Continuum Model of Localized States at a Domain Wall

- Envelope-Function Approximation
- EFA for 1D chain
- EFA for metallic SSH and the masleess 1D Dirac equation
- EFA for gaped SSH and bound states at interfaces
- EFA for QWZ

Envelope-Function Approximation: Recipie

- 1. Rely on "spatially slowly varying" wave functions
- 2. Find relevant energy/momentum range
- 3. Expand the Hamiltonian around relevant momenta
- 4. Replace relevant momentum by derivatives

EFA for 1D chain



$$H_i = H_{per} + V o rac{p^2}{2m} + V(x)$$

EFA for metallic SSH

$H(k) = [v + w \cos(k)] \sigma_x + w \sin(k) \sigma_y$ -1 (c) $H(k_0+q)pprox -wq\sigma_w$ v = u"masless Dirac fermion" π

EFA for gapped SSH



"massive Dirac Hamiltonian"



This language gives a single, sublattice polarized zero energy state localized on the interface also!

$$arphi(x) = \left(egin{array}{c} 0 \ 1 \end{array}
ight) f(x) \ f(x) \propto e^{-rac{1}{w}\int_0^x dx' M(x')}$$

EFA for QWZ



 $\hat{H}(\mathbf{k}_0+\mathbf{q})pprox(u+2)\sigma_z+q_x\sigma_x+q_y\sigma_y$ M

EFA for QWZ



$$arphi(x,y)=\left(egin{array}{c}1\-1\end{array}
ight)e^{iq_xx}f(y)$$

$$f(y)=e^{-\int_0^y dy' M(y')}$$



Envelope-function Hamiltonian in one dimension (1)

Consider the SSH model. Let the intercell hopping w = 1 be homogeneous. The intracell hopping v changes smoothly in space, described by the function v(x). The system is in the nearly metallic case everywhere, that is, $|v(x) - 1| \ll 1$. Which one is the low-energy effective Hamiltonian of the system?

(a)
$$\hat{H} = v(x)\hat{\sigma}_x + \hat{p}\,\hat{\sigma}_y$$

(b) $\hat{H} = [v(x) + 1]\hat{\sigma}_x + \hat{p}\,\hat{\sigma}_y$
(c) $\hat{H} = [v(x) - 1]\hat{\sigma}_x - \hat{p}\,\hat{\sigma}_y$

(d) None of the above.



Envelope-function Hamiltonian in one dimension (2)

Consider the SSH model. Let the intracell hopping v = 1 be homogeneous. The intercell hopping w changes smoothly in space, described by the function w(x). The system is in the nearly metallic case everywhere, that is, $|1 - w(x)| \ll 1$. Which one is the low-energy effective Hamiltonian of the system?

(a)
$$\hat{H} = \hat{\sigma}_x + w(x)\hat{p}\,\hat{\sigma}_y$$

(b) $\hat{H} = [1 + w(x)]\hat{\sigma}_x + w(x)\hat{p}\,\hat{\sigma}_y$
(c) $\hat{H} = [1 - w(x)]\hat{\sigma}_x - w(x)\hat{p}\,\hat{\sigma}_y$
(d) $\hat{H} = [1 - w(x)]\hat{\sigma}_x - \frac{1}{2}\left\{w(x), \hat{p}\right\}\,\hat{\sigma}_y$



Envelope-function Hamiltonian in two dimensions (1)

The bulk momentum-space Hamiltonian of the Qi-Wu-Zhang model reads

$$\hat{H} = \sin(k_x)\hat{\sigma}_x + \sin(k_y)\hat{\sigma}_y + \left[u + \cos(k_x) + \cos(k_y)\right]\hat{\sigma}_z$$

For u = 2, which one is the low-energy envelope-function Hamiltonian?

(a)
$$\hat{H}_{\text{EFA}} = \hat{p}_x \hat{\sigma}_x + \hat{p}_y \hat{\sigma}_y$$

(b)
$$\hat{H}_{\text{EFA}} = -\hat{p}_x\hat{\sigma}_x - \hat{p}_y\hat{\sigma}_y$$

(c)
$$\hat{H}_{\text{EFA}} = \hat{p}_x \hat{\sigma}_x - \hat{p}_y \hat{\sigma}_y$$

(d) None of them.



Envelope-function Hamiltonian in two dimensions (2)

The bulk momentum-space Hamiltonian of the Qi-Wu-Zhang model reads

$$\hat{H} = \sin(k_x)\hat{\sigma}_x + \sin(k_y)\hat{\sigma}_y + \left[u + \cos(k_x) + \cos(k_y)\right]\hat{\sigma}_z$$

For u = 0, which one is the low-energy envelope-function Hamiltonian?

(a)
$$\hat{H}_{\text{EFA}} = \hat{p}_x \hat{\sigma}_x + \hat{p}_y \hat{\sigma}_y$$

(b) $\hat{H}_{\text{EFA}} = -\hat{p}_x \hat{\sigma}_x - \hat{p}_y \hat{\sigma}_y$

(c) None of them.

(d) Both (a) and (b).



Scattering in one dimension (1)

An electron is moving in a nearly metallic SSH chain. It is described by the 1D massive Dirac Hamiltonian $\hat{H} = M\hat{\sigma}_x - w\,\hat{p}\,\hat{\sigma}_y$. It is scattered by a high, smooth potential barrier, $\hat{U} = V(x)\hat{\sigma}_0$. What is the probability of reflection from the barrier?



(c) between 0 and 1

(d) surprisingly, it is greater than 1, known as the 'Klein paradox'

Scattering in one dimension (2)

An electron is moving in a metallic SSH chain. It is described by the 1D massless Dirac Hamiltonian $\hat{H} = -w \hat{p} \hat{\sigma}_y$. It is scattered by a high, smooth potential barrier, $\hat{U} = V(x)\hat{\sigma}_0$. What is the probability of reflection from the barrier?



(c) between 0 and 1

(d) surprisingly, it is greater than 1, known as the 'Klein paradox'

Scattering in one dimension (3)

An electron is moving in a nearly metallic, inhomogeneous SSH chain. It is described by the 1D massive Dirac Hamiltonian $\hat{H} = M(x)\hat{\sigma}_x - w\,\hat{p}\,\hat{\sigma}_y$. The spatial dependence of the mass is shown in the figure. What is the probability of reflection from the barrier?



(c) between 0 and 1

(d) surprisingly, it is greater than 1, known as the 'Klein paradox'

Scattering in two dimensions (1)

An electron is moving in a metallic QWZ lattice along x. It is described by a 2D massless Dirac Hamiltonian $\hat{H} = \hat{p}_x \hat{\sigma}_x + \hat{p}_y \hat{\sigma}_y$. It is scattered by a high, smooth potential barrier, $\hat{U} = V(x)\hat{\sigma}_0$. What is the probability of reflection from the barrier?



(a) 0

(b) 1

(c) between 0 and 1, and the value depends on the details of V(x)

(d) between 0 and 1, but the value does not depend on the details of V(x)

Scattering in two dimensions (2)

An electron is moving in a metallic QWZ lattice along an arbitrary direction. It is described by a 2D massless Dirac Hamiltonian $\hat{H} = \hat{p}_x \hat{\sigma}_x + \hat{p}_y \hat{\sigma}_y$. It is scattered by a high, smooth potential barrier, $\hat{U} = V(x)\hat{\sigma}_0$. What is the probability of reflection from the barrier?



(a) 0

(b) 1

(c) between 0 and 1, and the value depends on the details of V(x)

(d) between 0 and 1, but the value does not depend on the details of V(x)

Domain wall and the structure of the energy spectrum (1)

Consider the massive 1D Dirac Hamiltonian, with a step-like mass domain wall as depicted.

$$\hat{H} = M(x)\hat{\sigma}_x + \hat{p}\hat{\sigma}_y$$

(a)

energy

 $\left(\right)$

What is the structure of the energy spectrum of this system? (black line: discrete level; blue region: continuum)

(b)



Domain wall and the structure of the energy spectrum (2)

Consider the massive 1D Dirac Hamiltonian, with a gradual mass domain wall as depicted, $M(x) = \alpha x$.

M(x)

 $\hat{H} = M(x)\hat{\sigma}_x + \hat{p}\hat{\sigma}_y$

energy

 $\left(\right)$

What is the structure of the energy spectrum of this system?



Domain wall and the structure of the energy spectrum (3)

Consider the massive 1D Dirac Hamiltonian, with the mass domain wall as depicted.



Fate of a bound state after a sudden change (1)



(b) It escapes from the bound state and spreads away from its original position.

(c) It remains confined in the vicinity of its original position, but starts to oscillate.

(d) None of the above.

Fate of a bound state after a sudden change (2)

Consider an electron in one dimension. It is described by the Hamiltonian $\hat{H} = \frac{\hat{p}^2}{2m} + V(x)$. Initially, we have the blue confinement potential, and the electron occupies the ground state of the Hamiltonian, which is a bound state. Suddenly, the potential changes to the red one. What happens to the electron?

(a) Nothing, it remains in the same state.

(b) It escapes from the bound state and spreads away from its original position.

(c) It remains confined in the vicinity of its original position, but starts to oscillate.

(d) Part of it escapes, part of it remains localized and starts to oscillate.



Fate of a bound state after a sudden change (3)

Consider an electron in one dimension.

It is described by the one-dimensional massive Dirac equation:

 $\hat{H} = M(x)\hat{\sigma}_z - w\hat{p}\hat{\sigma}_y$

Initially, we have the blue mass domain wall, and the electron

occupies the zero-energy bound state.

Suddenly, the mass profile changes to the red one.

What happens to the electron?

(a) Nothing, it remains in the same state.



(b) It escapes from the bound state and spreads away from its original position.

(c) It remains confined in the vicinity of its original position, but starts to oscillate.

(d) Part of it escapes, part of it remains localized and starts to oscillate.

Fate of a bound state after a sudden change (4)

Consider an electron in one dimension. It is described by the one-dimensional massive Dirac equation: $\hat{H} = M(x)\hat{\sigma}_z - w\hat{p}\hat{\sigma}_y$ Initially, we have the blue mass domain wall, and the electron occupies the zero-energy bound state. Suddenly, the mass profile changes to the red one. V(x)What happens to the electron? initia Х tina (a) Nothing, it remains in the same state.

(b) It escapes from the bound state and spreads away from its original position.

(c) It remains confined in the vicinity of its original position, but starts to oscillate.

(d) Part of it escapes, part of it remains localized and starts to oscillate.

Fate of a bound state after a sudden change (5)

Consider an electron in one dimension. It is described by the one-dimensional SSH model. Initially, we have a domain wall between a trivial and a topological half-chain, both in the fully dimerized limit, and an electron occupies the zero-energy bound state. Suddenly, the hoppings are rearranged such that the trivial part becomes topological and the topological part becomes trivial, again both fully dimerized. What happens to the electron?



- (a) Nothing, it remains in the same state.
- (b) It escapes from the bound state and spreads away from its original position.
- (c) It remains confined in the vicinity of its original position, but starts to oscillate.
- (d) Part of it escapes, part of it remains localized and starts to oscillate.