Condensed Matter Theory problem set 3

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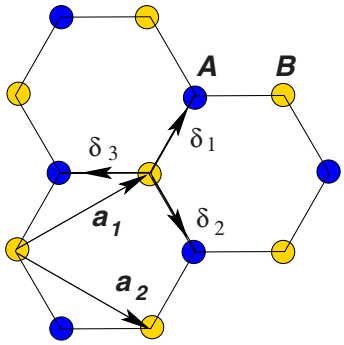
Background: Graphene consists of a planar hexagonal Bravais lattice with a basis of two Carbon atoms, labeled A and B, see figure below (taken from Castro Neto *et al.*, Rev. Mod. Phys. **81**, 109 (2009)). Strong covalent σ bonds are formed by planar sp^2 orbitals of the carbon atoms. In this figure, blue circles indicate carbon atoms on the A sublattice, while yellow circles indicate carbon atoms on the B sublattice. The vectors $\mathbf{a}_1$ and $\mathbf{a}_2$ are the lattice unit vectors. The carbon-carbon distance in graphene is $a \approx 0.142$ nm.

The remaining p_z orbitals, standing perpendicular to the lattice plane, form a band of mobile electrons. Graphene features a number of fascinating properties (e.g., high electron mobility, gapless semiconductor, ...) that can be traced back to its band structure. Furthermore, electrons in graphene behave like massless two-dimensional Dirac fermions.



Problem 6: Band structure of graphene and Dirac electrons

The tight-binding Hamiltonian for the mobile electrons in graphene makes the assumption that electrons can hop with hopping amplitude t between neighboring sites with nearest neighbor vectors

$$\boldsymbol{\delta}_1 = \frac{a}{2}(1,\sqrt{3}), \quad \boldsymbol{\delta}_2 = \frac{a}{2}(1,-\sqrt{3}), \quad \boldsymbol{\delta}_3 = -a(1,0), \tag{1}$$

and therefore it reads

$$H = -t \sum_{\langle i,j\rangle,\sigma} (a^\dagger_{\sigma,i} b_{\sigma,j} + \text{H.c.}), \tag{2}$$

where $a_{i,\sigma}$ ($a^\dagger_{i,\sigma}$) annihilates (creates) an electron with spin $\sigma \in \{\uparrow, \downarrow\}$ on site $\boldsymbol{R}_i$ on sublattice A (and equivalently for sublattice B). The brackets $\langle\cdot\rangle$ denote a summation over nearest neighbors. Furthermore, we define the Fourier transform of the ladder operators by $c_{\sigma,i} = \frac{1}{N}\sum_{\boldsymbol{k}} e^{-i\boldsymbol{k}\cdot\boldsymbol{R}_i} c_{\sigma,\boldsymbol{k}}$ where $c \in \{a, b\}$.

(a) From the information given in the figure above, derive explicit expressions for the lattice vectors $\boldsymbol{a}_1$ and $\boldsymbol{a}_2$ and also determine the reciprocal lattice vectors $\boldsymbol{b}_1$ and $\boldsymbol{b}_2$.

(b) Plot the first Brillouin zone and give explicit expressions for the positions of the corners of the Brillouin zone. There are two inequivalent corners, typically denoted by $\boldsymbol{K}$ and $\boldsymbol{K}'$, that cannot be connected by reciprocal lattice vectors. You should find

$$\boldsymbol{K} = \left(\frac{2\pi}{3a}, \frac{2\pi}{3\sqrt{3}}\right), \quad \boldsymbol{K}' = \left(\frac{2\pi}{3a}, -\frac{2\pi}{3\sqrt{3}}\right). \tag{3}$$

(c) Use the Fourier transform to write the tight-binding Hamiltonian in momentum space and determine its energy eigenvalues $E_\pm(\boldsymbol{k})$. Note that due to the lattice structure with a basis of two atoms you will obtain two energy bands. You should find a result of the form

$$E_\pm(\boldsymbol{k}) = \pm t\sqrt{3 + f(\boldsymbol{k})} \tag{4}$$

$$\text{with} \quad f(\boldsymbol{k}) = 2\cos(\sqrt{3}k_y a) + 4\cos\left(\frac{\sqrt{3}}{2}k_y a\right)\cos\left(\frac{3}{2}k_x a\right). \tag{5}$$

(d) Optional, in case you have access to Mathematica or Maple: Plot the energy dispersion in momentum space in the first Brillouin zone. It looks quite pretty, so please try!

(e) Calculate the points in momentum space where the energy vanishes. These points are called 'Dirac points' for reasons that become clear below.

(f) Expand the full energy band structure calculated in (c) close to the $\boldsymbol{K}$ (or $\boldsymbol{K}'$) vector with $\boldsymbol{k} = \boldsymbol{K} + \boldsymbol{q}$ with $|\boldsymbol{q}| \ll |\boldsymbol{K}|$ and give the linearized energy dispersion close to $\boldsymbol{K}$ as $E_\pm(\boldsymbol{q})$.

(g) Extra (and more difficult): Show that the linearized version of the Hamiltonian close to the $\boldsymbol{K}$ and $\boldsymbol{K}'$ points corresponds to a sum of two two-dimensional Dirac- (or Weyl-) Hamiltonians which be can written as $\sim \pm\boldsymbol{\tau}^{(*)}\cdot\boldsymbol{k}$ with Pauli matrices $\tau_{x,y}$ in sublattice space.

Problem 7: Bloch/Wannier Functions for Cold Atoms in Optical Lattices

We consider neutral atoms confined to one dimension. The atoms are subject to a periodic standing wave inducing the following potential to the atoms

$$V(x) = V_0 \sin^2(k_L x) \tag{6}$$

with $k_L = \pi/d$ and d is the distance between two minima. The eigenvalue problem for a single particle in this periodic potential with energy eigenvalue $\varepsilon_{n,k}$ is given by

$$-\frac{\hbar^2}{2M}\frac{\partial^2}{\partial x^2}\phi_{n,k}(x) + V(x)\phi_{n,k}(x) = \varepsilon_{n,k}\phi_{n,k}(x)\,. \tag{7}$$

(a) Use the Bloch ansatz $\phi_{n,k}(x) = u_{n,k}(x)e^{ikx}$ with $u_{n,k}(x+d) = u_{n,k}(x)$ and rewrite the above eigenvalue problem in terms of $u_{n,k}(x)$.

(b) Fourier expand $u_{n,k}$ with coefficients $c_{n,k}(l)$ and derive the following recurrence relation

$$E_R\left(2l + \frac{k}{k_L}\right)^2 c_{n,k}(l) - \frac{V_0}{4}\left[c_{n,k}(l+1) - 2c_{n,k}(l) + c_{n,k}(l-1)\right] = \varepsilon_{n,k}(l)c_{n,k}(l) \tag{8}$$

where we introduced the recoil energy $E_R = \hbar^2 k_L^2/(2M)$.

(c) In order to obtain the spectrum one truncates the system (8) for $|l| \leq l_{max}$ and solves the remaining eigenvalue problem numerically. Choose the parameters $V_0 = 6E_R$, $l_{max} = 10$ and sketch the first three bands over the Brillouin zone.

(d) For a deep lattice, Taylor expand the potential to second order at $x = 0$, i.e., $V(x) = M\omega^2 x^2/2$, and determine the spectrum of the single well. Give a criterion for the validity of the deep lattice approximation.

(e) For deep optical lattices we use the ground-state function of the harmonic oscillator to approximate the Wannier functions for the first band,

$$w_1(x - x_n) = \left(\sqrt{\pi}a\right)^{-1/2} \exp\left[-\frac{(x-x_n)^2}{2a^2}\right], \tag{9}$$

with $x_n = nd$ and oscillator length $a = \sqrt{\hbar/(M\omega)}$. Calculate the tunnel matrix element in the deep-lattice limit

$$J = \int_{-\infty}^{\infty} dx\, w_1^*(x - x_n)\left(-\frac{\hbar^2}{2M}\frac{\partial^2}{\partial x^2} + V(x)\right) w_1(x - x_{n+1})\,. \tag{10}$$