Report Problems

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In these problems, we explore the *Bloch electrons* in a 1D periodic potential.

I. SHORT SUMMARY OF BLOCH THEOREM

Let us consider the Schrödinger equation for a single electron with mass m in a potential $U(x)$:

$$\begin{aligned} H\psi(x) &= \left[-\frac{\hbar^2}{2m}\left(\frac{\partial}{\partial x}\right)^2 + U(x)\right]\psi(x) \\ &= \varepsilon\psi(x), \end{aligned} \tag{1}$$

where H is the Hamiltonian, ε is the eigenenergy, $\psi(x)$ is the eigenstate, and $U(x)$ is the periodic potential with the periodicity a, that is,

$$U(x+a) = U(x), \tag{2}$$

of N periods in a linear arrangement with periodic boundary conditions. Then, the celebrated *Bloch theorem* [1–3] states that $\psi(x)$, the eigenstates of the periodic Hamiltonian H in Eq. (1), can be written as

$$\psi_k(x) = e^{ikx}u_k(x), \tag{3}$$

where $u_k(x)$ is a periodic function,

$$u_k(x+a) = u_k(x). \tag{4}$$

Here, the index k is the *wave number*, which is written as

$$k = \frac{2\pi}{Na}n = \frac{2\pi}{L}n. \tag{5}$$

When L is finite (where $L = Na$, the total length) $\{k\}$ are taking discrete values with $n = 0, \pm 1, \pm 2, \cdots, \pm\frac{N}{2}$. With $L \to \infty$, that is, in the thermodynamic limit, k becomes continuum taking values from $-\frac{\pi}{a}$ to $\frac{\pi}{a}$, that is, values inside the *Brillouin zone*.

The Bloch theorem stated in Eq. (3) with Eq. (4) is equivalent to saying [1, 2]

$$\psi_k(x+a) = e^{ika}\psi_k(x). \tag{6}$$

II. 1D TIGHT-BINDING MODEL WITH SECOND QUANTIZATION [3]

Let us consider the following *1D tight-binding* Hamiltonian,

$$H = \sum_m \hbar\omega\left(\hat{a}_m^\dagger\hat{a}_m - \frac{1}{2}\right) - t\sum_m \hat{a}_m^\dagger\hat{a}_{m+1}, \tag{7}$$

which can be considered as an example of H in Eq. (1) after the second quantization [3], where $\hat{a}_m^\dagger$ and $\hat{a}_m$ are the fermionic creation and annihilation operators with the commutation relation:

$$\left\{\hat{a}_m, \hat{a}_{m'}^\dagger\right\} = \hat{a}_m\hat{a}_m^\dagger + \hat{a}_{m'}^\dagger\hat{a}_m = \delta_{mm'}. \tag{8}$$

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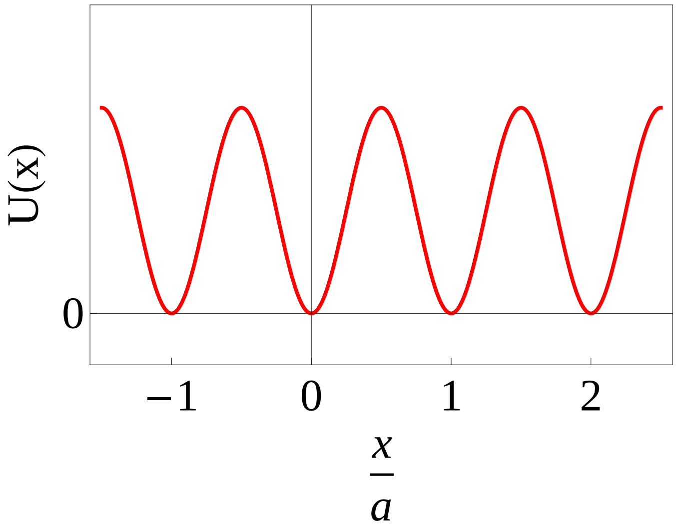

FIG. 1: A periodic potential $U(x)$.

Here the first term is the energies of isolated *fermionic* oscillators indexed by m with the *fermionic vacuum energy* of "$-\frac{1}{2}\hbar\omega$" (as opposed to the bosonic vacuum energy of "$+\frac{1}{2}\hbar\omega$") and the second term appears as a result of the tonneling between *nearest neighbors*, e.g., the m-th and the $(m+1)$-th fermionic oscillators. According to the Bloch theorem, the eigenstates of Eq. (7) are the Bloch states,

$$\psi_k(x) = \langle x|k\rangle = \langle x|\hat{a}_k^\dagger|0\rangle. \tag{9}$$

The relation between the isolated harmonic oscillator states (the *Wannier states*)

$$\psi_m(x) = \langle x|m\rangle = \langle x|\hat{a}_m^\dagger|0\rangle, \tag{10}$$

which must be the eigenstates if there were no tunneling, and the Bloch states $\psi_k(x)$ in Eq. (9) are

$$|k\rangle = \hat{a}_k^\dagger|0\rangle = \frac{1}{\sqrt{N}}\sum_m e^{ik(ma)}\hat{a}_m^\dagger|0\rangle = \frac{1}{\sqrt{N}}\sum_m e^{ik(ma)}|m\rangle \tag{11}$$

$$|m\rangle = \hat{a}_m^\dagger|0\rangle = \frac{1}{\sqrt{N}}\sum_k^{B.Z.} e^{-ik(ma)}\hat{a}_k^\dagger|0\rangle = \frac{1}{\sqrt{N}}\sum_k^{B.Z.} e^{-ik(ma)}|k\rangle. \tag{12}$$

Problem 1

Show that the Hamiltonian Eq. (7) can be diagonalized with $\hat{a}_k$ and $\hat{a}_k^\dagger$ to become

$$H = \sum_{k\geq 0}\left[(\hbar\omega - 2t\cos ka)\,\hat{a}_k^\dagger\hat{a}_k - \frac{1}{2}\hbar\omega\right]. \tag{13}$$

With one election in the *mode* k, that is, $\hat{a}_k^\dagger\hat{a}_k = 1$, we have an eigenenergy

$$\varepsilon_k = \frac{1}{2}\hbar\omega - 2t\cos ka. \tag{14}$$

III. 1D TIGHT-BINDING MODEL WITH INSTANTONS [4]

Let us see how the result in the section II can be obtained by instanton methods. Figure 1 shows the periodic potential $U(x)$, while Figure 2 shows the inverted one $-U(x)$. The instntons living there are thus more or less the

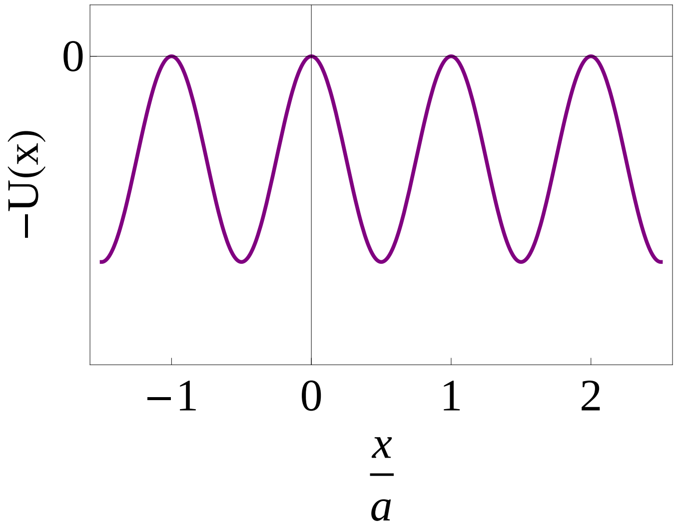

FIG. 2: An inverted periodic potential $-U(x)$.

same as in the double-well case we have learned. Here the probability $G(a,-a;\tau)$ of finding particle go from $-a$ to a was given by (*note 2017-10-16: Eq. (21)*)

$$G(a,-a;\tau)=\sqrt{\frac{m\omega}{\pi\hbar}}e^{-\frac{\omega\tau}{2}}\sum_{\text{n:odd}}\frac{1}{n!}\left(\tau K e^{-\frac{nS_{in}}{\hbar}}\right)^n. \tag{15}$$

Now, the difference is that the instantons can start at any position, $x=am$, and go to the next one, $x=(m+1)a$; likewise, the anti-instantons can start at $x=am$, and go to the next one, $x=(m-1)a$. We thus have the probability $G(j_f,j_i;\tau)$ of finding an electron go from the j_i-th site at $x=j_ia$ to the j_f-th site at $x=j_fa$ as

$$G(j_f,j_i;\tau)=\sqrt{\frac{m\omega}{\pi\hbar}}e^{-\frac{\omega\tau}{2}}\sum_{n=0}^{\infty}\underbrace{\frac{1}{n!}\left(\tau K e^{-\frac{nS_{in}}{\hbar}}\right)^n}_{n\ \text{instanton}}\sum_{\bar{n}=0}^{\infty}\underbrace{\frac{1}{\bar{n}!}\left(\tau K e^{-\frac{nS_{in}}{\hbar}}\right)^{\bar{n}}}_{\bar{n}\ \text{anti-instanton}}\ \delta_{(n-\bar{n})-(j_f-j_i)}. \tag{16}$$

Problem 2

Using the following identity with a dummy index θ

$$\delta_{ab}=\int_0^{2\pi}\frac{d\theta}{2\pi}e^{i\theta(a-b)}, \tag{17}$$

show that

$$G(j_f,j_i;\tau)=\int_0^{2\pi}\frac{d\theta}{2\pi}\left(\sqrt{\frac{m\omega}{\pi\hbar}}e^{i(j_f-j_i)\theta}\right)\exp\left[-\frac{\tau}{\hbar}\left(\frac{1}{2}\hbar\omega-2\hbar K e^{-\frac{S_{in}}{\hbar}}\cos\theta\right)\right]. \tag{18}$$

Since $G(j_f,j_i;\tau)$ is originally meant to be

$$\begin{aligned} G(j_f,j_i;\tau) &= \langle j_f|e^{-\frac{\tau}{\hbar}H}|j_i\rangle \\ &= \int_0^{2\pi} d\theta\langle j_f|\theta\rangle e^{-\frac{\tau}{\hbar}\varepsilon_\theta}\langle\theta|j_i\rangle, \end{aligned} \tag{19}$$

from Eq. (18) we have

$$\varepsilon_\theta=\frac{1}{2}\hbar\omega-2\hbar K e^{-\frac{S_{in}}{\hbar}}\cos\theta \tag{20}$$

and

$$\langle j|\theta\rangle=\left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}}\frac{1}{\sqrt{2\pi}}e^{ij\theta}. \tag{21}$$

Now we see that ε_θ in Eq. (20) corresponds to Eq. (14) with

$$ka \sim \theta \tag{22}$$

and

$$t \sim \hbar K e^{-\frac{S_{in}}{\hbar}}, \tag{23}$$

while $\langle j|\theta\rangle$ in Eq. (21) corresponds to Eq. (9). Indeed,

$$\begin{aligned}
\langle x|k\rangle &= \langle x|\frac{1}{\sqrt{N}}\sum_{m'} e^{ikm'a}|m'\rangle \\
&\sim \langle x|\frac{1}{\sqrt{2\pi}}\int dx'_m e^{ikx'_m}|x'_m\rangle = \frac{1}{\sqrt{2\pi}}\int dx'_m e^{ikx'_m} \underbrace{\langle x|x'_m\rangle}_{\sim\delta_{xx'_m}\langle x|0\rangle} \\
&\sim \frac{1}{\sqrt{2\pi}}e^{ikx}\langle x|0\rangle = \frac{1}{\sqrt{2\pi}}e^{ij\theta}\left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}}
\end{aligned} \tag{24}$$

with $m'a \sim x'_m$ and $x \sim ja$.

[1] M. Tinkham, *Group theory and Quantum Mechanics* (Dover, New York, 2003).
[2] N. W. Ashcroft and N. D. Mermin, *Solid State Physics* (Brooks/Cole, Belmont, 1976).
[3] A. Altland and B. D. Simons, *Condensed Matter Field Theory*, 2nd ed. (Cambridge University Press, Cambridge, 2010).
[4] Sidney Coleman, *Aspect of Symmetry*, (Cambridge University Press, Cambridge 1985), Chapter 7.