

An algebraic geometry method for calculating DOS for 2D tight binding models

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Abstract

An algebraic geometry method is used to calculate the moments of the electron density of states as a function of the energy for lattices in the tight binding approximation. Interpreting the moments as the Mellin transform of the density allows writing down a formula for the density as an inverse Mellin transform. The method is illustrated by working out the density function for the two-dimensional square and honeycomb lattices.

The tight binding model is a widely used scheme for studying electronic band structure of solids [1]. The model is defined by a Hamiltonian quadratic in the electron creation and destruction operators indexed by a set of points in the D -dimensional Euclidean space \mathbf{R}^D , called sites. The sites

form a lattice Λ , taken to model a crystal. The physical picture underpinning the model supposes that the electrons are tightly bound to a site but may hop from a given site to its neighbouring ones, which, for the purpose of the present discussion, are restricted to the nearest neighbours only, with proximity defined with respect to distances measured along lattice paths. Thus each physical system is defined by its specific lattice description. The translation symmetry of the lattice permits restricting the quasi-momenta \mathbf{k} , that is the variables on the reciprocal lattice $\tilde{\Lambda}$, dual to Λ , to a closed subset of the dual \mathbf{R}^D . The convex hull of this closed subset is called the Brillouin zone. The eigenvalues of the tight binding Hamiltonian are invariant functions defined on the Brillouin zone.

We consider a related variant of the tight binding approximation wherein the energy eigenvalues of electrons are those of a discrete Laplacian associated with the lattice [2]. The discrete Laplacian is defined on complex-valued functions f on \mathbf{R}^D as

$$\nabla f(\mathbf{v}) = \sum_{\mathbf{a}, \mathbf{b} \in \mathcal{A} \subset \Lambda} c_{\mathbf{a}} c_{\mathbf{b}} f(\mathbf{v} + \mathbf{a} - \mathbf{b}),$$

where the set \mathcal{A} generates the lattice Λ . The parameters c are taken to be unity on every site. The eigenvalues of the Laplacian for this variant are the square of the energy eigenvalues obtained from the usual tight binding model.

Given a lattice Λ in \mathbf{R}^D and the energy eigenvalues of the single electron states, its associated Green's function, often referred to as the lattice Green's function, can be evaluated and has found diverse applications [3–6]. The electronic density of states (DOS) as well as a host of other physical quantities of the crystalline solid can be obtained from the Green's function. For example, the DOS of the system can be determined from the imaginary part of the Green's function G as $\rho(\epsilon) = -(1/\pi) \lim_{\eta \rightarrow 0^+} \text{Im } G(\epsilon + i\eta)$, ϵ denoting the energy eigenvalue. This follows from the definition of the DOS as a sum over delta functions $\delta(E - E_n)$ over energies, where E_n is an electron energy eigenvalue. Various techniques have been developed to determine the DOS as it contains important physical information, such as electron conductivity in solids [7–9].

We use standard methods of algebraic geometry to determine the moments of the DOS for the tight binding model in two dimensions. There is a certain naturality in this formulation. First, the Laplacian is a natural operator and second, periodic functions of two variables, like the single electron eigenvalues obtained here, is a means to define a well-studied object in algebraic geometry, namely a complex algebraic surface, also called an elliptic

curve. Thus all two-dimensional (2D) lattice systems with energy eigenvalues periodic in both directions represent elliptic curves. Let us mention that although we restrict to 2D models only, the technique used here generalizes to higher dimensions.

The DOS in this approach can be written solely in terms of the combinatorial data of the lattice, without requiring the knowledge of electronic wave functions and sum over delta functions. There exist algebraic geometry methods for studying elliptic curves using differential equations, known as Picard–Fuchs equations. The solutions to these equations provide an alternative way to describe an elliptic curve. From this algebraic geometry insight the electronic DOS can also be related to these solutions of the Picard–Fuchs equation which, in our case, is a single second-order differential equation [10]. Circuits around the singular points of the Picard–Fuchs equation are related to the (co)homological properties of the curve. Indeed, the derivation of the Picard–Fuchs equation follows from these topological properties. A surface, such as the Brillouin zone, which is doubly periodic, is topologically a torus, with two linearly independent closed one-forms that are not exact. Let us recall that a closed one-form on a space is one that vanishes when operated on by the differential operator d . It can be written locally, though not necessarily globally, as df where f is a function on the space. An exact one-form is one that can be globally written as df . Such a form becomes identically zero when operated on by the operator d . The dimension of the first cohomology group of the space is the number of linearly independent closed but not exact one-forms. It is a topological invariant. In the 2D examples that we discuss, there are two linearly independent closed but not exact one-forms present. Thus, if we start with an arbitrary local expression for a family of one-forms on the surface and differentiate with respect to the family parameter z , then every differentiation produces a new one-form. Thus, the first and second derivatives along with the original one make three one-forms. If all of these one-forms are further constructed to be closed then we know that there must be a linear relationship between these three since the first cohomology group has dimension two. This linear relationship is the Picard–Fuchs equation. The procedure of constructing the one-forms on algebraic surfaces through differentiation with respect to the family parameter and discarding exact one-forms at each step has been used earlier in various contexts [10–12].

We illustrate this approach in two examples, namely, the 2D tight binding model for the square and honeycomb lattices. The honeycomb case represents graphene which is a system of considerable current interest. In these two cases we show the two steps used to determine the electron energy DOS. First, algebraic geometry is used to determine the energy moments of the DOS which are interpreted as Mellin transforms. Next, we use the

powerful techniques of inverting Mellin transforms to determine an analytic expression for the DOS. Indeed, the advantage of the present approach lies in obtaining the DOS as an inverse Mellin transform, simplifying numerical evaluations for any value of the energy.

Let us start by briefly discussing the general combinatorial setup to fix notation. We shall also identify the physical quantities, in particular, the DOS, in terms of the combinatorial data. We restrict the discussion to 2D cases. Generalization to higher dimensions may be considered following known results [2]. The model we consider is described by a finite subset \mathcal{A} of \mathbf{Z}^2 . The lattice Λ is then obtained by taking the \mathbf{Z} -span of the difference of points in \mathcal{A} , that is,

$$\Lambda = \mathbf{Z}\text{-span}\{\mathbf{a} - \mathbf{b} \mid \mathbf{a}, \mathbf{b} \in \mathcal{A}\}. \quad (1)$$

In other words, the set \mathcal{A} is obtained as marking one of the lattice points of the model as the origin and collecting the points connected to it by a single path in the lattice. For example, the set $\mathcal{A} = \{(-1, 0), (1, 0), (0, -1), (0, 1)\}$ for the square lattice, while $\mathcal{A} = \{(1, 0), (0, 1), (-1, -1)\}$ for the honeycomb lattice in two dimensions. The lattice constant is taken to be unity throughout.

On the points of \mathcal{A} we consider the distribution given by a sum of Dirac deltas as

$$\mathcal{D} = \sum_{\mathbf{a} \in \mathcal{A}} \delta_{\mathbf{a}}. \quad (2)$$

Being supported solely on the lattice points, this embodies a crystal in the tight binding approximation. The delta functions may, in principle, have different weights at different points, but we shall not consider that here. The Fourier transform of \mathcal{D} is given by

$$\widehat{\mathcal{D}}(\mathbf{k}) = \sum_{\mathbf{a} \in \mathcal{A}} e^{-2\pi i \mathbf{k} \cdot \mathbf{a}}, \quad (3)$$

where the quasi-momenta $\mathbf{k} = (k_1, k_2)$ are valued in the reciprocal lattice

$$\widetilde{\Lambda} = \{\mathbf{k} \in \mathbf{R}^2 \mid \mathbf{k} \cdot (\mathbf{a} - \mathbf{b}) \in \mathbf{Z}, \forall \mathbf{a}, \mathbf{b} \in \mathcal{A}\} \quad (4)$$

dual to Λ . The eigenvalues of the discrete Laplacian ∇ based on Λ are then written in terms of the quasi-momenta as the dispersion relation

$$E(\mathbf{k})^2 := |\widehat{\mathcal{D}}(\mathbf{k})|^2 = \sum_{\mathbf{a}, \mathbf{b} \in \mathcal{A}} \cos 2\pi \mathbf{k} \cdot (\mathbf{a} - \mathbf{b}). \quad (5)$$

The energy E is periodic with period lattice $\tilde{\Lambda}$ thus descending to a function on the Brillouin zone $U^\Lambda \sim \mathbf{R}^2/\tilde{\Lambda}$, which has the topology of a torus. Let us introduce complex variables x, y and define a Laurent polynomial [2]

$$W(x, y) = \sum_{\mathbf{a}, \mathbf{b} \in \mathcal{A}} \mathbf{x}^{\mathbf{a}-\mathbf{b}} \quad (6)$$

associated to the set \mathcal{A} , satisfying $|\widehat{\mathcal{D}}(\mathbf{k})|^2 = W(e^{2\pi i k_1}, e^{2\pi i k_2})$, where $\mathbf{x} = (x_1, x_2) = (x, y)$ and $\mathbf{x}^\lambda = x_1^{\lambda_1} x_2^{\lambda_2}$, for $\lambda \in \Lambda$. The number of states, denoted $V(\epsilon)$, is given by the normalized volume of the Brillouin zone such that $|\widehat{\mathcal{D}}(\mathbf{k})|^2 \leq \epsilon$. Let us remark that, as mentioned before, by equation (5), the parameter ϵ is the square of the energy obtained from an usual tight binding model. The Hilbert transform of the differential dV is defined as the integral of the resolvent $1/(z - \epsilon)$ with respect to the measure defined by dV over the real line as

$$H(z) = \int_{\mathbf{R}} \frac{dV(\epsilon)}{z - \epsilon} \quad (7)$$

$$= \frac{1}{(2\pi i)^2} \int_{|x|=|y|=1} \frac{1}{z - W(x, y)} \frac{dx dy}{x y}, \quad (8)$$

where z is a complex parameter.

The function $H(z)$ in (8) is the period of a differential one-form along a one-cycle on the hypersurface given by $z = W(x, y)$ in $(\mathbf{C}^*)^2$. It is obtained as a solution to a Picard–Fuchs equation in the form of a Laurent series in the complex variable z which, according to (7), is given in terms of moments a_n as

$$H(z) = \sum_{n=0}^{\infty} a_n z^{-1-n}. \quad (9)$$

The moments can be calculated by either substituting (9) in the Picard–Fuchs equation or by using the residue theorem in (8) as

$$a_n = \text{constant term of the Laurent polynomial } W(x, y)^n.$$

From the moments one can calculate the lattice Green's function and hence the DOS [7, 8]. Although these methods do not yield explicit formulas, they lead to systematic approximation schemes that can be numerically implemented in an efficient manner. We shall consider a different way to

obtain the DOS from $H(z)$ which yields explicit formulas. The idea is to expand (7) in a geometric series in ϵ/z as

$$H(z) = \frac{1}{z} \sum_{n=0}^{\infty} \int_{\mathbf{R}} \frac{dV}{d\epsilon} \left(\frac{\epsilon}{z}\right)^n d\epsilon \quad (10)$$

$$= \sum_{n=0}^{\infty} z^{-1-n} \int_{\mathbf{R}} \rho(\epsilon) \epsilon^n d\epsilon, \quad (11)$$

where we defined the DOS $\rho(\epsilon) = dV/d\epsilon$. Comparing with (9) we conclude

$$a_n = \int_{\mathbf{R}} \rho(\epsilon) \epsilon^n d\epsilon. \quad (12)$$

We now make our simple but important observation, namely, the moments a_n of the DOS $\rho(\epsilon)$ can be interpreted as the Mellin transform of $\epsilon\rho(\epsilon)$ if we replace the integers n by a complex variable s . An immediate consequence of this remark is, as emphasized before, that an expression for the DOS can be easily written down as the inverse Mellin transform of $a_n = a(s)$. We have the formula

$$\rho(\epsilon) = \frac{1}{2\pi i} \int_{c_0-i\infty}^{c_0+i\infty} \epsilon^{-1-s} a(s) ds, \quad (13)$$

where the line integral is evaluated along a vertical line in the complex plane and c_0 is an appropriate real constant. This approach thus gives an explicit formula for the DOS in terms of a function determined by the methods of algebraic geometry. Moreover, it allows us to calculate the DOS for any value of ϵ , large or small, by choosing appropriate contours in the s -plane. In order to use this method we need to be able to replace the discrete set a_n by a function $a(s)$ of a complex variable s . For the cases that we study there is a natural way of doing this. We shall now consider two examples.

Example 1 (Square lattice). For the square lattice the set of generating points in \mathbf{Z}^2 is $\mathcal{A} = \{(-1, 0), (1, 0), (0, -1), (0, 1)\}$. This corresponds to the polynomial

$$W = (x + 1/x + y + 1/y)^2 \quad (14)$$

in the coordinate ring $\mathbf{C}[x, x^{-1}, y, y^{-1}]$. Then the dispersion relation is obtained to be

$$E(\mathbf{k})^2 = 4 + 2 \cos 2\pi k_1 + 2 \cos 2\pi k_2. \quad (15)$$

We shall evaluate the resolvent $H(z)$ defined in (8). Writing the complex variables x, y in terms of the homogeneous coordinates of a 2D complex projective space \mathbf{P}^2 as $x = v_1/v_0$ and $y = v_2/v_0$, $v_0 \neq 1$, we rewrite H as

$$\begin{aligned}
 H(z) &= \int \frac{v_0 v_1 v_2 \Omega}{z(v_0 v_1 v_2)^2 - (v_1 + v_2)^2 (v_1 v_2 + v_0^2)^2} \\
 &= \frac{1}{2z} \left(\int \frac{\Omega}{(v_0 v_1 v_2) - t(v_1 + v_2)(v_1 v_2 + v_0^2)} \right. \\
 &\quad \left. + \int \frac{\Omega}{(v_0 v_1 v_2) + t(v_1 + v_2)(v_1 v_2 + v_0^2)} \right), \tag{16}
 \end{aligned}$$

where $\Omega = v_0 dv_1 \wedge dv_2 - v_1 dv_0 \wedge dv_2 + v_2 dv_0 \wedge dv_1$ is the canonical two-form on \mathbf{P}^2 and we defined $t = 1/\sqrt{z}$. The Picard–Fuchs equations of both the varieties

$$t(v_1 + v_2)(v_1 v_2 + v_0^2) \pm v_0 v_1 v_2 = 0 \tag{17}$$

are the same, namely

$$\frac{d^2 \varpi}{dt^2} + \frac{1 - 48t^2}{t - 16t^3} \frac{d\varpi}{dt} + \frac{16\varpi}{16t^2 - 1} = 0. \tag{18}$$

Thus, series solutions with only the terms with even powers of t survive. This Fuchsian equation has two solutions which can be obtained as series in t by the Frobenius’ method. The two solutions are

$$\varpi_1(t) = {}_2F_1(1/2, 1/2; 1; 16t^2), \tag{19}$$

$$\begin{aligned}
 \varpi_2(t) &= (\log t + 2 \log 2) {}_2F_1(1/2, 1/2; 1; 16t^2) \\
 &\quad + \frac{1}{2\pi} \sum_{n=0}^{\infty} \frac{d}{d\alpha} \left[\frac{\Gamma(\alpha + n + 1/2)^2}{\Gamma(\alpha + m + 1)^2} \right]_{\alpha=0} (16t^2)^n. \tag{20}
 \end{aligned}$$

Here ${}_2F_1(a_1, a_2; b_1; x)$ represents a hypergeometric function defined by the series

$${}_2F_1(a_1, a_2; b_1; x) = \sum_{n=0}^{\infty} \frac{(a_1)_n (a_2)_n}{(b_1)_n n!} x^n, \tag{21}$$

where $(a)_n = a(a + 1) \dots (a + n - 1)$ is the Pochhammer symbol. The two integrals in H are then linear combinations of the two solutions, namely

$$\begin{aligned}
 H(z) &= \frac{c_1}{2z} {}_2F_1\left(1/2, 1/2; 1; \frac{16}{z}\right) \\
 &+ \frac{c_2}{2z} (\log z - 4 \log 2) {}_2F_1\left(1/2, 1/2; 1; \frac{16}{z}\right) \\
 &- \frac{c_2}{4\pi z} \sum_{n=0}^{\infty} \frac{d}{d\alpha} \left[\frac{\Gamma(\alpha + n + 1/2)^2}{\Gamma(\alpha + n + 1)^2} \right]_{\alpha=0} \left(\frac{16}{z}\right)^n,
 \end{aligned} \tag{22}$$

where c_1 and c_2 are arbitrary constants. Instead of trying to determine the constants from boundary conditions, we shall recourse to the calculation of moments to determine the DOS. This entails direct evaluation of the integral (8) using residues. Since the constant term in the expansion of W^n is $\binom{2n}{n}^2$, we have

$$\begin{aligned}
 a_n &= \binom{2n}{n}^2 \\
 &= \frac{\Gamma(2n + 1)^2}{\Gamma(1 + n)^4} \\
 &= \frac{(2n)^2 \Gamma(2n)^2}{n^2 \Gamma(n)^2 \Gamma(1 + n)^2} \\
 &= \frac{1}{\pi} \frac{\Gamma(n + 1/2)^2}{\Gamma(1 + n)^2} 16^n,
 \end{aligned} \tag{23}$$

where we used the duplication formula $\pi^{1/2} \Gamma(2x) = 2^{2x-1} \Gamma(x) \Gamma(x + 1/2)$ in the last step. By (9) this gives the resolvent H as

$$\begin{aligned}
 H(z) &= \sum_{n=0}^{\infty} a_n z^{-1-n} \\
 &= \frac{1}{2z} {}_2F_1\left(1/2, 1/2; 1; \frac{16}{z}\right).
 \end{aligned} \tag{24}$$

By (13), the DOS is then obtained as the inverse Mellin transform

$$\rho(\epsilon) = \frac{1}{2\pi i} \frac{1}{\pi} \int_{c_0 - i\infty}^{c_0 + i\infty} \frac{\Gamma(s + 1/2)^2}{\Gamma(1 + s)^2} 16^s \epsilon^{-1-s}, \tag{25}$$

where the integrand is derived from (23) by substituting s for n .

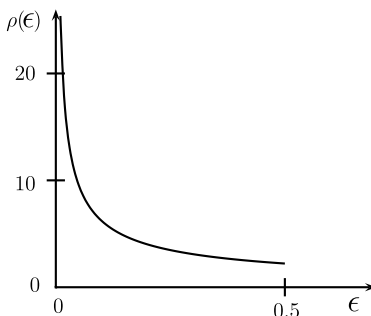


Figure 1: Behaviour of DOS $\rho(\epsilon)$ near $\epsilon = 0$ for the square lattice.

Choosing $c_0 = 0$ and closing the contour with a semicircular arc on the left so as to obtain an expression valid near $\epsilon = 0$, we get

$$\rho(\epsilon) = \frac{4 \log 2 - \log \epsilon}{4\sqrt{\epsilon}} {}_2F_1(1/2, 1/2; 1; \epsilon/16) + \frac{\pi}{4\sqrt{\epsilon}} \sum_{n=0}^{\infty} \frac{d}{ds} \left[\frac{1}{\Gamma(1+s)^2 \Gamma(1/2-s)^2} \right]_{s=-1/2-n} \left(\frac{\epsilon}{16} \right)^n \quad (26)$$

whose leading behaviour near $\epsilon = 0$ is shown in figure 1. Let us point out that there is a lower limit to the admissible range of energy ϵ determined by the sample geometry. The DOS plotted integrated over the whole range of energy does not depend on this physical cut off since the integral is finite even without a cutoff. The same holds good for the honeycomb lattice as well to which we now turn as our next example.

Example 2 (Honeycomb lattice). For the honeycomb lattice we have $\mathcal{A} = \{(1, 0), (0, 1), (-1, -1)\}$, leading to the Laurent polynomial

$$W(x, y) = \left(x + y + \frac{1}{xy} \right) \left(\frac{1}{x} + \frac{1}{y} + xy \right) \quad (27)$$

in $\mathbf{C}[x, x^{-1}, y, y^{-1}]$. The dispersion relation is

$$E(\mathbf{k})^2 = 3 + \cos(2\pi(k_1 - k_2)) + \cos(2\pi(2k_1 + k_2)) + \cos(2\pi(k_1 + 2k_2)) \quad (28)$$

which upon a change of basis of the reciprocal lattice

$$k_1 = (\sqrt{3}\kappa_x + 3\kappa_y)/6, \quad k_2 = (\sqrt{3}\kappa_x - 3\kappa_y)/6 \quad (29)$$

yields the more usual form [13]

$$E(\boldsymbol{\kappa})^2 = 1 + 4 \cos^2 \pi \kappa_y + 4 \cos \pi \kappa_y \cos \pi \sqrt{3} \kappa_x. \quad (30)$$

Let us define the homogeneous coordinates of a \mathbf{P}^2 , namely $[v_0 : v_1 : v_2]$, related to x, y by

$$x^2y = v_1/v_0, \quad xy^2 = v_0/v_2. \tag{31}$$

Substituting these in (8) we obtain the resolvent

$$H(z) = \int \frac{\Omega}{zv_0v_1v_2 - (v_0 + v_1 + v_2)(v_0v_1 + v_1v_2 + v_2v_0)} \tag{32}$$

solving the Picard–Fuchs equation

$$\frac{d^2\varpi}{dz^2} + \frac{9 - 20z + 3z^2}{z(9 - 10z + z^2)} \frac{d\varpi}{dz} + \frac{(z - 3)\varpi}{z(9 - 10z + z^2)} = 0. \tag{33}$$

Again, instead of writing down all the solutions of this equation, it suffices for our purposes to consider the moments. The constant term in the expansion of W gives the moments [2]

$$\begin{aligned} a_n &= \sum_{j=0}^n \binom{n}{j}^2 \binom{2j}{j} \\ &= \sum_{j=0}^n \frac{\Gamma(1+n)^2 \Gamma(2j+1)}{\Gamma(1+n-j)^2 \Gamma(1+j)^4} \\ &= \frac{1}{\sqrt{\pi}} \sum_{j=0}^n \frac{\Gamma(1+n)^2 \Gamma(j+1/2)}{\Gamma(1+n-j)^2 \Gamma(1+j)^3} 4^j \\ &= \frac{1}{\sqrt{\pi}} \sum_{j=0}^{\infty} \frac{\Gamma(1+n)^2 \Gamma(j+1/2)}{\Gamma(1+n-j)^2 \Gamma(1+j)^3} 4^j, \tag{34} \\ &= {}_3F_2(1/2, -n, -n; 1, 1; 4), \tag{35} \end{aligned}$$

where ${}_3F_2(a_1, a_2, a_3; b_1, b_2; x)$ is the generalized hypergeometric function defined by the series

$${}_3F_2(a_1, a_2, a_3; b_1, b_2; x) = \sum_{n=0}^{\infty} \left(\frac{(a_1)_n (a_2)_n (a_3)_n}{(b_1)_n (b_2)_n n!} \right) x^n. \tag{36}$$

The duplication formula has been used in deriving the expression (34) and the sum has been extended to all integral values of j since $1/\Gamma(1+n-j)$

vanishes for all $j \geq n + 1$. As before, equation (33) is solved with

$$H(z) = \sum_{n=0}^{\infty} a_n z^{-1-n}. \tag{37}$$

Then the DOS is expressed in terms of the inverse Mellin transform of $a(s)$ as

$$\rho(\epsilon) = \frac{1}{\sqrt{\pi}} \frac{1}{2\pi i} \sum_{k=0}^{\infty} \int_{c_0-i\infty}^{c_0+i\infty} \frac{\Gamma(1+s)^2 \Gamma(k+1/2)}{\Gamma(1+s-k)^2 \Gamma(1+k)^3} 4^k \epsilon^{-1-s}. \tag{38}$$

We can also write the sum over k as an integral, as

$$\rho(\epsilon) = \frac{1}{\sqrt{\pi}} \left(\frac{1}{2\pi i} \right)^2 \int_{\mathcal{C}} dt \int_{c_0-i\infty}^{c_0+i\infty} ds \frac{\Gamma(1+s)^2 \Gamma(t+1/2) \Gamma(-t)}{\Gamma(1+s-t)^2 \Gamma(1+k)^2} 4^t \epsilon^{-1-s}, \tag{39}$$

where the contour \mathcal{C} is chosen so as to go parallel to the imaginary axis and closing on the right to enclose integers $t = 0, 1, 2, \dots$ on the t -plane. Now reversing the order of the integrations we first evaluate the integral over t by closing the contour on the left, $\text{Re}(t) < 0$, so that we pick up contributions from the poles of $\Gamma(1/2 + t)$ at $t = -1/2 - k$, for positive integers k . This leads to

$$\rho(\epsilon) = \frac{1}{2\sqrt{\pi}} \frac{1}{2\pi i} \sum_{k=0}^{\infty} \int_{c_0-i\infty}^{c_0+i\infty} \frac{\Gamma(1+s)^2 \Gamma(k+1/2)}{\Gamma(3/2+k+s)^2 \Gamma(1/2-k)^2 \Gamma(1+k)} 4^{-k} \epsilon^{-1-s}. \tag{40}$$

In order to derive a power series in ϵ , we note that $\Gamma(1+s)^2$ has double poles at $s = -1 - n$, for positive integral n . Thus, performing the integral by closing the contour on the left we obtain

$$\rho(\epsilon) = \frac{1}{2\sqrt{\pi}} \sum_{n=0}^{\infty} \sum_{k=0}^{\infty} \frac{d}{ds} \left[\frac{\Gamma(k+1/2) 4^{-k} \epsilon^{-1-s}}{\Gamma(3/2+k+s)^2 \Gamma(1/2-k)^2 \Gamma(1+k) \Gamma(-s)} \right]_{s=-1-n} \tag{41}$$

which can be rewritten as

$$\rho(\epsilon) = \frac{1}{2\sqrt{\pi}} \sum_{n=0}^{\infty} \sum_{k=0}^{\infty} \frac{(1/4)^k \Gamma(1/2+k)}{\Gamma(1/2-k)^2 \Gamma(1+k)} \epsilon^n \left(- \frac{1}{\Gamma(1/2+k-n)^2 \Gamma(1+n)^2} \log \epsilon + \frac{d}{ds} \left[\frac{1}{\Gamma(3/2+k+s)^2 \Gamma(-s)^2} \right]_{s=-1-n} \right). \tag{42}$$

The behaviour of the DOS near $\epsilon = 0$ is plotted in figure 2.

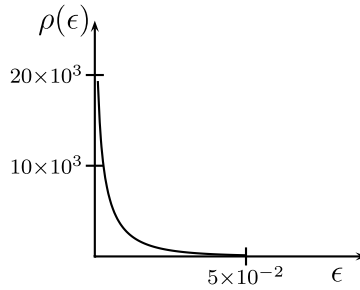


Figure 2: Behaviour of DOS $\rho(\epsilon)$ near $\epsilon = 0$ for the honeycomb lattice.

To summarize, we have discussed the DOS of the 2D nearest-neighbour tight binding Hamiltonian from an algebraic geometry viewpoint. We have discussed two examples based on the 2D square and honeycomb lattices. The DOS is obtained as a function of energy. The Hilbert transform of the DOS is the resolvent that satisfies Picard–Fuchs equations of algebraic varieties that correspond to the lattices in a combinatorial fashion. Explicit expressions are given for small energies in terms of infinite series, involving hypergeometric functions. Let us note that the Brillouin zone corresponding to each of the lattices is a topological torus. Thus, qualitative features of the results may be understood in topological terms. We intend to present details of these topological arguments in a future work. A practical advantage of this approach is that it allows evaluation of DOS in any domain of energy by appropriate choice of contours suitably in the integrals. The resulting infinite series obtained converge rather fast and may be easily evaluated numerically. Finally, let us mention that we have presented our calculations in the context of electrons in a crystalline medium but the results obtained are also applicable for the DOS of a system of phonons where a tight binding nearest-neighbour model is appropriate [14].

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