Modern Topics in Solid-State Theory: Exercise 1.

Polyacetylene

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1. Energy spectrum and symmetries

The Su-Schrieffer-Heeger (SSH) model describes the low-energy electron physics of polyacetylene. It is defined on a chain with two sites in the unit cell denoted by A/B. In real space the Hamiltonian of this model is given by

$$\mathcal{H} = \sum_i \left[(t+\delta t) c_{Ai}^\dagger c_{Bi} + (t-\delta t) c_{Ai+1}^\dagger c_{Bi} + \text{h.c.} \right], \tag{1}$$

where δt parametrizes the dimerization, and c_{Ai} describes the electron annihilation operator on the lattice site (A, i).

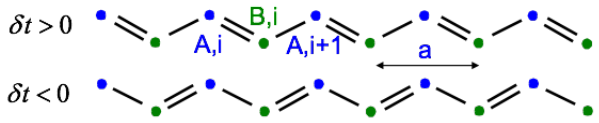

Figure 1: Dimerization patterns occurring in polyacetylene.

(a) Performa a Fourier transform and show that in momentum space the Hamiltonian is given by

$$\mathcal{H} = \sum_k \begin{pmatrix} c_{Ak}^\dagger & c_{Bk}^\dagger \end{pmatrix} h(k) \begin{pmatrix} c_{Ak} \\ c_{Bk} \end{pmatrix}.$$

Determine the form of $h(k)$.

(b) Show that the Hamiltonian $h(k)$ satisfies the following symmetries

$$\begin{aligned} &\text{Time-reversal symmetry:} && u_T h^T(-k) u_T^\dagger = +h(k), \quad \text{with } u_T = \sigma_0, \\ &\text{Particle-hole symmetry:} && u_C h^T(-k) u_C^\dagger = -h(k), \quad \text{with } u_C = \sigma_3, \\ &\text{Sublattice symmetry:} && Sh(k) + h(k)S = 0, \quad \text{with } S = u_T u_C = \sigma_3. \end{aligned} \tag{2}$$

Using the sublattice symmetry, show that the energy spectrum of $h(k)$ is symmetric with respect to zero energy. I.e., show that $\Psi(-E) = S\Psi(E)$, where Ψ and E are the eigenfunctions and eigenvalues of $h(k)$, respectively.

(c) Compute the energy spectrum of model (1) with open boundary conditions by numerically diagonalizing the Hamiltonian. Plot the energy spectrum as a function of dimerization δt.

(d) Compute the local density of states of the Hamiltonian and show that in the topological phase there are zero-energy end states.

2. Topological invariant and domain wall states

(a) The winding number is given by

$$\nu = \frac{i}{2\pi} \int dk \left[q^{-1} \partial_k q \right], \tag{3}$$

with $q(k) = \hat{h}(k)/\lambda(k)$, where $\lambda(k)$ denotes the positive energy eigenvalues and $\hat{h}(k)$ is the off-diagonal part of the Hamiltonian. Compute the winding number ν as a function of δt and show that ν is non-zero whenever there is a zero-energy end state.

(b) Close to the topological phase transition point, at $\delta t = 0$, the Hamiltonian $h(k)$ can be expanded around $k_0 = \pi$. Show that this low-energy expansion gives

$$h_{\text{eff}}(k) = vk\sigma_y + m(x)\sigma_x, \tag{4}$$

with $m(x) = 2\delta t$ and $v = (t - \delta t)$. At a domain wall the mass $m(x)$ changes from positive to negative, for example $m(x) = m_0 \tanh x$. Using the wavefunction ansatz $\psi_0 = \chi e^{-\int_0^x m(x')dx'}$ derive the form of the domain wall bound state with energy $E = 0$.

3. Fractional charge (optional)

A charge one-half fraction is bound at domain walls that separate the two different dimerization patterns in polyacetylene (see Fig. 1). To show this, consider the following two Hamiltonians

$$\begin{aligned} h_{\text{eff}} &= k\sigma_y + m(x)\sigma_x, \qquad \lim_{x\to\pm\infty} m(x) = \pm m_0, \qquad x \in \mathbb{R}. \\ h^0_{\text{eff}} &= k\sigma_y + m_0\sigma_x, \end{aligned} \tag{5}$$

where h_0 is a reference Hamiltonian that does not have any domain walls (m_0 does not depend on x). We introduce the two complete sets of orthonormal eigenfunctions

$$h^0_{\text{eff}}\Psi_0(E_0, x) = E_0\Psi_0(E_0, x), \qquad E_0 \in \mathbb{R},$$

and

$$h_{\text{eff}}\Psi(E, x) = E\Psi(E, x), \qquad E \in \mathbb{R},$$

for any $x \in \mathbb{R}$. The charge at the domain wall is measured relative to that without the domain wall,

$$Q = \int_{-\infty}^{+\infty} dx \int_{-\infty}^{0} dE \left[\rho(E, x) - \rho_0(E, x) \right], \tag{6}$$

with the charge densities

$$\rho_0(E_0, x) = \Psi_0^\dagger(E_0, x)\Psi_0(E_0, x), \qquad \rho(E, x) = \Psi^\dagger(E, x)\Psi(E, x), \tag{7a}$$

for any $x \in \mathbb{R}$.

(a) By numerically diagonalizing a lattice version of the Hamitlonians in Eq. (5) compute the charge Q at the domain wall.

(b) Using an analytical derivation, show that the value $Q = 1/2$ follows from the spectral symmetry, $\Psi(-E) = S\Psi(E)$, of the Hamiltonian.