Wigner Crystal State in Twisted Bilayer Graphene

An ongoing research project in solid-state physics
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draft, updated randomly

General scenario

In this project, we consider an infinitely large twisted bilayer graphene and a ton of electrons poured onto it. ***The aim of this project is to find the critical value of the electron density, or the charge carrier density, for which the Wigner crystal state melts on the twisted bilayer graphene (tBLG).*** The first step is to do such job in vacuum. Note that the state we are interested in comes with three lattice on a same two-dimensional plane: two honeycomb lattices of carbon atoms with a twisted angle and the equilateral triangle lattice of electrons. See Fig.1.

General logic

Let $\mathbf{R}_{i,j}$ be the Bravais lattice of the triangle lattice, and let $\mathbf{r}_{i,j}$ be displacement from the lattice point $\mathbf{R}_{i,j}$, see the figure below. Due to the electrostatic force, any small displacement feels a storing force; for the extremely small displacement, each electron can thus be considered as a harmonic oscillator. The Hamiltonian, in the real position space, of the Wigner crystal state is thus the sum of total kinetic energy, total mechanical energy, and total electrostatic energy

$$H = \sum_{i,j\in\mathbb{Z}} -\frac{\hbar^2}{2m_\mathrm{e}}\Delta_{i,j} \; + \; \sum_{i,j\in\mathbb{Z}} \frac{1}{2}m_\mathrm{e}\omega_{i,j}^2 r_{i,j}^2 \; + \; \frac{1}{2}\sum_{i,j\in\mathbb{Z}} (-e)V_{i,j}(\mathbf{r}_{i,j} = \mathbf{0}_{i,j}) \tag{1}$$

where $\Delta_{i,j}$ is Laplacian taken in the frame of the electron at $\mathbf{R}_{i,j}$, and $V_{i,j}$ is the electrostatic potential of the electron at $\mathbf{R}_{i,j} + \mathbf{r}_{i,j}$. The last term is from the law that the total electrostatic energy of a charge distribution is " $\frac{1}{2}\sum_{\text{all}}$ (charge) (potential at this charge). "

Here, we can see that the total potential energy—the sum of the last two terms—at zero displacement is not zero but is equal to the electrostatic energy of the triangle lattice. In other words, each electron is a two-dimensional harmonic oscillator with a background $(-e)V_{i,j}(\mathbf{r}_{i,j} = \mathbf{0}_{i,j})$.

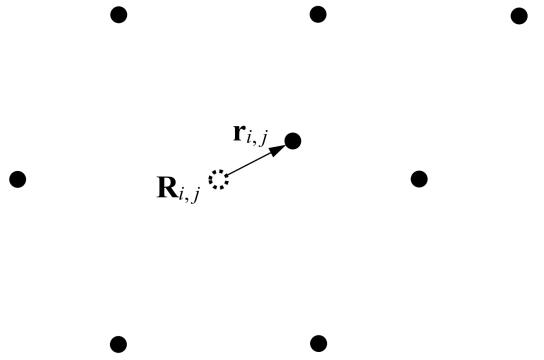

FIG. 1 The small displacement from the lattice point. The black dot represents an electron.

Assume the plane is infinitely large, $V_{i,j}(\mathbf{0}_{i,j}) = V$ and $\omega_{i,j} = \omega$ for all $i, j \in \mathbb{Z}$, then

$$\boxed{H = \sum_{i,j\in\mathbb{Z}} \left(-\frac{\hbar^2}{2m_\mathrm{e}}\Delta_{i,j} + \frac{1}{2}m_\mathrm{e}\omega^2 r_{i,j}^2\right) + \frac{1}{2}\sum_{i,j\in\mathbb{Z}} (-e)V} \tag{2}$$

The first term is the sum of the Hamiltonian of a two-dimensional harmonic oscillator, and now the background of every harmonic oscillator is the same.

We need to find the minimal expectation of (2) per electron since the Wigner crystal state is the state with lowest energy. For the first term, "per electron" means we can get rid of the sum since every electron is identical. Its minimal expectation per electron is then obtained by using the ground state:

$$\left\langle -\frac{\hbar^2}{2m_\mathrm{e}}\Delta + \frac{1}{2}m_\mathrm{e}\omega^2 r^2 \right\rangle_{\min} = \left\langle \psi_{\mathrm{gs}}(r) \middle| -\frac{\hbar^2}{2m_\mathrm{e}}\Delta + \frac{1}{2}m_\mathrm{e}\omega^2 r^2 \middle| \psi_{\mathrm{gs}}(r) \right\rangle = E_{\mathrm{gs}} = \hbar\omega = \frac{\hbar^2}{m_\mathrm{e}w^2}\,, \tag{3}$$

where $w = \sqrt{\dfrac{\hbar}{m_\mathrm{e}\omega}}$ has the unit of length and the ground state is

$$\psi_{\mathrm{gs}}(r) = \frac{w}{\sqrt{\pi}}e^{-\frac{1}{2}w^2r^2}, \qquad \psi_{\mathrm{gs}}(p) = \sqrt{\frac{w}{\pi\hbar}}e^{-\frac{w^2}{2\hbar^2}p^2} \tag{4}$$

In general, $E = (n + 1)\hbar\omega$ for the eigenstate $\psi_n(r)$; the ground state is the state with $n = 0$.

The second term is actually a constant as V is a constant. The elementary electrostatics again tells us that the expected electrostatic energy per charge is " $\frac{1}{2}$ (charge) (potential at this charge)." So, the expectation of the second term per electron is $\frac{1}{2}(-e)V$.

We now conclude that the minimal expectation of the Hamiltonian per electron is

$$\boxed{\langle H \rangle_{\text{min, one}} = \frac{\hbar^2}{m_e w^2} + \frac{1}{2}(-e)V} \tag{5}$$

Obviously, the remaining task is to find V.

Geometry of the electron lattice

Let the length $R = |\mathbf{R}_{1,0}|$ be the lattice constant of the equilateral triangle lattice. The lattice can be described by the Bravais lattice with the primitive vectors

$$\mathbf{a}_1 = \mathbf{R}_{1,0} = R\mathbf{e}_1,$$
$$\mathbf{a}_2 = \mathbf{R}_{0,1} = \frac{R}{2}\mathbf{e}_1 + \frac{\sqrt{3}R}{2}\mathbf{e}_2;$$

so, the position of each electron can be labeled as

$$\mathbf{R}_{i,j} = i\mathbf{a}_1 + j\mathbf{a}_2, \quad i, j \in \mathbb{Z} \tag{6}$$

One can easily find the corresponding reciprocal lattice

$$\mathbf{K}_{l,m} = l\mathbf{b}_1 + m\mathbf{b}_2, \quad l, m \in \mathbb{Z} \tag{7}$$

with primitive vectors

$$\mathbf{b}_1 = \frac{2\pi}{R}\left(\mathbf{e}_1 - \frac{1}{\sqrt{3}}\mathbf{e}_2\right), \qquad \mathbf{b}_2 = \frac{2\pi}{R}\frac{2}{\sqrt{3}}\mathbf{e}_2. \tag{8}$$

of course we have

$$|\mathbf{K}_{l,m}| = \frac{4\pi}{\sqrt{3}R}\sqrt{l^2 + m^2 - lm} \tag{9}$$

Further, $\mathrm{d}^2\mathbf{R}_{i,j}$ and $\mathrm{d}^2\mathbf{K}_{i,j}$ stand for the area elements in Bravais lattice and reciprocal lattice space. Think about Riemann sum and integration in calculus

$$\int_D f(\mathbf{x})\mathrm{d}^2\mathbf{x} = \iint_D f(x, y)\mathrm{d}x\mathrm{d}y = \sum_{x^*}\sum_{y^*} f(x^*, y^*)\mathrm{d}x\mathrm{d}y$$

$\mathrm{d}\mathbf{x}$ is a area element of the partition of the integrating area D and each such area element contain only one point (x^*, y^*) at which the f assumed, see figure below. Similarly, $\mathrm{d}\mathbf{R}_{i,j}$ and $\mathrm{d}\mathbf{K}_{i,j}$ must be an area element of a partition of the lattice space and each one contains only a single lattice point. This kind of area element is called the **Wigner-Seitz cell**. By elementary Euclidean geometry, we have

$$\mathrm{d}^2\mathbf{R}_{i,j} = \frac{\sqrt{3}}{2}R^2, \qquad \mathrm{d}^2\mathbf{K}_{i,j} = \frac{8\pi^2}{\sqrt{3}R^2} \tag{10}$$

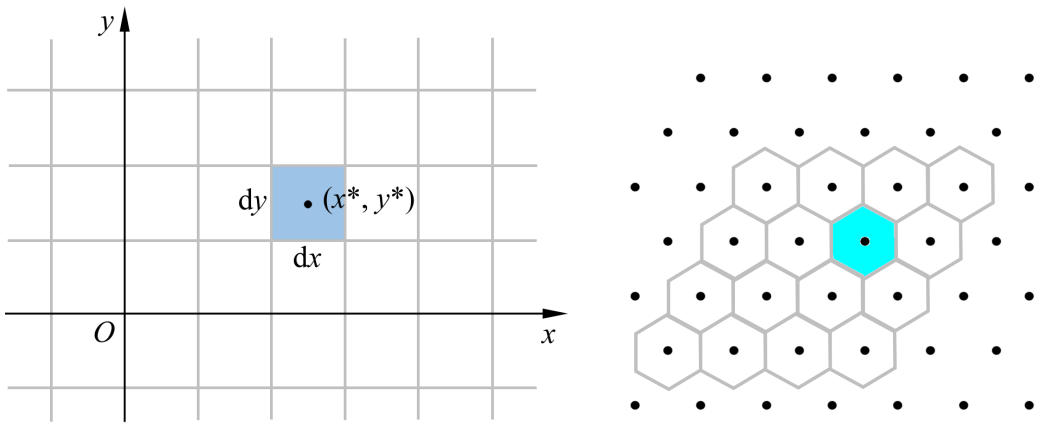

FIG. 2 (left) The partition and the unit cell of $\mathbb{R}^2$ of the Riemann sum; (right) the partition and the unit cell of the lattice space.

A ill-defined partition: The following partition is not a well-defined one since each cell is not identical. The yellow one has a lattice point at the lower left vertex but the green one does not.

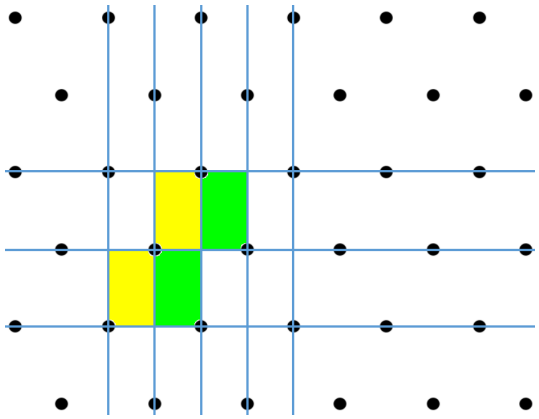

FIG. 3 An ill-defined partition and the unit cell of the lattice space.

The total potential energy per electron

In this section, we are going to find V in formula (4), the total potential energy per electron.

Since we assumed the plane is an infinitely large square which means its side length $L \to \infty$, the electrostatic energy of the electron at $\mathbf{R}_{i,j}$ is approximately equal to that of the electron at $\mathbf{R}_{0,0} = \mathbf{0}$. So, our task is to first find the electrostatic potential at $\mathbf{R}_{0,0}$.

Let $V(\mathbf{R}_{i,j})$ *be the electrostatic potential at* $\mathbf{0}$ *due to the electron at* $\mathbf{R}_{i,j}$, then the total (net) electrostatic potential at $\mathbf{0}$ is just the scalar sum of all $V(\mathbf{R}_{i,j})$ except $V(\mathbf{R}_{0,0})$; namely,

$$V = \sum_{\substack{i,j\in\mathbb{Z} \\ (i,j)\neq(0,0)}} V(\mathbf{R}_{i,j}) \tag{11}$$

The direct calculation will end up with a diverge series since the plane is assumed to be infinitely large and the potential is inverse proportional to the distance.

Our approach is to utilize the Fourier transform

$$\tilde{V}(\mathbf{k}) := \int_{-\infty}^{\infty} V(\mathbf{r}) e^{-i\mathbf{k}\cdot\mathbf{r}} \mathrm{d}^2\mathbf{r}, \quad V(\mathbf{r}) := \frac{1}{(2\pi)^2} \int_{-\infty}^{\infty} \tilde{V}(\mathbf{k}) e^{i\mathbf{r}\cdot\mathbf{k}} \mathrm{d}^2\mathbf{k}.$$

where $\mathbf{r}$ is a vector in $\mathbf{R}_{i,j}$ space and $\mathbf{k}$ is a vector in the corresponding reciprocal space $\mathbf{K}_{i,j}$. We are interested in the potential at $\mathbf{r} = \mathbf{R}_{i,j}$, so

$$V(\mathbf{R}_{i,j}) = \frac{1}{(2\pi)^2} \int_{-\infty}^{\infty} \tilde{V}(\mathbf{k}) e^{i\mathbf{R}_{i,j}\cdot\mathbf{k}} \mathrm{d}^2\mathbf{k}. \tag{12}$$

So,

$$V = \sum_{\substack{i,j\in\mathbb{Z} \\ (i,j)\neq(0,0)}} \frac{1}{(2\pi)^2} \int_{-\infty}^{\infty} \tilde{V}(\mathbf{k}) e^{i\mathbf{R}_{i,j}\cdot\mathbf{k}} \mathrm{d}^2\mathbf{k} = \frac{1}{(2\pi)^2} \int_{-\infty}^{\infty} \tilde{V}(\mathbf{k}) \sum_{\substack{i,j\in\mathbb{Z} \\ (i,j)\neq(0,0)}} e^{i\mathbf{R}_{i,j}\cdot\mathbf{k}} \, \mathrm{d}^2\mathbf{k} \tag{13}$$

The double sum inside the integrand is

$$\sum_{\substack{i,j\in\mathbb{Z} \\ (i,j)\neq(0,0)}} e^{i\mathbf{R}_{i,j}\cdot\mathbf{k}} = -e^{i\mathbf{R}_{0,0}\cdot\mathbf{k}} + \sum_{i,j\in\mathbb{Z}} e^{i\mathbf{R}_{i,j}\cdot\mathbf{k}} = -1 + \frac{2(2\pi)^2}{\sqrt{3}} \frac{1}{R^2} \sum_{l,m\in\mathbb{Z}} \delta(\mathbf{k} - \mathbf{K}_{l,m}) \tag{14}$$

where we use the Fourier series of Dirac delta function δ in the last step. Then, invoke the number density n of electron

$$n = \frac{1}{\text{area of one Wigner-Seitz cell}} = \frac{1}{\frac{\sqrt{3}}{2}R^2} = \frac{2}{\sqrt{3}R^2}; \tag{15}$$

and the surface charge density will be $\sigma = (-e)n$, we have

$$\sum_{\substack{i,j\in\mathbb{Z} \\ (i,j)\neq(0,0)}} e^{i\mathbf{R}_{i,j}\cdot\mathbf{k}} = -1 + (2\pi)^2 n \sum_{l,m\in\mathbb{Z}} \delta(\mathbf{k} - \mathbf{K}_{l,m}) \tag{16}$$

Derivation of Fourier series of Dirac delta function and the unit-consistency First consider the following two identities

$$\int_{-\infty}^{\infty} e^{ikx} \mathrm{d}x = 2\pi\delta(k)^{[1]}$$

$$\sum_{x\in\mathbb{Z}} e^{ixk} = 2\pi\delta(k) \quad \text{in the weak sense on } k \in (-\pi, \pi)^{[2]}$$

The first one is unit-consistent since both sides has unit of x, but the second one is not since the left hand side is dimensionless yet the right hand side is of unit x. Both of them are mathematically correct, but in physics we always want the unit to be consist. So, we re-write the second one as

$$\sum_{x\in\mathbb{Z}} e^{ixk}\mathrm{d}x = 2\pi\delta(k) \quad \text{in the weak sense on } k\in(-\pi,\pi)$$

where $\mathrm{d}x$ is a unit, or the smallest allowable, step in $\mathbb{Z}$; of course, it is $+1$. Further,

$$\sum_{x\in\mathbb{Z}} e^{ixk}\mathrm{d}x = 2\pi\delta(k-2\pi) \quad \text{in the weak sense on } k\in(\pi,3\pi)$$
$$\sum_{x\in\mathbb{Z}} e^{ixk}\mathrm{d}x = 2\pi\delta(k-4\pi) \quad \text{in the weak sense on } k\in(3\pi,5\pi)$$
$$\cdots$$

To conclude,

$$\sum_{x\in\mathbb{Z}} e^{ixk}\mathrm{d}x = 2\pi\sum_{n\in\mathbb{Z}}\delta(k-2n\pi) \quad \text{for all } k \tag{17}$$

One can also treat it as an approximation of the first equation or the discrete inverse Fourier transform of $\{...,1,1,...\}$ of which the result is discrete values of Dirichlet kernel and becomes the Dirac delta function when treat k as a continuous variable.

In our case, we have the unit-consistent formula

$$\sum_{i,j\in\mathbb{Z}} e^{i\mathbf{R}_{i,j}\cdot\mathbf{k}}\mathrm{d}^2\mathbf{R}_{i,j} = (2\pi)^2\sum_{l,m\in\mathbb{Z}}\delta(\mathbf{k}-\mathbf{K}_{l,m}) \quad \text{for all } \mathbf{k}$$

where $\mathrm{d}^2\mathbf{R}_{i,j} = \dfrac{\sqrt{3}}{2}R^2$ is the area element in the lattice plane; plug it back into the last formula, we can then get Eq. (14).

After the calculation of the double sum, we can now plug it into (13),

$$\begin{aligned} V &= \frac{1}{(2\pi)^2}\int_{-\infty}^{\infty}\tilde{V}(\mathbf{k})\left(-1+(2\pi)^2 n\sum_{l,m\in\mathbb{Z}}\delta(\mathbf{k}-\mathbf{K}_{l,m})\right)\mathrm{d}^2\mathbf{k} \\ &= -\frac{1}{(2\pi)^2}\int_{-\infty}^{\infty}\tilde{V}(\mathbf{k})\mathrm{d}^2\mathbf{k} \;+\; n\int_{-\infty}^{\infty}\tilde{V}(\mathbf{k})\sum_{l,m\in\mathbb{Z}}\delta(\mathbf{k}-\mathbf{K}_{l,m})\mathrm{d}^2\mathbf{k} \\ &= -\frac{1}{(2\pi)^2}\int_{-\infty}^{\infty}\tilde{V}(\mathbf{k})\mathrm{d}^2\mathbf{k} \;+\; n\sum_{l,m}\tilde{V}(\mathbf{K}_{l,m}) \end{aligned} \tag{18}$$

Check the unit again: both terms are of unit $\mathrm{unit}(V)\cdot\mathrm{unit}(k)^2 = \mathrm{unit}(V)\cdot\mathrm{unit}(r)^{-2}$; in second term n is of $\mathrm{unit}(r)^{-2}$.

This is the simplest form of V we can get. To keep going, we need to invoke the actual expression of the electrostatic potential V. In Bravais lattice space, let $r=|\mathbf{r}|$, then it is

$$V(r) = -\frac{1}{4\pi\varepsilon_0}\frac{e}{r} \quad \text{with } \lim_{r\to\infty}V(r)=0; \tag{19}$$

let $k=|\mathbf{k}|$, the Fourier transform in polar coordinate [3] then gives its form in the reciprocal lattice space,

$$\tilde{V}(k) = -\frac{1}{4\pi\varepsilon_0}\frac{2\pi e}{k} \quad \text{with } \lim_{k\to\infty}\tilde{V}(k)=0; \tag{20}$$

[1] W. Strauss, *Partial Differential Equations, An Introduction*, 2nd ed (John Wiley & Sons, 2008), p.345.
[2] *ibid.*, p.334.
[3] N. Baddour, Adv. Imaging Electron Phys. **165**, 1 (2011).

We see $\tilde{V}$ is still inverse proportional to the distance in the reciprocal lattice space. This means we cannot avoid the the divergence of $\int_0^\infty \frac{1}{k} k \mathrm{d}k = \int_0^\infty \mathrm{d}k$; we need to find a proper way to deal with it.

The first term in (18) looks really like the inverse Fourier transform of $\tilde{V}(\mathbf{k})$, but we will not add the kernel $e^{i\mathbf{r}\cdot\mathbf{k}}$ and take the limit $\mathbf{r} \to \mathbf{0}$ to actually transform it since it will come back to where we leave. Instead, we add a Gaussian phase term centered at zero $e^{-\frac{1}{2}w^2k^2}$, where $\mathrm{unit}(w) = \mathrm{unit}(k)^{-1}$, and take the limit $w \to 0$;

$$V = \lim_{w\to 0}\left(-\frac{1}{(2\pi)^2}\int_{-\infty}^{\infty}\tilde{V}(\mathbf{k})e^{-\frac{1}{2}w^2k^2}\mathrm{d}^2\mathbf{k} \;+\; n\sum_{l,m}\tilde{V}(\mathbf{K}_{l,m})e^{-\frac{1}{2}w^2K_{l,m}^2}\right) \tag{21}$$

where $K_{l,m} = |\mathbf{K}_{l,m}|$.

The Gaussian phase term is added to make the integral convergent; the infinite sum of discrete variables can be approximated by the corresponding integral which is also made to be convergent.

Assume the expression of V is independent of angle θ, the formula can be simplified as

$$V = \lim_{w\to 0}\left(-\frac{1}{2\pi}\int_{0}^{\infty}\tilde{V}(k)e^{-\frac{1}{2}w^2k^2}k\mathrm{d}k \;+\; n\sum_{l,m}\tilde{V}(K_{l,m})e^{-\frac{1}{2}w^2K_{l,m}^2}\right) \tag{22}$$

and so

$$\boxed{E_{\mathrm{one}} = \lim_{w\to 0}\frac{\hbar^2}{m_e w^2} + \frac{-e}{2}\left(-\frac{1}{2\pi}\int_{0}^{\infty}\tilde{V}(k)e^{-\frac{1}{2}w^2k^2}k\mathrm{d}k \;+\; n\sum_{l,m}\tilde{V}(K_{l,m})e^{-\frac{1}{2}w^2K_{l,m}^2}\right)} \tag{23}$$

note that w in kinetic energy is the same as the Gaussian packet we used in potential energy.

Comment 1: (23) **in terms of** η **and** r_s

We are interested in expressing E_{one} only in terms of the Wigner-Seitz radius r_s and the ratio η of w to the lattice constant. The Wigner-Seitz radius r_s is defined to satisfy

$$\pi r_s^2 := \text{average area per electron} = \frac{\text{area of one Wigner-Seitz cell}}{1} = \frac{1}{n}$$

So,

$$n = \frac{1}{\pi r_s^2} \tag{24}$$

and based on (15) and (9)

$$R = \sqrt{\frac{2\pi}{\sqrt{3}}}\, r_s, \quad K_{l,m} = \sqrt{\frac{8\pi}{\sqrt{3}}(l^2 + m^2 - lm)}\,\frac{1}{r_s} \tag{25}$$

and based on the definition of η

$$w = \eta R = \eta\sqrt{\frac{2\pi}{\sqrt{3}}}\, r_s \tag{26}$$

Comment 2: Try to find (23) **analytically**

Plug (20) into it, the first term becomes

$$-\frac{1}{2\pi}\frac{-2\pi e}{4\pi\varepsilon_0}\int_0^\infty \frac{1}{k}e^{-\frac{1}{2}w^2k^2}k\,\mathrm{d}k = \sqrt{\frac{\pi}{2}}\frac{e}{4\pi\varepsilon_0}\frac{1}{w}, \tag{27}$$

and the second term is

$$\begin{aligned} n\sum_{l,m}\tilde{V}(K_{l,m})e^{-\frac{1}{2}w^2K_{l,m}^2} &= n\frac{-2\pi e}{4\pi\varepsilon_0}\frac{\sqrt{3}R}{4\pi}\sum_{l,m}\frac{1}{\sqrt{l^2+m^2-lm}}e^{-\frac{1}{2}w^2\frac{16\pi^2}{3R^2}(l^2+m^2-lm)} \\ &= -\frac{e}{4\pi\varepsilon_0}\frac{1}{R}\sum_{l,m}\frac{1}{\sqrt{l^2+m^2-lm}}e^{-\frac{8\pi^2w^2}{3R^2}(l^2+m^2-lm)} \end{aligned}$$

This infinite sum converges since it takes the form $\sum_a \frac{e^{-a}}{\sqrt{a}}$. Thus,

$$V(w) = \frac{e}{4\pi\varepsilon_0}\left(\sqrt{\frac{\pi}{2}}\frac{1}{w} - \frac{1}{R}\sum_{l,m\in\mathbb{Z}}\frac{1}{\sqrt{l^2+m^2-lm}}e^{-\frac{8\pi^2w^2}{3R^2}(l^2+m^2-lm)}\right) \tag{28}$$

Immediately, we can find the *total potential energy per electron*

$$\frac{1}{2}(-e)V(w) = -\frac{e^2}{4\pi\varepsilon_0}\left(\sqrt{\frac{\pi}{8}}\frac{1}{w} - \frac{1}{2R}\sum_{l,m\in\mathbb{Z}}\frac{1}{\sqrt{l^2+m^2-lm}}e^{-\frac{8\pi^2w^2}{3R^2}(l^2+m^2-lm)}\right) \tag{29}$$

Combine the formula (**??**) and (29), we have *total energy per electron*

$$\boxed{E_{\text{one}} = \frac{\hbar^2}{m_e w^2} - \frac{e^2}{4\pi\varepsilon_0}\left(\sqrt{\frac{\pi}{8}}\frac{1}{w} - \frac{1}{2R}\sum_{l,m\in\mathbb{Z}}\frac{1}{\sqrt{l^2+m^2-lm}}e^{-\frac{8\pi^2w^2}{3R^2}(l^2+m^2-lm)}\right)} \tag{30}$$

We present the exact result here but it is hard to continue doing it analytically due to the double sum. Instead, we are going to do it numerically. ***We abandon the formula*** (29) ***and choose to code the second term in formula*** (23) ***directly. A more general computer program will compute both two terms in*** (23) ***directly; such a program will contain a function that carries the form of the potential*** $\tilde{V}(k)$ ***indicated by users.***

The total energy per electron

Before evaluating E_{one} numerically, we want to

Another thing is the values of constants. We name a new set of units: 1 hbar := 1 $\hbar$, 1 emass := 1 m_{e}, 1 e := 1 e, and 1 econst := $\dfrac{1}{4\pi\varepsilon_0}$. They define a unit of length

$$1\,\text{Bohr} = 1\,\frac{4\pi\varepsilon_0\hbar^2}{m_{\text{e}}e^2} = 1\frac{\text{hbar}^2}{\text{econst}\cdot\text{emass}\cdot\text{e}^2}$$

Instead of using "meter," we will measure the length in unit of Bohr radius, and in this case, $\hbar$, m_{e}, e, and $\dfrac{1}{4\pi\varepsilon_0}$ can be assigned to 1.0 in the code.

In addition, since $l = m = 0$ will typically give a divergent summand in the second term, we have to remove it intentionally.

In our case, we need to code E_{one} as a function of η and r_s,

$$\texttt{Eone}(w, r_s) = \texttt{T} - \frac{1}{2}\,(\,\texttt{Vint} + \texttt{Vsum}\,) \qquad \text{[in computer]}$$

where

$$\texttt{T} = \frac{1}{w^2} \qquad \text{[in computer]}$$

$$\texttt{Vint} = -\frac{1}{2\pi}\int_0^\infty \tilde{V}(k)e^{-\frac{1}{2}w^2k^2}k\,\mathrm{d}k \qquad \text{[in computer]}$$

$$\texttt{Vsum} = \frac{1}{\pi r_s^2}\sum_{(l,m)\neq(0,0)} \tilde{V}(K_{l,m})e^{-\frac{1}{2}w^2K_{l,m}^2} \qquad \text{[in computer]}$$

Of course, we have to define the function of potential $\tilde{V}(k)$ globally in our code.

Here is an example in Python.

```
def Eone(w, r_s):
    # T: kinetic energy
    T = 1/(w*w)


    # Vint: the integral in the expression of V
    def integrand(k):
        return Vtilde(k) * np.exp(-0.5*w*w*k*k) * k
    I = integrate.nquad(integrand, [[0, np.inf]])
    Vint = -I[0] / (2.0*np.pi)


    # Vsum: the summation in the expression of V
    def K(l,m):
        return np.sqrt((8.0*np.pi/np.sqrt(3)) * (l*l + m*m - l*m)) / r_s
    S = 0
    for l in range(-1000, 1001):
        for m in range(-1000, 1001):
            if l==0 and m==0:
                S = S + 0
            else:
                S = S + Vtilde(K(l,m))*np.exp(-0.5*w*w*K(l,m)*K(l,m))
    Vsum = S / (np.pi*r_s*r_s)


    # returns Eone
    return T - 0.5*(Vint + Vsum)
```

In vacuum,

$$\tilde{V}(k) = -\frac{2\pi}{k} \quad \text{with} \lim_{k\to\infty} V(k) = 0 \qquad \text{[in computer];} \tag{31}$$

some outputs are

if we treat Eone is a function of eta and n, then
E(5,1)=-0.08533141373155004
E(1,1) = 0.3733429313326011
E(0.1,1)= 90.10665293889625
E(0.01, 0.001)=9937.281847266722
E(0.01, 0.01)=9936.809834459207
E(0.01, 0.1)=9932.08970638404
E(0.01, 1)=9884.88842563238
E(0.01, 5)=9675.104955625
E(0.01, 10)=9412.875618115773
E(0.01, 15)=9150.646280606548
E(0.01, 100)=4692.7475429497135

however, if we set R=1, then n=2/sqrt(3) and Eone is a function only of eta:
E(eta=0.01) = 9997.893564574373

E(eta=0.1) = 97.9212699456691
E(eta=1) = 0.3733429313533917
E(eta=10) = -0.05266570686577501
E(eta=100) =-0.006166570686577503

another way: only terms of R since n is related to R:
E(R=0.01) = 9792.12699456691
E(R=0.1) = 979.212699456691
E(R=1) = 97.92126994566911
E(R=10) = 9.79212699456691
E(R=100) = 0.9792126994566911

????

Quantum melting criterion

Combine

and then use the unit “Bohr”,

$$r_s = b\,\text{Bohr}, \quad b := \frac{r_s}{1\text{ Bohr radius}}$$

So,

$$n = \frac{1}{\pi b^2}\text{Bohr}^{-2} \tag{32}$$

and let

$$w = \frac{1}{\pi b^2}\text{Bohr}^{-2} \tag{33}$$

and then use the unit “Bohr”,

$$r_s = b\,\text{Bohr}, \quad b := \frac{r_s}{1\text{ Bohr radius}}$$

So,

$$n = \frac{1}{\pi b^2}\text{Bohr}^{-2} \tag{34}$$

and let

$$w = \frac{1}{\pi b^2}\text{Bohr}^{-2} \tag{35}$$

When we say $R = b\,\text{Bohr}$, we means $R = b\dfrac{4\pi\varepsilon_0\hbar^2}{m_e e^2}$ (unit: meter), and b itself is dimensionless.

In twisted bilayer graphene (tBLG), the dielectric constant and the formalism of potential are different from they are in vacuum. The electric potential energy is given by [4]

$$\tilde{U}(k) = \frac{\tilde{U}_0(k)}{1 - \tilde{U}_0(k)\Pi(k)} \tag{36}$$

where $\Pi(\mathbf{k}, \omega) = -\frac{|\mathbf{k}|^2}{\pi}\left(\frac{m}{k^2} + \frac{1}{2k}\left(1 - \frac{4m^2}{k^2}\right)\arctan\frac{k}{2m}\right)$ and $k = \sqrt{|\mathbf{k}|^2 - \omega^2}$

[4] V. N. Kotov, V. M. Pereira, and B. Uchoa, Phys. Rev. B **78**, 075433 (2008).