

Green's Functions and DOS for Some 2D Lattices

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Abstract

In this presentation we present the Green's functions and density of states for the most frequently encountered 2D lattices: square, triangular, honeycomb, kagome, and Lieb lattice. Though the results are well known, we hope that its derivation performed in a uniform way provides some pedagogical value.

Keywords

2D Lattices

1. Introduction

Fermionic lattice models are widely used not only as a purely theoretical tool but also as a basis for investigation and modelling of physical properties of real materials [1]. Despite their relative formal simplicity—the Hamiltonians of many of them can be written down as bilinears of fermionic operators—analytical calculation of the lattice Green's functions can present substantial difficulties.

In general, the lattice Green's functions of systems are ubiquitous [2] [3] [4] in solid state physics, appearing in problems of lattice vibrations, spin wave theory of magnetic systems, localized oscillation modes at lattice defects, combinatorial problems in lattices [5], and flux calculations in lattice percolation [6]. Lattice Green's functions are also central to the theory of random walks on a lattice [7] [8], and to the calculation of the effective resistance of resistor networks [9].

The lattice Green's functions are of central importance for understanding the electronic behavior of perfect crystalline solids. It also provides the basis for understanding the electronic properties of real, imperfect crystalline solids, since

the imperfections can be treated as a perturbation. Lattice Green's functions are also important for calculating RKKY interaction [10] [11] [12] [13].

We will now consider several popular 2D lattices calculate Green's functions and density of states (DOS). Yielding the same results, the derivation of these results performed in a uniform way and being presented in one place delivers some pedagogical value.

In all cases we'll consider the models with the nearest neighbour hopping only, the amplitude of the hopping we'll take to be 1, so the Hamiltonian will be

$$H = \sum_{\langle ij \rangle} c_i^\dagger c_j \tag{1}$$

where c^\dagger and c are electron creation and annihilation operators, and the summation in Equation (1) is with respect to nearest neighbor pairs. The period of the lattice we'll also take to be equal to 1.

2. Square Lattice

In the wave vector representation, the Hamiltonian for the square lattice is

$$H_{\square}(\mathbf{k}) = \epsilon_{\square}(\mathbf{k}) = 2 \cos k_x + 2 \cos k_y. \tag{2}$$

The site diagonal matrix element of the Green's function is

$$\begin{aligned} g_{\square}(E) &= \frac{1}{(2\pi)^2} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \frac{dk_x dk_y}{E - \epsilon_{\square}(\mathbf{k})} \\ &= \frac{1}{(2\pi)^2} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \frac{dk_x dk_y}{E - 2 \cos k_x - 2 \cos k_y}. \end{aligned} \tag{3}$$

Employing the identity

$$\frac{1}{2\pi} \int_{-\pi}^{\pi} \frac{d\theta}{a + b \cos \theta} = \frac{\text{sign}(a)}{\sqrt{a^2 - b^2}} \quad (|a| > |b|) \tag{4}$$

to perform integration with respect to k_y , we obtain for $E < -4$ or $E > 4$

$$\begin{aligned} g_{\square}(E) &= \frac{1}{2\pi} \int_{-\pi}^{\pi} \frac{dk_x}{\sqrt{(E - 2 \cos k_x)^2 - 4}} \\ &= \frac{\text{sign}(E)}{2\pi} \int_{-1}^1 \frac{dx}{\sqrt{(1-x^2)(x-c)(x-d)}}, \end{aligned} \tag{5}$$

where $c = 1 + \frac{E}{2}$, $d = -1 + \frac{E}{2}$. For $E < -4$ we may use the identity [14]

$$\int_b^a \frac{dx}{\sqrt{(a-x)(x-b)(x-c)(x-d)}} = \frac{2}{\sqrt{(a-c)(b-d)}} K(k), \tag{6}$$

where $a > b > c > d$, K is the complete elliptic integral of the first kind, and

$$k = \sqrt{\frac{(a-b)(c-d)}{(a-c)(b-d)}}. \tag{7}$$

In our case $a = 1$, $b = -1$; hence we obtain

$$(a-b)(c-d) = 4$$

$$(a-c)(b-d) = \frac{E^2}{4}. \tag{8}$$

Thus we get for $E > 4$

$$g_{\square}(E) = \frac{2}{\pi E} K\left(\frac{4}{E}\right). \tag{9}$$

We can analytically continue the Green function from the part of real axis $E < -4$. For $-4 < E < 4$ we have $k > 1$. Hence we should put $E = \epsilon + i0^+$, that is k acquires infinitesimal imaginary part $i0^+$, and we may use the identities [4]

$$\text{Im}\left[K(k + i0^+)\right] = -\frac{1}{k} K\left(\sqrt{1 - \frac{1}{k^2}}\right) \tag{10}$$

$$\text{Re}\left[K(k + i0^+)\right] = \frac{1}{k} K\left(\frac{1}{k}\right) \tag{11}$$

to get [4]

$$\rho_{\square}(\epsilon) = -\frac{1}{\pi} \text{Im}\left[g(\epsilon + i0^+)\right] = \frac{1}{2\pi^2} K\left(\sqrt{1 - \frac{\epsilon^2}{16}}\right). \tag{12}$$

The DOS is presented on **Figure 1**.

3. Triangular Lattice

Let \mathbf{a}_1 , \mathbf{a}_2 and \mathbf{a}_3 be the three periods of the triangular lattice adding up to zero. The Hamiltonian in the wave vector representation is

$$H_{\Delta}(\mathbf{k}) = \epsilon_{\Delta}(\mathbf{k}) = 2 \cos k_1 + 2 \cos k_2 + 2 \cos k_3, \tag{13}$$

where $k_i \equiv \mathbf{a}_i \cdot \mathbf{k}$. The site diagonal matrix element of the Green's function is (k_1 and k_2 are the components of \mathbf{k} in the oblique coordinate system)

$$\begin{aligned} g_{\Delta}(E) &= \frac{1}{(2\pi)^2} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \frac{dk_1 dk_2}{E - \epsilon_{\Delta}(\mathbf{k})} \\ &= \frac{1}{(2\pi)^2} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \frac{dk_1 dk_2}{E - 2 \cos k_1 - 4 \cos\left(k_2 + \frac{k_1}{2}\right) \cos\left(\frac{k_1}{2}\right)}. \end{aligned} \tag{14}$$

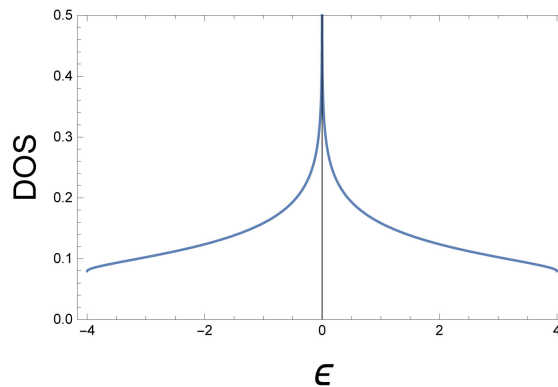


Figure 1. DOS for the square lattice.

(We used the transformation suggested in Ref. [8]). Employing the identity (4) to perform integration with respect to k_2 we obtain for $E > 6$ or $E < -2$

$$\begin{aligned}
 g_{\Delta}(E) &= \frac{\text{sign}(E)}{2\pi} \int_{-\pi}^{\pi} \frac{dk_1}{\sqrt{(E - 2 \cos k_1)^2 - 8 - 8 \cos k_1}} \\
 &= \frac{\text{sign}(E)}{8\pi} \int_{-\pi}^{\pi} \frac{dk_1}{\sqrt{(a - \cos k_1)(b - \cos k_1)}} \\
 &= \frac{\text{sign}(E)}{4\pi} \int_{-1}^1 \frac{dx}{\sqrt{(1-x^2)(a-x)(b-x)}},
 \end{aligned}
 \tag{15}$$

where [15]

$$\begin{aligned}
 a &= 1 + \frac{E}{2} + \sqrt{3 + E} \\
 b &= 1 + \frac{E}{2} - \sqrt{3 + E}
 \end{aligned}
 \tag{16}$$

For $E > 6$ we may use the identity [14]

$$\int_d^c \frac{dx}{\sqrt{(a-x)(b-x)(c-x)(x-d)}} = \frac{2}{\sqrt{(a-c)(b-d)}} K(k),
 \tag{17}$$

where $a > b > c > d$, and

$$k = \sqrt{\frac{(a-b)(c-d)}{(a-c)(b-d)}}.
 \tag{18}$$

From Equation (16) follows

$$\begin{aligned}
 (a-b)(c-d) &= 4r \\
 (a-c)(b-d) &= \frac{1}{4}(r-1)^3(r+3),
 \end{aligned}
 \tag{19}$$

where

$$r = \sqrt{3 + E}.
 \tag{20}$$

Thus we get for $E > 6$ [16] [17]

$$g_{\Delta}(E) = \frac{1}{\pi(r-1)^{3/2}(r+3)^{1/2}} K\left(\frac{4r^{1/2}}{(r-1)^{3/2}(r+3)^{1/2}}\right).
 \tag{21}$$

We can analytically continue the Green function from the part of real axis $E > 6$. For $-2 < E < 6$ we have $k > 1$. Hence we should put $E = \epsilon + i0^+$, that is k acquires infinitesimal imaginary part $i0^+$, we may use the identities (10), (11) and take into account that

$$1 - \frac{1}{k^2} = \frac{(3-r)(r+1)^3}{16r}.
 \tag{22}$$

For $-3 < E < 2$ the value of k become imaginary. We may use the identity [18]

$$K(ik) = \kappa' K(\kappa),
 \tag{23}$$

where

$$\kappa = \frac{k}{\sqrt{k^2 + 1}}, \quad \kappa' = \frac{1}{\sqrt{k^2 + 1}}. \quad (24)$$

In our case

$$\kappa = \sqrt{\frac{4r}{(3-r)(r+1)^{3/4}}}, \quad (25)$$

and we reproduce DOS for the triangular lattice [16]

$$\rho_{\Delta}(\epsilon) = -\frac{1}{\pi} \text{Im} \left[g(\epsilon + i0^+) \right] = \frac{1}{\pi^2 \sqrt{z_0}} K \left(\sqrt{\frac{z_1}{z_0}} \right), \quad (26)$$

where

$$z_0 = \begin{cases} \frac{(3-r)(r+1)^3}{4} & \text{for } -3 \leq \epsilon \leq -2, \\ 4r & \text{for } -2 \leq \epsilon \leq 6 \end{cases}, \quad (27)$$

$$z_1 = \begin{cases} 4r & \text{for } -3 \leq \epsilon \leq -2 \\ \frac{(3-r)(r+1)^3}{4} & \text{for } -2 \leq \epsilon \leq 6 \end{cases} \quad (28)$$

The DOS is presented on **Figure 2**.

4. Honeycomb Lattice

The honeycomb lattice can be considered as a triangular lattice with a basis of two lattice points. The tight binding Hamiltonian for the electrons is

$$\hat{H} = \sum_n a_n^\dagger (b_{n+\delta_1} + b_{n+\delta_2} + b_{n+\delta_3}) + \text{H.c.}, \quad (29)$$

where $\delta_1, \delta_2, \delta_3$ are the vectors connecting an atom with its nearest neighbors.

Going to wave vector representation we obtain

$$\hat{H} = \sum_k \Psi_k^\dagger \hat{H}(\mathbf{k}) \Psi_k, \quad (30)$$

where

$$\hat{H}(\mathbf{k}) = \begin{pmatrix} 0 & \sum_i e^{-ik \cdot \delta_i} \\ \sum_i e^{ik \cdot \delta_i} & 0 \end{pmatrix}. \quad (31)$$

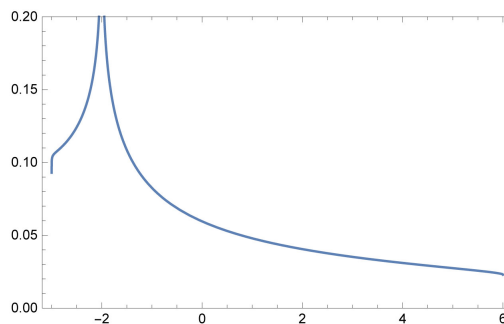


Figure 2. DOS for the triangular lattice.

Taking into account that $\delta_1 - \delta_2 = a_3$, $\delta_2 - \delta_3 = a_1$, $\delta_3 - \delta_1 = a_2$, we obtain the spectrum as

$$\epsilon_\nu(\mathbf{k}) = \nu\sqrt{X_k}, \tag{32}$$

where $\nu = \pm 1$, and

$$X_k \equiv 2(\cos k_1 + \cos k_2 + \cos k_3) + 3. \tag{33}$$

The dispersion law can be written in the form

$$\epsilon_\nu(\mathbf{k}) = \nu\sqrt{3 + \epsilon_\Delta(\mathbf{k})}. \tag{34}$$

The Green's function is

$$g_H(E) = \frac{1}{2\pi^2} \int_{-\pi}^{\pi} dk_1 \int_{-\pi}^{\pi} dk_2 \frac{E}{E^2 - 3 - \epsilon_\Delta(k)}. \tag{35}$$

Thus we obtain

$$g_H(E) = 2Eg_\Delta(E^2 - 3). \tag{36}$$

For the density of states we obtain

$$\rho_H = 2|\epsilon| \rho_\Delta(\epsilon^2 - 3). \tag{37}$$

Actually, Equations (36) and (37) become completely obvious after we square the Hamiltonian (31) to get

$$\hat{H}^2(\mathbf{k}) = \begin{pmatrix} \epsilon_\Delta(\mathbf{k}) + 3 & 0 \\ 0 & \epsilon_\Delta(\mathbf{k}) + 3 \end{pmatrix}. \tag{38}$$

The DOS is presented on **Figure 3**.

5. Kagome Lattice

The kagome lattice can be considered as a triangular lattice (which we consider to be identical to the lattice introduced above for the honeycomb lattice) with a basis of three lattice points. The Hamiltonian is

$$\hat{H} = \sum_n \left[a_n^\dagger (b_{n+\delta_3} + b_{n-\delta_3}) + a_n^\dagger (c_{n+\delta_2} + c_{n-\delta_2}) + b_{n+\delta_1}^\dagger (c_{n+\delta_1} + c_{n-\delta_1}) + \text{H.c} \right], \tag{39}$$

where $\delta_i = a_i/2$ are the vectors connecting the nearest neighbors.

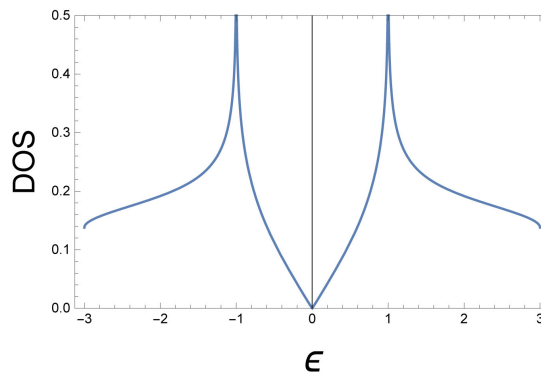


Figure 3. DOS for the honeycomb lattice.

Going to wave vector representation we obtain

$$\hat{H} = \sum_{\mathbf{k}} \Psi_{\mathbf{k}}^{\dagger} \hat{H}(\mathbf{k}) \Psi_{\mathbf{k}}, \quad (40)$$

where

$$\hat{H}(\mathbf{k}) = 2 \begin{pmatrix} 0 & \cos\left(\frac{k_3}{2}\right) & \cos\left(\frac{k_2}{2}\right) \\ \cos\left(\frac{k_3}{2}\right) & 0 & \cos\left(\frac{k_1}{2}\right) \\ \cos\left(\frac{k_2}{2}\right) & \cos\left(\frac{k_1}{2}\right) & 0 \end{pmatrix}. \quad (41)$$

The spectrum is found from the equation

$$\det(\epsilon \hat{I} - \hat{H}) = 0. \quad (42)$$

Calculating the determinant and taking into account that $k_1 + k_2 + k_3 = 0$ we may present the dispersion equation as

$$[\epsilon(\mathbf{k}) + 2][\epsilon^2(\mathbf{k}) - 2\epsilon(\mathbf{k}) - X_{\mathbf{k}} + 1] = 0. \quad (43)$$

Thus we have a flat band $\epsilon_F(\mathbf{k}) = -2$, and two dispersive bands

$$\epsilon_{\nu}(\mathbf{k}) = 1 + \nu \sqrt{X_{\mathbf{k}}}. \quad (44)$$

The Green's function is

$$g_K(E) = \frac{1}{(2\pi)^2} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \frac{dk_1 dk_2}{E + 2} + \frac{1}{2\pi^2} \int_{-\pi}^{\pi} dk_1 \int_{-\pi}^{\pi} dk_2 \frac{E - 1}{E^2 - 2E - 2 - \epsilon_{\Delta}(k)}. \quad (45)$$

Comparing Equations (45) and (14) we obtain

$$g_K(E) = \frac{1}{E + 2} + 2(E - 1)g_{\Delta}[(E - 1)^2 - 3] \quad (46)$$

Hence

$$\rho_K = \delta(\epsilon + 2) + 2|\epsilon - 1|\rho_{\Delta}[(\epsilon - 1)^2 - 3]. \quad (47)$$

We see that apart from the δ -function peak, the DOS for the Kagome lattice is the DOS for the honeycomb lattice shifted by 1. The DOS is presented on **Figure 4**.

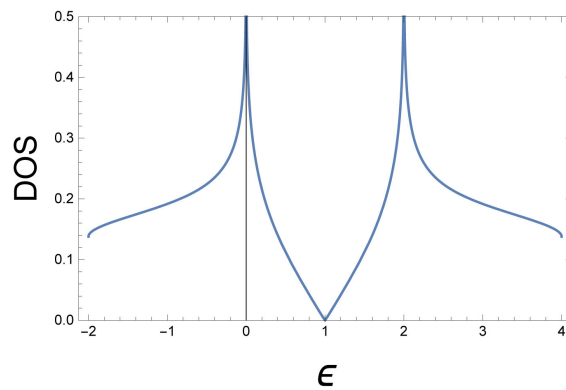


Figure 4. DOS for the kagome lattice. (The δ -function peak is omitted).

6. Lieb Lattice

Consider now the Lieb lattice with the Hamiltonian

$$\hat{H}(\mathbf{k}) = 2 \begin{pmatrix} 0 & \cos\left(\frac{k_x}{2}\right) & 0 \\ \cos\left(\frac{k_x}{2}\right) & 0 & \cos\left(\frac{k_y}{2}\right) \\ 0 & \cos\left(\frac{k_y}{2}\right) & 0 \end{pmatrix}. \tag{48}$$

The spectrum of the Hamiltonian (48) is

$$\epsilon_F(\mathbf{k}) = 0, \quad \epsilon_V(\mathbf{k}) = 2v \sqrt{\cos^2\left(\frac{k_x}{2}\right) + \cos^2\left(\frac{k_y}{2}\right)}. \tag{49}$$

The Green's function is

$$g_L(E) = \frac{1}{(2\pi)^2} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \frac{dk_1 dk_2}{E} + \frac{1}{2\pi^2} \int_{-\pi}^{\pi} dk_1 \int_{-\pi}^{\pi} dk_2 \frac{2E}{E^2 - 4 - \epsilon_{\square}(\mathbf{k})}. \tag{50}$$

Comparing Equations (50) and (3) we obtain

$$g_L(E) = \frac{1}{E} + 2Eg_{\square}(E^2 - 4). \tag{51}$$

Hence

$$\rho_K = \delta(\epsilon) + 2|\epsilon| \rho_{\square}(\epsilon^2 - 4) = \delta(\epsilon) + \frac{|\epsilon|}{\pi^2} K \left(\sqrt{1 - \frac{(\epsilon^2 - 4)^2}{16}} \right). \tag{52}$$

The DOS is presented on **Figure 5**.

7. Conclusions

To summarize, we have expressed lattice Green's functions and density of states for triangular and square lattice through the complete elliptic integral of the first kind in a uniform way. The Green's functions were calculated analytically as functions of energy on the part of real axis, and then continued analytically on the whole complex plane.

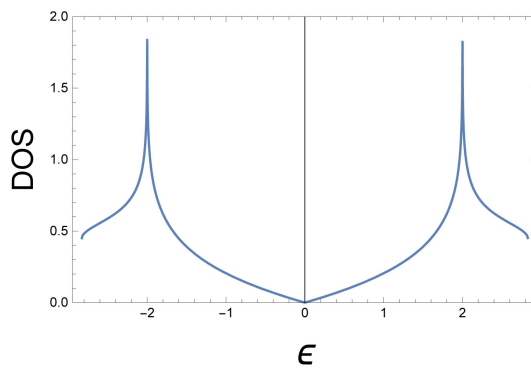


Figure 5. DOS for the Lieb lattice. (The δ -function peak is omitted).

We connected lattice Green's functions and density of states for honeycomb and kagome lattices with those of the triangular lattice, and Green's functions and density of states for Lieb lattice with those of square lattice. Exact expressions for lattice density of states ought to be useful in dynamical mean field theory calculations [19].

We have also shown that the well known results for the wave functions of electrons in the vicinity of the Dirac points in the honeycomb lattice are not connected with the nearest-neighbor hopping approximation, but follow from the symmetry of the model.

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Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

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Appendix A: Why the Wave Functions of Electrons in Honeycomb Lattice Define What They Are?

The results for the wave functions of electrons in the vicinity of the Dirac points in the honeycomb lattice (Equations (A9) and (A10) below) are well known [20]. In this appendix we want to emphasise the fact that these results are not connected, as it is sometimes erroneously stated, with the nearest-neighbor hopping approximation, but follow from the symmetry of the model.

Looking at Equation (33) we understand that to find minimal value of $X_{\mathbf{k}}$ we should find minimal value of the sum of cosines of three numbers which add up to zero. This value is equal to $-3/2$ and is achieved when two of the numbers are $2\pi/3$ and the third number is $-4\pi/3$ (the point \mathbf{K}), or when two of the numbers are $-2\pi/3$ and the third number is $4\pi/3$ (the point \mathbf{K}'). The bands touch each other at these points.

The wave functions can be presented as

$$\Psi_{\nu}(\mathbf{k}) = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{-i\tilde{\theta}_{\mathbf{k}}/2} \\ \nu e^{i\tilde{\theta}_{\mathbf{k}}/2} \end{pmatrix}, \quad (\text{A1})$$

where

$$\tilde{\theta}_{\mathbf{k}} = \text{Arg}\left(\sum_i e^{i\boldsymbol{\delta}_i \cdot \mathbf{k}}\right). \quad (\text{A2})$$

Making substitution

$$\mathbf{k} = \mathbf{K} + \mathbf{q}, \quad (\text{A3})$$

expanding with respect to \mathbf{q} and keeping only the linear terms we obtain

$$X_{\mathbf{q}} = \frac{1}{2} \sum_i (\mathbf{a}_i \cdot \mathbf{q})^2 = \frac{3}{4} q^2. \quad (\text{A4})$$

Thus we have the conic point in the spectrum.

In the same approximation

$$\sum_i e^{i\boldsymbol{\delta}_i \cdot \mathbf{k}} = \sum_i e^{i\boldsymbol{\delta}_i \cdot \mathbf{K}} (\boldsymbol{\delta}_i \cdot \mathbf{q}) = (\mathbf{n} + i\mathbf{m}) \cdot \mathbf{q}, \quad (\text{A5})$$

where

$$\mathbf{n} = \sum_i \boldsymbol{\delta}_i \cos(\boldsymbol{\delta}_i \cdot \mathbf{K}), \quad \mathbf{m} = \sum_i \boldsymbol{\delta}_i \sin(\mathbf{K} \boldsymbol{\delta}_i). \quad (\text{A6})$$

One can easily check up that

$$\mathbf{n} \perp \mathbf{m}, \quad |\mathbf{n}| = |\mathbf{m}|. \quad (\text{A7})$$

Hence $\tilde{\theta}_{\mathbf{q}} = \theta_{\mathbf{q}}$, where $\theta_{\mathbf{q}}$ is the polar angle of \mathbf{q} , the X axis being chosen in the direction of \mathbf{n} . If we chose

$$\begin{aligned} \boldsymbol{\delta}_1 &= \frac{1}{2} \left(\frac{1}{\sqrt{3}}, 1 \right), & \boldsymbol{\delta}_2 &= \frac{1}{2} \left(\frac{1}{\sqrt{3}}, -1 \right), \\ \boldsymbol{\delta}_3 &= -\left(\frac{1}{\sqrt{3}}, 0 \right), & \mathbf{K} &= \left(\frac{2\pi}{\sqrt{3}}, \frac{2\pi}{3} \right), \end{aligned} \quad (\text{A8})$$

then X axis is in the direction of $\boldsymbol{\delta}_2$. Hence Equation (A1) can be written as

$$\Psi_{\nu, \mathbf{K}}(\mathbf{q}) = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{-i\theta_{\mathbf{q}}/2} \\ \nu e^{i\theta_{\mathbf{q}}/2} \end{pmatrix}. \quad (\text{A9})$$

For the \mathbf{K}' point, the wavefunctions are obtained from those in Equation (A9) by permutation of the sublattices

$$\Psi_{\nu, \mathbf{K}'}(\mathbf{q}) = \Psi_{\nu, \mathbf{K}}^*(\mathbf{q}). \quad (\text{A10})$$

The natural question appears: are Equations (A9) and (A10) connected to the simplest possible tight-binding model we have used? The answer is: No, these equations are general, and follow from the symmetry of the problem. In fact, the general tight-binding Hamiltonian for the honeycomb lattice is

$$\hat{H} = \begin{pmatrix} \sum_{\mathbf{a}} t'(\mathbf{a}) e^{i\mathbf{k}\cdot\mathbf{a}} & \sum_{\mathbf{a}} t(\mathbf{a} + \boldsymbol{\delta}) e^{i\mathbf{k}\cdot(\mathbf{a} + \boldsymbol{\delta})} \\ \sum_{\mathbf{a}} t^*(\mathbf{a} + \boldsymbol{\delta}) e^{-i\mathbf{k}\cdot(\mathbf{a} + \boldsymbol{\delta})} & \sum_{\mathbf{a}} t'(\mathbf{a}) e^{i\mathbf{k}\cdot\mathbf{a}} \end{pmatrix}, \quad (\text{A11})$$

where the summation is with respect to all lattice vectors \mathbf{a} , and $\boldsymbol{\delta}$ is some arbitrary, but fixed $\boldsymbol{\delta}_i$. The selection rule for matrix elements [21] gives

$$\sum_{\mathbf{a}} t(\mathbf{a} + \boldsymbol{\delta}) e^{i\mathbf{K}\cdot(\mathbf{a} + \boldsymbol{\delta})} = 0. \quad (\text{A12})$$

In fact, we are dealing with the product of two functions. The function $t(\mathbf{a} + \boldsymbol{\delta})$ realizes the unit representation of the point symmetry group C_3 (the full symmetry group of the inter-sublattice hopping is C_{3v} , but the restricted symmetry is enough to prove the cancelation). As far as the function $e^{i\mathbf{K}\cdot(\mathbf{a} + \boldsymbol{\delta})}$ is concerned, rotation of the lattice by the angle $2\pi/3$, say anticlockwise, is equivalent to rotation of the vector \mathbf{K} in the opposite direction that is substitution of the three equivalent corners of the Brillouin zone. Thus the exponent $e^{i\mathbf{K}\cdot(\mathbf{a} + \boldsymbol{\delta})}$ realizes $x - iy$ representation of the group C_3 . Because each of the multipliers in Equation (A12) realizes different irreducible representation of the symmetry group, the matrix element is equal to zero. Simply speaking, at a point \mathbf{K} the sublattices become decoupled, and this explains the degeneracy of the electron states in this point (these points) or, in other words, merging of the two branches of the single Brillouin zone.

Hence, for a general tight-binding model, the nondiagonal matrix element of the Hamiltonian (A11) is a linear function of \mathbf{q} : $(\mathbf{c} + i\mathbf{d}) \cdot \mathbf{q}$, invariant with respect to rotation of \mathbf{q} by $2\pi/3$ up to a \mathbf{q} independent constant. It immediately leads to the demands $|\mathbf{c}| = |\mathbf{d}|$, and $\mathbf{c} \perp \mathbf{d}$ and we recover Equation (A9). Equation (A10) follows from Equation (A9) because of invariance of the system with respect to mirror reflections.