

Reply to Our manuscript ncomms-14-09433/Dong et al

Now considering the following time-dependent model

$$H(t) = \mathcal{H} + \cos(\omega t)A + \cos(2\omega t + \theta)B + \cos(3\omega t + \phi)C \quad (1)$$

where \mathcal{H} , A , B and C are 4×4 time-independent Hamiltonian. The above model is also a function of \mathbf{k} , but this parameter is not shown explicitly here.

Obviously,

$$H(t) = H(t + T), \quad \omega T = 2\pi \rightarrow T = 2\pi/\omega \quad (2)$$

PH symmetry of this model: Assume

$$\Sigma H(\mathbf{k}, t) \Sigma^{-1} = -H(-\mathbf{k}, t) \quad (3)$$

for any t — this is because PH symmetry is an intrinsic symmetry of superconducting model because we have written the Hamiltonian in BdG form. Moreover, $\Sigma = \sigma_x K$ is independent of time, thus

$$\Sigma \mathcal{H}(\mathbf{k}, t) \Sigma^{-1} = -\mathcal{H}(-\mathbf{k}, t), \quad \Sigma A(\mathbf{k}, t) \Sigma^{-1} = -A(-\mathbf{k}, t), \quad (4)$$

$$\Sigma B(\mathbf{k}, t) \Sigma^{-1} = -B(-\mathbf{k}, t), \quad \Sigma C(\mathbf{k}, t) \Sigma^{-1} = -C(-\mathbf{k}, t) \quad (5)$$

Now we try to expand the time-dependent model to time-independent model using Bloch basis, that is we assume

$$\psi(t) = e^{-i\epsilon t} \mathcal{U}(t), \quad \mathcal{U}(t) = \mathcal{U}(t + T) \quad (6)$$

We can expand \mathcal{U} using the following wavefunction

$$\mathcal{U}(t) = \sum_n e^{in\omega t} \psi_n \quad (7)$$

Insert this wavefunction to the following Schrodinger Equation

$$i\partial_t \psi(t) = H(t) \psi(t) \quad (8)$$

Then we have

$$\epsilon \psi_n = (\mathcal{H} + n\omega) \psi_n + \frac{1}{2}(A\psi_{n-1} + A\psi_{n+1}) + \frac{1}{2}(B\psi_{n-2}e^{i\theta} + B\psi_{n+2}e^{-i\theta}) + \frac{1}{2}(C\psi_{n-3}e^{i\phi} + C\psi_{n+3}e^{-i\phi}) \quad (9)$$

Thus the model can be written in the following form

$$H_{4N \times 4N} = \begin{pmatrix} H_{-2} & A' & B' & C' & & & \\ A' & H_{-1} & A' & B' & C' & & \\ B' & A' & H_0 & A' & B' & C' & \\ C' & B' & A' & H_1 & A' & B' & C' \\ & C' & B' & A' & H_2 & A' & B' & C' \\ & & C' & B' & A' & H_3 & A' & B' & C' \\ & & & C' & B' & A' & H_4 & A' & B' \\ & & & & C' & B' & A' & H_5 & A' \end{pmatrix} \quad (10)$$

where $H_n = n\omega + \mathcal{H}$, $A' = A/2$, $B' = B/2$ and $C' = C/2$. The basis is then

$$\Psi = (\cdots, \psi_{-1}, \psi_0, \psi_1, \cdots)^T \quad (11)$$

The true wavefunction of the time-dependent Eq can be constructed using the above wavefunction, but is not necessary for us.

Now we try to calculate the Berry phase using the following method

$$C = \int F_{12} dk_x dk_y = \sum_i F_i \delta A = d^2 \sum_i F_i \quad (12)$$

where F is the Berry of the occupied between $[-\pi/T, 0]$. When $T \rightarrow \infty$, we have $-\pi/T = -\infty$, that is, all the occupied bands.

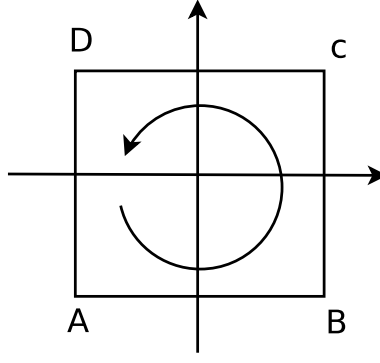


FIG. 1. Calculation of Berry phase numerically.

Now we try to calculate the loop around a loop, see the above figure, we have

$$F\delta A = \int_{\partial S} A \cdot dl = \int_{A \rightarrow B} + \int_{B \rightarrow C} + \int_{C \rightarrow D} + \int_{D \rightarrow A} A \cdot dl \quad (13)$$

For $A \rightarrow B$, we have

$$\int_{A \rightarrow B} A \cdot dl = \langle \psi(x) | \partial_x | \psi(x) \rangle d = \langle \psi(x) | \frac{|\psi(x+d)\rangle - |\psi(x)\rangle}{d} d = \langle \psi(A) | \psi(B) \rangle - 1 \quad (14)$$

Notice that $\langle \psi(A) | \psi(B) \rangle \sim 1$, thus $\langle \psi(A) | \psi(B) \rangle - 1 = x \sim 0$. For small x , we have

$$\ln(x+1) = x \quad (15)$$

Thus we have

$$\int_{\partial S} A \cdot dl = \ln \langle \psi(A) | \psi(B) \rangle \quad (16)$$

Thus for the whole loop, we have

$$FdA = \ln \langle \psi(A) | \psi(B) \rangle \langle \psi(B) | \psi(C) \rangle \langle \psi(C) | \psi(D) \rangle \langle \psi(D) | \psi(A) \rangle \quad (17)$$

which is obviously gauge invariant.

Calculation of Berry phase. Now assume that $\Psi_{n\mathbf{k}}$ is the Eigenvalue of the time-independent Hamiltonian $H_{4N \times 4N}$, with eigenvalues $E_{n\mathbf{k}}$ in $[-\pi/T, 0]$. In this case we have

$$F_{12} = \sum_{n|E_{n\mathbf{k}} \in [-\pi/T, 0]} F_{12}^{(n)}, \quad (18)$$

which is the major equation used to study the Chern number of the whole system.

Summary

1. In time-dependent model, the time-dependent wavefunction is $\psi = \sum_n c_n e^{-i\epsilon t + n\omega t} \psi_n$. In time-dependent model, the wavefunction is $\Psi = (\dots, \psi_{-1}, \psi_0, \psi_1, \dots)$.

2. In the time-independent model, we do not need to worry about the frequency $n\omega$ in the time-dependent model. You can treat these frequencies as index in realistic calculations.

Of course, it is also Ok if you want to calculate the Chern number using the time-dependent wavefunction $\psi(t)$ instead of Ψ . You can find that

$$\int_0^T \langle \psi(t) | \partial | \psi(t) \rangle = \langle \Psi | \partial | \Psi \rangle. \quad (19)$$

The above result can resolve all your concerns. It is also correct if you plot the wavefunction using $\psi(t)$ instead of Ψ .

3. When $T \rightarrow 0$, $[-\pi/T, 0] \rightarrow [-\infty, 0]$, thus we naturally recover the result obtained in stationary condition.

Sorry do not worry about it. This method is well-defined in math.