PHYS 6211: HW 2

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1 Problem 1

(a) The Hamiltonian for the tight-binding model is

$$\hat{H} = -t \sum_{i,j} \sum_{\sigma} (c^{\dagger}_{i\sigma} c_{j\sigma} + c^{\dagger}_{j\sigma} c_{i\sigma}).$$

Using the Fourier transforms

$$c_{i\sigma} = \frac{1}{\sqrt{N}} \sum_{k} c_{k\sigma} e^{ik\cdot R_i}$$

$$c^{\dagger}_{i\sigma} = \frac{1}{\sqrt{N}} \sum_{k} c^{\dagger}_{k\sigma} e^{-ik\cdot R_i}$$

we can rewrite the Hamiltonian as

$$-\frac{t}{N} \sum_{i,j} \sum_{\sigma} \sum_{kk'} (c^{\dagger}_{k\sigma} c_{k'\sigma} e^{-ik\cdot R_i} e^{ik'\cdot R_j} + c^{\dagger}_{k'\sigma} c_{k\sigma} e^{-ik'\cdot R_j} e^{ik\cdot R_i}).$$

Since we can traverse the reciprocal lattice by adding or subtract reciprocal vectors we can recast R_j as

$$R_j = R_i + G,$$

where G is a reciprocal lattice vector.

$$H = -\frac{t}{2N} \sum_{R_i} \sum_{\sigma} \sum_{kk'} (c^{\dagger}_{k\sigma} c_{k'\sigma} e^{i(k'-k)\cdot R_i} e^{ik'\cdot G} + c^{\dagger}_{k'\sigma} c_{k\sigma} e^{i(k'-k)\cdot R_i} e^{-ik'\cdot G}).$$

Here, we can use the identity

$$\sum_{R_i} e^{i(k'-k)\cdot R_i} = N\delta_{kk'}$$

to reduce the Hamiltonian to

$$H = -\frac{t}{2N} \sum_{k\sigma} 2c^{\dagger}_{k\sigma} c_{k\sigma} (e^{ik\cdot G} + e^{-ik\cdot G}) = \sum_{k\sigma} c^{\dagger}_{k\sigma} c_{k\sigma} \epsilon_k, \text{ where } \epsilon_k = -tcos(k \cdot G).$$

In the case of a 1D chain lattice with spacing $a = 1$, $G = \pm a\hat{e}_x$ and

$$\epsilon_{k,1D} = -tcos(ka) - tcos(-ka) = -2tcos(k).$$

In the case of a 2D square lattice with spacing $a = 1$, $G = \pm a\hat{e}_x \pm a\hat{e}_y$ and

$$\epsilon_{k,2D} = -tcos(k_x a) - tcos(-K - xa) - tcos(k_y a) - tcos(-k_y a) = -2t[cos(k_x) + cos(k_y)].$$

(b) For the 1D case, the density of states is

$$\rho_{1D}(\epsilon) = \int_{BZ} \frac{dk}{2\pi}\delta(\epsilon - \epsilon_k).$$

To make use of the property $\int \delta[f(x)]dx = \sum_i |f(x_i)|^{-1}$, where x_i are the zeros of f, we need to find the zeros of f.

$$f = \epsilon - \epsilon_k = 0 \rightarrow \epsilon = -2tcos(k) \rightarrow k = cos^{-1}\left(-\frac{\epsilon}{2t}\right)$$

$$f' = 2tsin(k) = 2tsin\left(cos^{-1}\left(-\frac{\epsilon}{2t}\right)\right) = 2t\sqrt{1 - \frac{\epsilon^2}{4t^2}} = \sqrt{4t^2 - \epsilon^2}, \text{ for } -1 \leq -\frac{\epsilon^2}{4t^2} \leq 1.$$

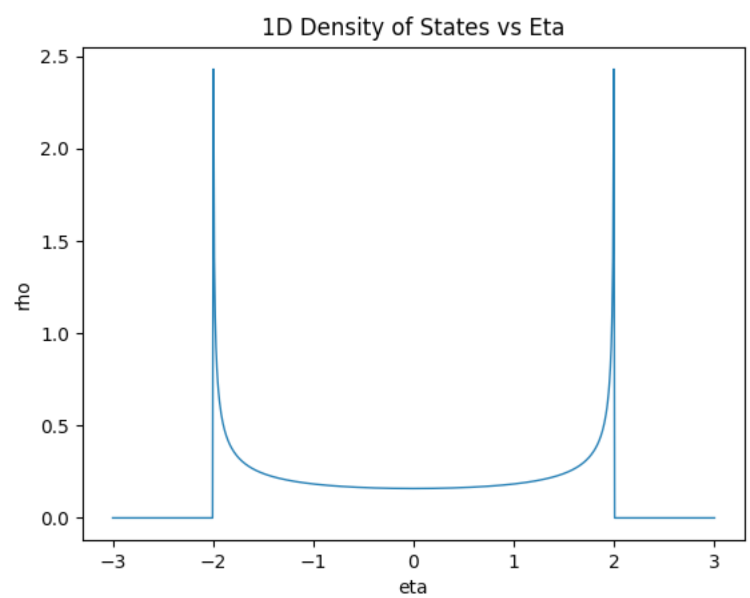
We can recast this as a step function to obey the condition $-1 \leq x \leq 1$ when we use $sin(cos^{-1}(x)) = \sqrt{1 + x^2}$,

$$\theta(2t - |\epsilon|).$$

Therefore,

$$\rho_{1D,\epsilon} = \frac{1}{2\pi}\frac{\theta(2t - |\epsilon|)}{\sqrt{4t^2 - \epsilon^2}}.$$

The plot of this function is



2 Problem 2

(a)

$$\hat{H} = -t\sum_{i,j}\sum_{\sigma}(a^{\dagger}_{i\sigma}b_{j\sigma} + b^{\dagger}_{j\sigma}a_{i\sigma}) = -\frac{t}{N}\sum_{ijkk'\sigma}(a^{\dagger}_{k\sigma}b_{k'\sigma}e^{ik\cdot R_i}e^{-ik'\cdot R_j} + b^{\dagger}_{k'\sigma}a_{k\sigma}e^{ik'\cdot R_j}e^{-ik\cdot R_i})$$

But we can replace R_j with nearest vectors,

$$R_j = R_i + \tau_i.$$

$$\hat{H} = -\frac{t}{N}\sum_{ikk'\sigma}(a^{\dagger}_{k\sigma}b_{k'\sigma}e^{i(k-k')\cdot R_i}e^{-ik'\cdot\tau_i} + b^{\dagger}_{k'\sigma}a_{k\sigma}e^{i(k'-k)\cdot R_j}e^{-ik\cdot\tau_i})$$

Using the identity

$$\sum_{R_i} e^{i(k'-k)\cdot R_i} = N\delta_{kk'},$$

$$\hat{H} = -t\sum_{k\sigma}\sum_{\tau_{1,2,3}}(a^{\dagger}_{k\sigma}b_{k\sigma}e^{-ik\cdot\tau} + b^{\dagger}_{k\sigma}a_{k\sigma}e^{-ik\cdot\tau})$$

(b) By defining quantum field operators we can easily rewrite the Hamiltonian as

$$\hat{H} = \sum_{k\sigma}\Psi^{\dagger}_{k\sigma}H_k\Psi_{k\sigma},\ \text{where}\ H_k = \begin{bmatrix} 0 & -te^{-ik\cdot\tau} \\ -te^{ik\cdot\tau} & 0 \end{bmatrix}.$$

$$\hat{H} = \sum_{k\sigma}\begin{bmatrix} a^{\dagger}_{k\sigma} b^{\dagger}_{k\sigma}\end{bmatrix}\begin{bmatrix} 0 & -te^{-ik\cdot\tau} \\ -te^{ik\cdot\tau} & 0 \end{bmatrix}\begin{bmatrix} a_{k\sigma} \\ b_{k\sigma}\end{bmatrix} = \sum_{k\sigma}\begin{bmatrix} a^{\dagger}_{k\sigma} b^{\dagger}_{k\sigma}\end{bmatrix}\begin{bmatrix} -te^{-ik\cdot\tau}b^{\dagger}_{k\sigma} \\ -te^{ik\cdot\tau}a^{\dagger}_{k\sigma}\end{bmatrix} =$$

$$= -t\sum_{k\sigma}\sum_{\tau_{1,2,3}}(a^{\dagger}_{k\sigma}b_{k\sigma}e^{-ik\cdot\tau} + b^{\dagger}_{k\sigma}a_{k\sigma}e^{-ik\cdot\tau}).$$

(c)

$$\det\begin{vmatrix} -\lambda & -te^{-ik\cdot\tau} \\ -te^{ik\cdot\tau} & -\lambda \end{vmatrix} = \lambda^2 - t^2e^{-ik\cdot\tau}e^{ik\cdot\tau} = 0$$

$$E_{\pm} = \pm t\sqrt{e^{-ik\cdot\tau}e^{ik\cdot\tau}}$$

$$e^{ik\cdot\tau} = e^{ik\cdot\tau_1} + e^{ik\cdot\tau_2} + e^{ik\cdot\tau_3} = e^{ik\cdot\tau_3}[1 + e^{ik\cdot(\tau_1-\tau_3)} + e^{ik\cdot(\tau_2-\tau_3)}] =$$

$$e^{-ik_xa}[1 + e^{i3k_xa/2}e^{i\sqrt{3}k_ya/2} + e^{i3k_xa/2}e^{-i\sqrt{3}k_ya/2}] = e^{-ik_xa}\left[1 + 2e^{i3k_xa/2}cos\left(\frac{\sqrt{3}k_ya}{2}\right)\right].$$

If we perform the same calculation for $e^{-ik\cdot\tau}$ and plug it into the expression for the energy bands we get

$$E_{\pm} = \pm t\sqrt{1 + 4cos\left(\frac{3k_x}{2}\right)cos\left(\frac{\sqrt{3}k_y}{2}\right) + 4cos^2\left(\frac{\sqrt{3}k_y}{2}\right)}.$$

So, there are clearly two energy bands that correspond to the upper and lower signs of $E_{\pm}$.