all c's) has been suppressed.

b) Neglecting the Fock term the mean field Hamiltonian can be written as

$$H_{\rm MF} = E_0 \sum_{i\sigma} c_{i\sigma}^\dagger c_{i\sigma} - t \sum_{\langle ij\rangle} c_{i\sigma}^\dagger c_{j\sigma} + \frac{U}{2} \sum_i [(N_i - M_i) n_{i\uparrow} + (N_i + M_i) n_{i\downarrow}], \tag{2}$$

where $N_i = \langle n_{i\uparrow}\rangle + \langle n_{i\downarrow}\rangle$ represents the average charge and $M_i = \langle n_{i\uparrow}\rangle - \langle n_{i\downarrow}\rangle$ average z-component of spin at site i.

c) For $N_i = N$ we can define new on-site energy $\tilde{E}_0 = E_0 + \frac{U}{2} N$ and write

$$H_{\rm MF} = \tilde{E}_0 \sum_{i\sigma} c_{i\sigma}^\dagger c_{i\sigma} - \frac{U}{2} M \sum_i (-1)^{i_x + i_y} (n_{i\uparrow} - n_{i\downarrow}) - t \sum_{\langle ij\rangle} c_{i\sigma}^\dagger c_{j\sigma}. \tag{3}$$

The M term acts as a staggered potential that is exactly opposite for the spin up and spin down electrons. Notice that in this mean field approximation the Hamiltonian can be written as $H_{\rm MF} = H_{\rm MF}^\uparrow + H_{\rm MF}^\downarrow$, i.e. the two orientations of spin are effectively decoupled. We can therefore focus, without loss of generality, on the spin up electrons. Dropping the spin index the relevant Hamiltonian is

$$H_{\rm MF}^\uparrow = \sum_i [\tilde{E}_0 - \frac{U}{2} M (-1)^{i_x + i_y}] c_i^\dagger c_i - t \sum_{\langle ij\rangle} c_i^\dagger c_j. \tag{4}$$

The Hamiltonian for the spin down is the same except the sign of M is reversed. To diagonalize this Hamiltonian notice that the unit cell now contains two lattice sites (Fig. 1). It is thus useful

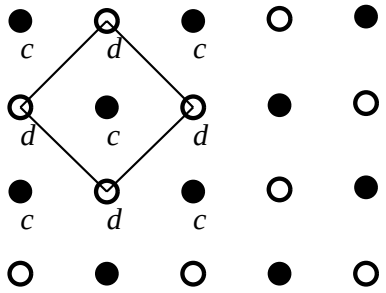

FIG. 2: The unit cell for the mean field Hamiltonian. Filled circles represent sites with M_i negative while open circles represent sites with M_i positive.

to define two new electron operators $c_i^\dagger$ and $d_i^\dagger$ that create electrons at the two inequivalent sites of the unit cell. In terms of these the Hamiltonian reads

$$H_{\rm MF}^{\uparrow} = \sum_i [\tilde{E}_0^- c_i^\dagger c_i + \tilde{E}_0^+ d_i^\dagger d_i] - t \sum_{i,\delta} (c_i^\dagger d_{i+\delta} + d_i^\dagger c_{i+\delta}), \tag{5}$$

where $\delta = \pm\hat{x}, \pm\hat{y}$ denotes the nearest neighbor vectors and $\tilde{E}_0^\pm = \tilde{E}_0 \pm \frac{U}{2}M$. Passing over to the Fourier space we can write

$$H_{\rm MF}^{\uparrow} = \sum_k \chi_{\mathbf{k}}^\dagger \begin{pmatrix} \tilde{E}_0^- & \epsilon_{\mathbf{k}} \\ \epsilon_{\mathbf{k}} & \tilde{E}_0^+ \end{pmatrix} \chi_{\mathbf{k}} \tag{6}$$

where $\epsilon_{\mathbf{k}} = -2t(\cos ak_x + \cos ak_y)$ and $\chi_{\mathbf{k}}^\dagger = (c_{\mathbf{k}}^\dagger, d_{\mathbf{k}}^\dagger)$. Now if we denote the 2×2 matrix appearing in the Eq. (6) $h_{\mathbf{k}}$ then we can write

$$H_{\rm MF}^{\uparrow} = \sum_k \chi_{\mathbf{k}}^\dagger h_{\mathbf{k}} \chi_{\mathbf{k}} = \sum_k (\chi_{\mathbf{k}}^\dagger U^\dagger)(U h_{\mathbf{k}} U^\dagger)(U\chi_{\mathbf{k}}) \equiv \sum_k \tilde{\chi}_{\mathbf{k}}^\dagger \tilde{h}_{\mathbf{k}} \tilde{\chi}_{\mathbf{k}} \tag{7}$$

where U is a unitary matrix ($U^\dagger U = 1$) that diagonalizes $h_{\mathbf{k}}$, i.e., $U h_{\mathbf{k}} U^\dagger = \begin{pmatrix} E_{\mathbf{k}}^- & 0 \\ 0 & E_{\mathbf{k}}^+ \end{pmatrix}$. The eigenvalues are obtained as usual from the solution of secular equation $\det(h_{\mathbf{k}} - E) = 0$ and read

$$E_{\mathbf{k}}^\pm = \tilde{E}_0 \pm \sqrt{(UM/2)^2 + \epsilon_{\mathbf{k}}^2}. \tag{8}$$

The Hamiltonian is diagonal, and can be written explicitly as

$$H_{\rm MF}^{\uparrow} = \sum_k [E_{\mathbf{k}}^- \tilde{c}_{\mathbf{k}}^\dagger \tilde{c}_{\mathbf{k}} + E_{\mathbf{k}}^+ \tilde{d}_{\mathbf{k}}^\dagger \tilde{d}_{\mathbf{k}}]. \tag{9}$$

Here $\tilde{c}_{\mathbf{k}}^\dagger$ and $\tilde{d}_{\mathbf{k}}^\dagger$ are the electron creation operators in the new basis and are related to the original electron operators by a unitary transformation $\tilde{\chi}_{\mathbf{k}}^\dagger \equiv (\tilde{c}_{\mathbf{k}}^\dagger, \tilde{d}_{\mathbf{k}}^\dagger) = \chi_{\mathbf{k}}^\dagger U^\dagger$. They represent the Bloch electrons occupying the upper and lower band, respectively.

For one electron per lattice site the lower band is completely filled while the upper band is empty. According to Eq. (8) the two bands are separated by a gap $\Delta = MU/2$ implying that the system is an insulator at half filling.