Van Hove singularities of surface states in crystalline topological insulator

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1 Introduction

In our physical model we considered a 2 dimensional surface states of crystalline topological insulator, trapped in parabolic potential. In such systems one can observe van Hove singularities. They are caused by reaching infinite values by the density of states function in several points on the lattice. These points refer to the saddle points of the potential.

Our goal was to evaluate eigenstates and eigenvalues in neighbourhood of the saddle points. We did this in two independent ways – theoretical and numerical. At the end we compared the obtained results for the particular Hamiltonian.

2 Theoretical derivation

2.1 Analytic solution

Let us consider 2 lattices of graphene twisted with respect to each other. We can solve a two dimensional problem of a particle close to the van Hove singularity trapped by an external potential. The potential results from a quadratic order

expansion around the saddle point. We modelled our system with following Hamiltonian:

$$\mathcal{H} = \tfrac{1}{2}\left(-p_x^2 + p_y^2\right) + V(x,y), \tag{1}$$

with a most general form for the potential described by 3-parameter parabolic function:

$$V(x,y) = \tfrac{1}{2}\left(-Ax^2 + 2Bxy + Cy^2\right), \tag{2}$$

where we assume $A, C > 0$

To find the eigenvalues of $\mathcal{H}$ we solved the problem by method of hyperbolic rotation, which will be described in the following section.

2.2 Exact solution by hyperbolic rotation

Consider a following change of spatial variables

$$\begin{pmatrix} x' \\ y' \end{pmatrix} = \begin{pmatrix} \cosh\vartheta & \sinh\vartheta \\ \sinh\vartheta & \cosh\vartheta \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}, \tag{3}$$

or the same inverted

$$\begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} \cosh\vartheta & -\sinh\vartheta \\ -\sinh\vartheta & \cosh\vartheta \end{pmatrix} \begin{pmatrix} x' \\ y' \end{pmatrix}. \tag{4}$$

The angle ϑ will be choosen such as to diagonalize the resulting Hamiltonian.

The derivatives transform as

$$\begin{pmatrix} \partial_x \\ \partial_y \end{pmatrix} = \begin{pmatrix} \cosh\vartheta & \sinh\vartheta \\ \sinh\vartheta & \cosh\vartheta \end{pmatrix} \begin{pmatrix} \partial_{x'} \\ \partial_{y'} \end{pmatrix}. \tag{5}$$

We find that the kinetic part doesn't change upon such a transformation, with the simple algebra

$$\begin{aligned} \partial_x^2 - \partial_y^2 &= \cosh^2\vartheta\partial_{x'}^2 + \sinh^2\vartheta\partial_{y'}^2 + 2\cosh\vartheta\sinh\vartheta\partial_{x'}\partial_{y'} - 2\cosh\vartheta\sinh\vartheta\partial_{x'}\partial_{y'} - \cosh^2\vartheta\partial_{y'}^2 - \sinh^2\vartheta\partial_{x'}^2 & (6)\\ &= \partial_{x'}^2 - \partial_{y'}^2. & (7) \end{aligned}$$

Then we transform the potential

$$\begin{aligned} V(x,y) &= \tfrac{1}{2}(x,y)\begin{pmatrix} -A & B \\ B & C \end{pmatrix}\begin{pmatrix} x \\ y \end{pmatrix} & (8)\\ &= \tfrac{1}{2}(x',y')\begin{pmatrix} -Ac^2 - 2Bcs + Cs^2 & Asc + Bs^2 + Bc^2 - Csc \\ Asc + Bs^2 + Bc^2 - Csc & -As^2 - 2Bcs + Cc^2 \end{pmatrix}\begin{pmatrix} x' \\ y' \end{pmatrix} & (9) \end{aligned}$$

where we use an obvious shorthand notation $c = \cosh\vartheta$, $s = \sinh\vartheta$. The condition to get a diagonal problem reads

$$(C - A)\sinh\vartheta\cosh\vartheta = B(\cosh^2\vartheta + \sinh^2\vartheta) \tag{10}$$

and is easily solved for ϑ:

$$\tanh 2\vartheta = \frac{2B}{C - A}. \tag{11}$$

We introduce $\Delta = (C-A)^2 - 4B^2$ and find that a solution exists for $\Delta > 0$. The explicit forms are $\cosh 2\vartheta = \frac{C-A}{\sqrt{\Delta}}$, $\sinh 2\vartheta = \frac{2B}{\sqrt{\Delta}}$.

The final formula follows

$$\mathcal{H} = \tfrac{1}{2}\left(-p_{x'}^2 + p_{y'}^2\right) + \tfrac{1}{2}\left(-\Omega_-^2 x'^2 + \Omega_+^2 y'^2\right), \tag{12}$$

where in terms of our original parameters we find

$$\Omega_-^2 = C + A - \sqrt{\Delta},$$

$$\Omega_+^2 = C + A + \sqrt{\Delta}.$$

This Hamiltonian describes two harmonic oscillators, where one is taken with the opposite sign for energy. The eigenenergies are then

$$E(n,m) = -\Omega_- \left(n + \tfrac{1}{2}\right) + \Omega_+ \left(m + \tfrac{1}{2}\right) \tag{13}$$

and for $n, m = 0, 1, 2, \ldots$.

2.3 Final equations

Final equations for calculating eigenenergies are:

$$E(n,m) = -\Omega_-(n + \frac{1}{2}) + \Omega_+(m + \frac{1}{2}), \tag{14}$$

where $n, m = 0, 1, 2, \ldots$ The constants Ω_-, Ω_+ contain the potential parameters:

$$\Omega_-^2 = C + A - \sqrt{\Delta}, \tag{15a}$$

$$\Omega_+^2 = C + A + \sqrt{\Delta}, \tag{15b}$$

$$\Delta = (C - A)^2 - 4B^2. \tag{15c}$$

2.4 Realistic model

2.4.1 Dirac cones

Parallelly, we considered energy described by relation of dispersion presented in [1]. We searched for the saddle points of the surface developed by intersection of two electron Dirac cones.

2.4.2 Taylor expansion

The relation of dispersion is the following:

$$E(k_x, k_y) = \sqrt{m^2 + \delta^2 + v_x^2 k_x^2 + v_y^2 k_y^2 \pm 2\sqrt{m^2 v_x^2 k_x^2 + (m^2 + \delta^2) k_y^2 v_y^2}}. \tag{16}$$

We were interested in its form in the neighbourhood of the saddle points. Therefore, we found the points k_{x0}, k_{y0}, for which:

$$\frac{\partial E(k_x, k_y)}{\partial k_x}|_{k_{x0}, k_{y0}} = 0,$$

$$\frac{\partial E(k_x, k_y)}{\partial k_y}|_{k_{x0}, k_{y0}} = 0,$$

and Taylor expanded $E(k_x, k_y)$ around them. We chose expansion, such that its first order vanishes and the second one is quadratic. The obtained dispersion is:

$$E(k_x, k_y) = \frac{(\delta^2 - m^2) v_x^2 k_x^2}{\sqrt{3}(\delta^2 + m^2)^{\frac{3}{2}}} + \frac{v_y^2 (k_y + \frac{\sqrt{\delta^2 + m^2}}{2v_y^2})^2}{\sqrt{3}\sqrt{\delta^2 + m^2}}, \tag{17}$$

3 Numerical evaluation

Open source software ,,KWANT" `https://kwant-project.org/` was our main tool for numerical calculations. We evaluated independently each Hamiltonian i.e we found eigenstates and eigenvalues. Full tutorial with obainted results is available on `https://github.com/urszulaoleszek/van-hove`.

4 Summary

For the lowest eigenstate the compatibility (ratio) of numerical and theoretical results was in the best case $\sim 95\%$. For the several higher states $(n, m \leq 1)$ we obtained fairness of $70\% - 80\%$.

References

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