THE UNIVERSITY OF HONG KONG
DEPARTMENT OF PHYSICS

Solution for Assignment 1

Course: *Quantum Many-body Computation (PHYS8202)* – Prof.*Zi Yang Meng*
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Due date: *1st October, 2025*

1. **Density of States(DOS) of square lattice derivation**

We learn from the class that the 2D dispersion relation of a square lattice tight-binding model is

$$\epsilon(\mathbf{k}) = -2t(\cos(k_1) + \cos(k_2))$$

In the book *Lecture Notes on Electron Correlation and Magnetism* by Patrik Fazekas, page 165, the DOS of the square lattice tight binding band is in a closed form:

$$\rho(\epsilon) = \frac{1}{2\pi^2 t}\Theta(4t - |\epsilon|)K\left(1 - \frac{\epsilon^2}{16t^2}\right)$$

where K is the complete elliptic integral of the first kind. We can observe two features: the step-like discontinuities at the band edges, and the logarithmic singularity in the center. The latter can be obtained from the small-ϵ expansion:

$$\rho(\epsilon) \sim \frac{1}{2\pi^2 t}\ln\frac{t}{|\epsilon|}$$

(a) Try to derive the DOS of square lattice tight-binding model.

Solution: 1
Consider the definition of DOS:

$$\rho(\epsilon) = \frac{1}{N}\sum_{\mathbf{k}}\delta\big(\epsilon - \epsilon_{\mathbf{k}}\big) = \frac{1}{(2\pi)^2}\int_{-\pi}^{\pi}dk_1\int_{-\pi}^{\pi}dk_2\,\delta\big(\epsilon + 2t\cos(k_1) + 2t\cos(k_2)\big)$$

make the substitution:

$$\alpha = \frac{k_1 + k_2}{2}, \quad \beta = \frac{k_1 - k_2}{2}$$

After the substitution, the integration range becomes$\{\alpha, \beta | |\alpha| + |\beta| < \pi\}$. But we can extend the region to $\alpha \in (-\pi, \pi), \beta \in (-\pi, \pi)$, then DOS becomes

$$\rho(\epsilon) = \frac{1}{(2\pi)^2}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi}d\alpha d\beta\ \delta(\epsilon + 4t\cos(\alpha)\cos(\beta))$$

First integrate the β part. Use the identity

$$\delta[f(x)] = \sum_{k=1}^{N} \frac{\delta(x-x_k)}{|f'(x_k)|}$$

where x_k are the roots of $f(x)$. We have

$$\rho(\epsilon) = \frac{1}{8\pi^2 t} \int\limits_{|\cos(\alpha)|>\frac{|\epsilon|}{4t}} \frac{d\alpha}{\sqrt{\cos^2(\alpha) - \frac{\epsilon^2}{16}}}$$

If we want the integration to be non-zero, we obtain this condition:

$$|\epsilon| < 4t$$

The integration becomes

$$\rho(\epsilon) = \frac{1}{2\pi^2 t}\Theta(4t-|\epsilon|)\int_0^{\alpha_0} \frac{d\alpha}{\sqrt{\cos^2(\alpha) - \frac{\epsilon^2}{16t^2}}}$$

where $\cos(\alpha_0) = \frac{|\epsilon|}{4t}$. Make the substitution:

$$\sin(\theta) = \frac{\sin(\alpha)}{\sqrt{1-(\frac{\epsilon}{4t})^2}}$$

we finally have:

$$\begin{aligned}
\rho(\epsilon) &= \frac{1}{2\pi^2 t}\Theta(4t-|\epsilon|)\int_0^{\frac{\pi}{2}} \frac{d\theta}{\sqrt{1-(1-(\frac{\epsilon}{4t})^2)\sin^2(\theta)}} \\
&= \frac{1}{2\pi^2 t}\Theta(4t-|\epsilon|)K(1-(\frac{\epsilon}{4t})^2)
\end{aligned}$$

Solution: 2

Consider the one-body Green function:

$$G(z) = \sum_{\mathbf{k}} \frac{|\mathbf{k}\rangle\langle\mathbf{k}|}{z-\epsilon_{\mathbf{k}}}$$

$$G(\mathbf{r},\mathbf{r};z) = \langle\mathbf{r}|G(z)|\mathbf{r}\rangle = \sum_{\mathbf{k}} \frac{1}{z-\epsilon_{\mathbf{k}}} = \frac{N}{(2\pi)^2}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi} \frac{dk_1 dk_2}{z-\epsilon_{\mathbf{k}}}$$

where $z = \epsilon + i\eta$ Using the condition:

$$\lim_{\eta\to 0} \frac{1}{z-\epsilon_{\mathbf{k}}} = P\Big(\frac{1}{\epsilon-\epsilon_{\mathbf{k}}}\Big) - i\pi\delta(\epsilon-\epsilon_{\mathbf{k}})$$

one can obtain

$$\rho(\epsilon) = -\frac{1}{\pi N}\lim_{\eta\to 0} Im(G(\mathbf{r},\mathbf{r};z))$$

Now calculate $G(\mathbf{r}, \mathbf{r}; z)$. Make the substitution $\alpha = \frac{k_1+k_2}{2}, \beta = \frac{k_1-k_2}{2}$, we have

$$G(\mathbf{r}, \mathbf{r}; z) = \frac{N}{(2\pi)^2} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \frac{d\alpha d\beta}{z + 4t\cos(\alpha)\cos(\beta)}$$

Using the identity

$$\int \frac{dx}{a + b\cos x} = \frac{2}{\sqrt{a^2 - b^2}} \arctan\left(\sqrt{\frac{a-b}{a+b}} \tan\frac{x}{2}\right) + C \quad (|a| > |b|)$$

for $|z| > 4t$, we have

$$\begin{aligned} G(\mathbf{r}, \mathbf{r}; z) &= \frac{N}{(2\pi)^2} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \frac{d\alpha\, d\beta}{z + 4t\cos\alpha\cos\beta} \\ &= \frac{N}{\pi z} \int_0^{\pi} \frac{d\alpha}{\sqrt{1 - (4t/z)^2 \cos^2\alpha}} \\ &= \frac{2N}{\pi z} K(16t^2/z^2) \end{aligned}$$

$G(\mathbf{r}, \mathbf{r}; z)$ and $\frac{2}{\pi z} K(16t^2/z^2)$ are analytical, according to the identical theorem in complex analysis, $G(\mathbf{r}, \mathbf{r}; z) = \frac{2}{\pi z} K(16t^2/z^2)$. For $z = \epsilon + i\eta \quad (\eta \to 0, |\epsilon| < 4t)$, Using analytic continuation of K(m):

$$K(m) = \frac{1}{\sqrt{m}} \left[K\left(\frac{1}{m}\right) - iK\left(1 - \frac{1}{m}\right) \right] \quad (|m| > 1)$$

We have

$$G(\mathbf{r}, \mathbf{r}; z) = \frac{N}{2\pi t} \Big(K\Big(\frac{z^2}{16t^2}\Big) - iK\Big(1 - \frac{z^2}{16t^2}\Big) \Big)$$

Finally,

$$\rho(\epsilon) = -\frac{1}{\pi N} \lim_{\eta \to 0} Im(G(\mathbf{r}, \mathbf{r}; z)) = \frac{1}{2\pi^2 t} \Theta(4t - |\epsilon|) K\left(1 - \frac{\epsilon^2}{16t^2}\right)$$

(b) Try to obtain the logarithmic asymptotic behavior of the DOS at $\epsilon \to 0$.

Solution:
When $m \to 1$

$$K(m) \sim \frac{1}{2} \ln \frac{16}{1 - m}$$

So

$$\rho(\epsilon) \sim \frac{1}{2\pi^2 t} \ln \frac{t}{|\epsilon|} \quad (\epsilon \to 0)$$

2. **The gap equation**

We learn from the class that the gap equation for square lattice Hubbard model is

$$1 = U \int_0^{4t} \frac{\rho(\epsilon) d\epsilon}{\sqrt{\epsilon^2 + \Delta^2}}$$

(a) try to derive the relation in Jorge E.Hirsch's paper([Hirsch, Phys. Rev. B 31, 4403 (1985)]):

$$\Delta \sim t e^{-2\pi\sqrt{\frac{t}{U}}} \quad (d=2).$$

Solution:
When $\epsilon \to 0$, $\rho(\epsilon)$ is logarithmically divergent, the dominant contribution comes from the low-energy region. Thus, we directly approximate $\rho(\epsilon)$ by $\frac{1}{2\pi^2 t}\ln\frac{t}{\epsilon}$. Then the gap equation becomes:

$$1 \simeq U \int_0^{4t} d\epsilon \frac{1}{\sqrt{\epsilon^2+\Delta^2}} \frac{1}{2\pi^2 t} \ln\frac{t}{\epsilon}.$$

Making the substitution $\epsilon = \Delta \sinh u$, The integration becomes

$$1 = \frac{U}{2\pi^2 t} \int_0^{u_m} du \ln\frac{t}{\Delta \sinh(u)} = \frac{U}{2\pi^2 t}\left(u_m \ln\frac{t}{\Delta} - \int_0^{u_m} du \ln(\sinh(u))\right)$$

where u_m satisfies

$$\sinh(u_m) = \frac{4t}{\Delta}$$

We only consider the region where $U \to 0$ and $\Delta \to 0$, we have

$$u_m \sim \ln\frac{8t}{\Delta} \gg 1$$

The second term is

$$\int_0^{u_m} \ln(\sinh u)\, du = \frac{u_m^2}{2} - u_m \ln 2 + \frac{1}{2}\,\mathrm{Li}_2(e^{-2u_m}) - \frac{\pi^2}{12} = \frac{1}{2}(\ln\frac{8t}{\Delta})^2 + O(u_m)$$

where $Li_2(x)$ is the polylogarithmic function. So, the gap equation becomes

$$1 \sim \frac{U}{2\pi^2 t}\left(\ln\frac{8t}{\Delta}\ln\frac{t}{\Delta} - \frac{1}{2}(\ln\frac{8t}{\Delta})^2\right) = \frac{U}{4\pi^2 t}(\ln\frac{t}{\Delta})^2 + O(\ln\frac{t}{\Delta})$$

It turns out that

$$\Delta \sim t e^{-2\pi\sqrt{\frac{t}{U}}}$$

This is a simple version of the derivation. For a more rigorous one, you can find in the paper: https://arxiv.org/abs/2501.18141.

(b) Try to perform the momentum-space mean-field simulation and verify such result with your numerical data.

Solution: see the code in the class.