Report Problems

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Through the following problems, we shall explore the celebrated *Su-Schrieffer-Heeger model* of polyacetylene [1].

I. TIGHT-BINDING HAMILTONIAN [2]

For electrons in 1D periodic lattice potential (length: L) the Bloch states diagonalize the Hamitonian H_0, that is,

$$H_0 = \sum_{k_l} \epsilon_{k_l} \hat{a}^\dagger_{k_l} \hat{a}_{k_l}, \tag{1}$$

where $\hat{a}_{k_l}$ and $\hat{a}^\dagger_{k_l}$ are the annihilation and creation operators for an electron in a Bloch state indexed by the wave vector $k_l = \frac{2\pi}{L} \times l$. Let us see this problem in the real space indexed by $R_n = a \times n$, a vector specifying an atomic site, as opposed to k_l. Note that the atomic site separation is $a = \frac{L}{N}$, where N is the number of the atomic sites within the length L.

It is helpful to introduce the so-called *Wannier states*, for which the annihilation and creation operators, $\hat{a}_n$ and $\hat{a}^\dagger_n$ are respectively defined by

$$\hat{a}_n = \frac{1}{\sqrt{N}} \sum_{k_l} e^{ik_l \cdot R_n} \hat{a}_{k_l} \tag{2}$$

$$\hat{a}^\dagger_n = \frac{1}{\sqrt{N}} \sum_{k_l} e^{-ik_l \cdot R_n} \hat{a}^\dagger_{k_l}. \tag{3}$$

The inverse of each expression reads

$$\hat{a}_{k_l} = \frac{1}{\sqrt{N}} \sum_{n} e^{-ik_l \cdot R_n} \hat{a}_n \tag{4}$$

$$\hat{a}^\dagger_{k_l} = \frac{1}{\sqrt{N}} \sum_{n} e^{ik_l \cdot R_n} \hat{a}^\dagger_n. \tag{5}$$

With these expressions the Hamiltonian Eq. (1) becomes

$$H_0 = \frac{1}{N} \sum_{ij} \sum_{k_l} e^{ik_l \cdot (R_n - R_m)} \epsilon_{k_l} \hat{a}^\dagger_n \hat{a}_m = \sum_{nm} \hat{a}^\dagger_n t_{nm} \hat{a}_m, \tag{6}$$

where we have defined the *hopping matrix* t_{nm} as

$$t_{nm} = \frac{1}{N} \sum_{k_l} \epsilon_{k_l} e^{ik_l \cdot (R_n - R_m)}. \tag{7}$$

Equation (6) is called *tight-binding Hamiltonian* and describes electrons hopping from one lattice site n to the other m, whose strength is dictated by the hopping matrix element t_{nm} in Eq. (7). You can see that when $\epsilon_{k_l} = \text{const.}$, that is, single-particle Hamiltonian H_0 merely represents isolated atom and index k_l is irrelevant, then $t_{nm} \propto \delta_{nm}$ and there are no hopping. The dispersion $\epsilon_{k_l} \neq \text{const.}$ is thus pertinent to realize the inter-atomic hopping.

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Problem 1

By setting

$$t_{nm} = -t\delta_{n,m\pm1}, \tag{8}$$

show that the tight binding Hamiltonian Eq. (6) can be diagonalized in terms of Bloch states and becomes

$$H_0 = \sum_{k_l} \left(-2t\cos(k_l a)\right) \hat{a}^\dagger_{k_l} \hat{a}_{k_l}. \tag{9}$$

II. PEIERLS INSTABILITY

Polyacetylene, $(CH)_x$, is the simplest linear conjugated polymer, which can be microscopically modeled as a simple Hamiltonian proposed by Su, Shrieffer, and Heeger as

$$H_{\rm SSH} = \sum_{n=-\frac{N}{2}}^{\frac{N}{2}} -t\left(1+u_n\right)\left(\hat{a}^\dagger_n \hat{a}_{n+1} + h.c.\right), \tag{10}$$

where

$$u_n = (-1)^n \alpha. \tag{11}$$

This Hamiltonian is the variant of H_0 given by Eq. (6) in a sense that the original symmetric hopping matrix $t_{nm} = -t\delta_{n,m\pm1}$ given by Eq. (8) is modulated by the lattice distortion and becomes asymmetric. By distinguishing the two atomic sites n =odd and n =even and doubling the size of the unit cell, the tight binding Hamiltonian Eq. (10) can be modified into

$$H_{\rm SSH} = \sum_{n=-\frac{N}{4}}^{\frac{N}{4}} (-t)\left\{(1+\alpha)\left(\hat{b}^\dagger_n \hat{c}_n + h.c.\right) + (1-\alpha)\left(\hat{c}^\dagger_n \hat{b}_{n+1} + h.c.\right)\right\}. \tag{12}$$

Problem 2

(1) Using the expressions

$$\hat{b}_{k_l} = \frac{1}{\sqrt{\frac{N}{2}}} \sum_n e^{-i2k_l\cdot R_n} \hat{b}_n \tag{13}$$

$$\hat{c}_{k_l} = \frac{1}{\sqrt{\frac{N}{2}}} \sum_n e^{-i2k_l\cdot R_n} \hat{c}_n, \tag{14}$$

and the similar expressions for $\hat{b}^\dagger_{k_l}$ and $\hat{c}^\dagger_{k_l}$, show that the Hamiltonian, Eq. (12), can be given by

$$H_{\rm SSH} = -t\sum_{k_l} \left[b^\dagger_{k_l}, c^\dagger_{k_l}\right] \begin{bmatrix} 0 & (1+\alpha)+(1-\alpha)\,e^{2ik_l a} \\ (1+\alpha)+(1-\alpha)\,e^{2ik_l a} & 0 \end{bmatrix} \begin{bmatrix} b_{k_l} \\ c_{k_l} \end{bmatrix} \tag{15}$$

(2) By diagonalizing the 2×2 matrix, show that the energy eigenvalues are

$$E(k_l)_\pm = \pm 2t\left[1+\left(\alpha^2-1\right)\sin^2(k_l a)\right]^{\frac{1}{2}}. \tag{16}$$

As shown in Fig. 1 the energy eigenvalues E_{k_l}/t show a gap for the asymmetric hopping due to lattice distortion (for $\alpha \neq 0$). It is known that the the distorted lattice system has the lower energy for half-filling (electrons occupy lower branch) and the lattice without distortion is unstable, the phenomenon known as *Peierls instability* [2].

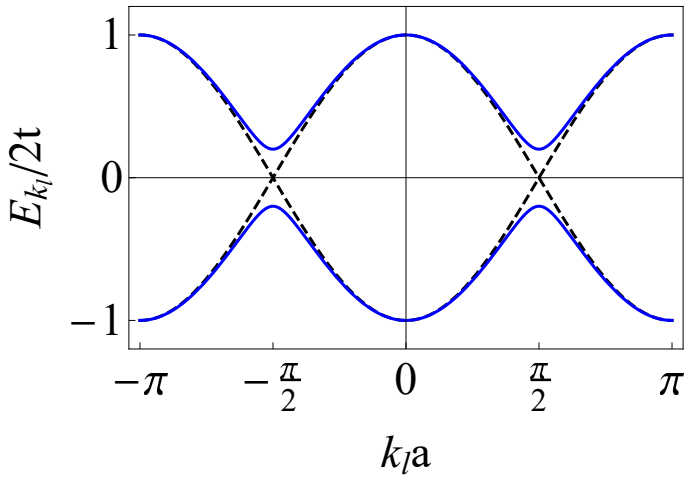

FIG. 1. Energy eigenvalues $E_{k_l}/2t$ given by Eq. (16) as a function of k_l. Black dotted line is for symmetric hopping, that is, no lattice distortion ($\alpha = 0$); Blue line is for asymmetric hopping due to lattice distortion ($\alpha = 0.2$).

III. BERRY PHASE AND ELECTRIC POLARIZATION [1–3]

Now let us seek the connection between the SSH model and the Berry phase, the later of which we have learned in the Lecture. To see this connection, we shall reverse the usual *second quantization* procedure, that is, from the second quantized Hamiltonian to the single-particle Hamiltonian. The single-particle Hamiltonian $H_{\text{Berry}}(\boldsymbol{R}(k_l))$ can be found in the second quantized Hamiltonian H_{SSH} given by Eq. (15) as

$$H_{\text{SSH}} = \sum_{k_l} \left[b_{k_l}^\dagger, c_{k_l}^\dagger \right] H_{\text{Berry}}(\boldsymbol{R}(k_l)) \begin{bmatrix} b_{k_l} \\ c_{k_l} \end{bmatrix}, \tag{17}$$

where

$$H_{\text{Berry}}(\boldsymbol{R}(k_l)) = -t \begin{bmatrix} 0 & (1+\alpha) + (1-\alpha)\, e^{2ik_l a} \\ (1+\alpha) + (1-\alpha)\, e^{-2ik_l a} & 0 \end{bmatrix} = \boldsymbol{R}(k_l) \cdot \boldsymbol{\sigma}. \tag{18}$$

Here, $\boldsymbol{\sigma} = \begin{bmatrix} \sigma_x \\ \sigma_y \\ \sigma_z \end{bmatrix}$ are the Pauli matrices and

$$\boldsymbol{R}(k_l) = \begin{bmatrix} X(k_l) \\ Y(k_l) \\ Z(k_l) \end{bmatrix} = -t \begin{bmatrix} (1+\alpha) + (1-\alpha)\cos(2k_l a) \\ -(1-\alpha)\sin(2k_l a) \\ 0 \end{bmatrix}. \tag{19}$$

Figure 2 shows the trajectories of $\boldsymbol{R}(k_k)/(-t)$ as k_l is swept from $-\frac{\pi}{2a}$ to $\frac{\pi}{2a}$ for various values of α.

The Berry curvature can then be calculated from the formula [see e.g., Eq. (B11) in the Lecture note 4: *Berry phase and Dirac monopole*]:

$$\begin{aligned}
\boldsymbol{\Omega}_+(k_l) &= \frac{i}{\left(E(k_l)_- - E(k_l)_-\right)^2} \left(\langle +(\boldsymbol{R}(k_l)) | \boldsymbol{\nabla} H_{\text{Berry}}(\boldsymbol{R}(k_l)) | -(\boldsymbol{R}(k_l)) \rangle \times \langle -(\boldsymbol{R}(k_l)) | \boldsymbol{\nabla} H_{\text{Berry}}(\boldsymbol{R}(k_l)) | +(\boldsymbol{R}(k_l)) \rangle \right) \\
&= \frac{i}{\left(E(k_l)_- - E(k_l)_-\right)^2} \begin{bmatrix} \left\langle +(\boldsymbol{R}(k_l)) \middle| \frac{\partial H_{\text{Berry}}(\boldsymbol{R}(k_l))}{\partial X} \middle| -(\boldsymbol{R}(k_l)) \right\rangle \\ \left\langle +(\boldsymbol{R}(k_l)) \middle| \frac{\partial H_{\text{Berry}}(\boldsymbol{R}(k_l))}{\partial Y} \middle| -(\boldsymbol{R}(k_l)) \right\rangle \\ \left\langle +(\boldsymbol{R}(k_l)) \middle| \frac{\partial H_{\text{Berry}}(\boldsymbol{R}(k_l))}{\partial Z} \middle| -(\boldsymbol{R}(k_l)) \right\rangle \end{bmatrix} \times \begin{bmatrix} \left\langle -(\boldsymbol{R}(k_l)) \middle| \frac{\partial H_{\text{Berry}}(\boldsymbol{R}(k_l))}{\partial X} \middle| +(\boldsymbol{R}(k_l)) \right\rangle \\ \left\langle -(\boldsymbol{R}(k_l)) \middle| \frac{\partial H_{\text{Berry}}(\boldsymbol{R}(k_l))}{\partial Y} \middle| +(\boldsymbol{R}(k_l)) \right\rangle \\ \left\langle -(\boldsymbol{R}(k_l)) \middle| \frac{\partial H_{\text{Berry}}(\boldsymbol{R}(k_l))}{\partial Z} \middle| +(\boldsymbol{R}(k_l)) \right\rangle \end{bmatrix} \\
&= \frac{i}{\left(E(k_l)_- - E(k_l)_-\right)^2} \begin{bmatrix} \langle +(\boldsymbol{R}(k_l)) | \sigma_x | -(\boldsymbol{R}(k_l)) \rangle \\ \langle +(\boldsymbol{R}(k_l)) | \sigma_y | -(\boldsymbol{R}(k_l)) \rangle \\ 0 \end{bmatrix} \times \begin{bmatrix} \langle -(\boldsymbol{R}(k_l)) | \sigma_x | +(\boldsymbol{R}(k_l)) \rangle \\ \langle -(\boldsymbol{R}(k_l)) | \sigma_y | +(\boldsymbol{R}(k_l)) \rangle \\ 0 \end{bmatrix},
\end{aligned} \tag{20}$$

where $|\pm(\boldsymbol{R}(k_l))\rangle$ are the instantaneous eigenstates of $H_{\text{Berry}}(\boldsymbol{R}(k_l))$.

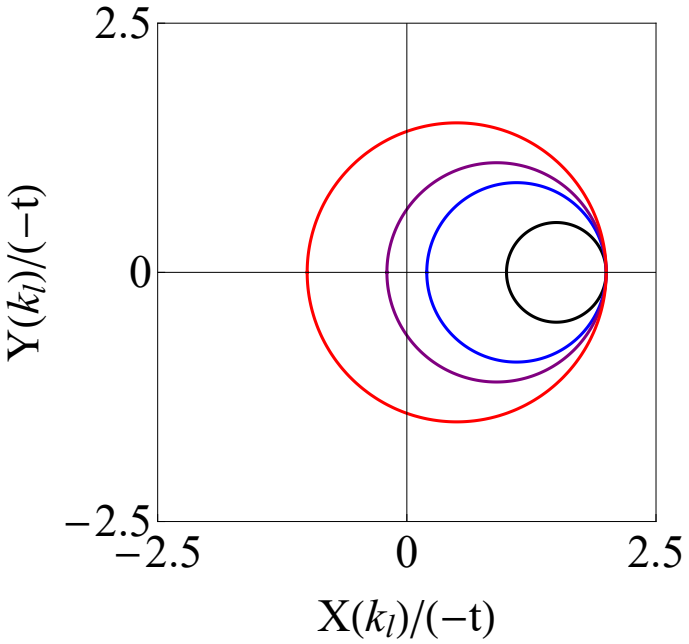

FIG. 2. Trajectory of $\boldsymbol{R}(k_k)/(-t)$ (within XY-plane) as k_l swept from $-\frac{\pi}{2a}$ to $\frac{\pi}{2a}$ for various values of α. Black: $\alpha = 0.5$; Blue: $\alpha = 0.1$; Purple: $\alpha = -0.1$, Red: $\alpha = -0.5$

Problem 3

Following the argument found in Sec. 3 of Berry's original paper [3] (or, otherwise, lengthy brute-force calculation), show that the Berry phase (Zak phase) can be given by

$$\gamma = \iint_{\mathcal{C}} \boldsymbol{\Omega}_+(k_l) \cdot d\boldsymbol{S} = \pi \tag{21}$$

for $\alpha < 0$, namely, the cases where the XY trajectories $\mathcal{C}$ [e.g., the purple and the red circles shown the in Fig. 2] encircles origin, that is, the degeneracy point, and

$$\gamma = \iint_{\mathcal{C}} \boldsymbol{\Omega}_+(k_l) \cdot d\boldsymbol{S} = 0 \tag{22}$$

for $\alpha > 0$, namely, the cases where the XY trajectories $\mathcal{C}$ [e.g., the black and the blue circles shown in Fig. 2] do not encircle the origin, that is, the degeneracy point. Here, the integrals are performed over the surfaces enclosing the XY trajectories $\mathcal{C}$.

This suggests that for polyacetylene with lattice distortion of $\alpha < 0$ there is the electric polarization of $\frac{e}{2}$ while for that with $\alpha > 0$ there is no electric polarization.

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[1] W. P. Su, J. R. Schrieffer, and A. J. Heeger, Phys. Rev. Lett. **42**, 1698 (1979).
[2] A. Altland and B. D. Simons, *Condensed Matter Field Theory*, 2nd ed. (Cambridge University Press, Cambridge, 2010).
[3] M. V. Berry, Proc. R. Soc. Lond. A **392**, 45 (1984).