



FIG. 1: An example of the Villain potential. The bottom tips can each be each approximated by a Gaussian.

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## Problem set - 5

Due: Nov. 18th by 5pm in TA box.

For full credit solve 3 and either 1 or 2. If you have time doing both 1 and 2 is recommended.

### 1. Villain Potential.

Consider a 2d lattice potential which is given by:

$$V(x, y) = -V_0 e^{-\lambda(2 - \cos kx - \cos ky)} \quad (1)$$

with  $k = 2\pi/a$ , and  $V_0 > 0$ , and  $\lambda \gg 1$ . According to Villain, we can approximate the rather complicated exponent of a cosine by a sum of Gaussians:

$$V(x, y) \approx - \sum_{n,m} e^{-\frac{1}{2}\lambda k^2((x-na)^2 + (y-ma)^2)}. \quad (2)$$

Below we assume that the potential is weak. Namely:  $V_0 \ll \frac{k_i^2}{2m}$ .

- What are the reciprocal lattice vectors of the lattice  $\vec{k}_1, \vec{k}_2$ ?
- In 2d momentum space, draw the first 4 Brillouin zones. Actually, I would encourage you to use a computer to draw the Brillouin zones. If you do (optional), try to plot the BZ's of the triangular lattice.
- Write  $V(x, y)$  in as an expansion in terms of harmonics of the reciprocal lattice vectors of the lattice:

$$V = \sum_{nm} V_{nm} e^{i(n\vec{k}_1 + m\vec{k}_2) \cdot \vec{r}}. \quad (3)$$

What are the components  $V_{nm}$ ?

- What are the band gaps that emerge at the BZ's linked by  $n\vec{k}_1 + m\vec{k}_2$ ?
- What is the effective mass of the bottom of the lowest band? Your answer should be accurate to order  $V_0^2$  (and within the Villain approximation).

### 2. Tight binding in a delta-function lattice.

Consider a potential given by an array of  $\delta$  functions in 1d:

$$V(x) = \sum_n -V_0 \delta(x - na). \quad (4)$$

Each potential has a negative-energy bound state. In this problem we will construct a tight-binding band out of these states.

- (a) Find the bound state (negative energy states) of one of the potential wells ignoring the others.

We would like to write Bloch waves with these states by creating the following superposition:

$$|p\rangle = \psi_p(x) = \sum_n \psi(x - na)e^{inap} \quad (5)$$

- (b) Show that  $|p\rangle$  indeed obeys Bloch theorem. Namely, if it is translated by the lattice constant, it returns to itself upto a phase:

$$\psi_p(x + a) = e^{ipa}\psi_p(x). \quad (6)$$

- (c) Overlap matrix. The exponentially decaying bound states found above clearly do not form an orthonormal set of states. Namely:

$$M_{nm} = \int_{-\infty}^{\infty} dx \psi(x - na)^* \psi(x - ma) \neq \delta_{nm} \quad (7)$$

Find the matrix  $M_{nm} = M_{n-m}$  (where the equality indicates that the matrix elements are only a function of the distance of the entry from the diagonal - which corresponds to the physical distance between wave functions).

- (d) Wannier wave functions construction. We would like to show that the following wave functions:

$$\phi_n(r) = \sum_m (M^{-1/2})_{nm} \psi(x - ma) \quad (8)$$

are orthogonal. We can do that directly first. Let me do this step for you:

$$\int_{-\infty}^{\infty} \phi_n(x)^* \phi_m(x) = \sum_{m,n} (M^{-1/2})_{n\ell}^* (M^{-1/2})_{mk} \int dx \psi(x - \ell a)^* \psi(x - ka). \quad (9)$$

This becomes:

$$= \sum_{m,n} (M^{-1/2})_{n\ell}^* (M^{-1/2})_{mk} M_{\ell k} = M_{n\ell}^{-1/2} M_{\ell k} M_{km}^{-1/2} = \delta_{nm}, \quad (10)$$

where we used the fact that  $M$  is hermitian.

Back to the problem!

Find  $M^{-1/2}$ . Instructions: Diagonalize  $M$  using plane wave ansatz  $e^{ipn}$ . This should give you  $M = UDU^\dagger$ . Then find  $M^{-1/2} = U \frac{1}{\sqrt{D}} U^\dagger$ .

What is  $\phi_n(x)$ ? They are called the Wannier basis for the lattice orbital.

- (e) Energy calculation. We now strongly suspect that

$$|p\rangle = \sum_n e^{inap} \phi_n(x) \quad (11)$$

are the true eigenstates of the problem. Let us confirm this and find the energy.

To calculate the energy, first find the hamiltonian in the

$$h_{nm} = \int_{-\infty}^{\infty} dx \psi(x - na)^* H(x) \psi(x - ma) \neq \delta_{nm} \quad (12)$$

Trick:  $H = H_m + V_{m,pert}$  with  $H_m = (p^2/2m - V_0\delta(x - ma))$  and  $V_{pert} = - \sum_{n \neq m} V_0\delta(x - na)$ . Use

$H_m\psi(x - ma) = -\epsilon\psi(x - ma)$  with  $\epsilon$  the binding energy of the state  $\psi(x)$ .

The Hamiltonian in the  $\phi_n$  basis is the one you found in PS4 variationally:

$$H_{eff} = \sum_{mn} \langle \phi_n | H | \phi_m \rangle | \phi_n \rangle \langle \phi_m | = [M^{-1/2} H M^{-1/2}]_{nm} \quad (13)$$

What are the energy eigenstates of  $H_{eff}$ ? Hint: Do the calculation in Fourier basis, Eq. (11).

3. Carriers and chemical potential in n-type semiconductor.

Consider an n-type semiconductor with donor density  $N_D$ , and the donor states appearing an energy  $\delta$  below the bottom of the conduction band. Assume that the density of states  $\rho(\epsilon) = \rho_0$  is constant for the conduction band, and that the valence band is so far in energy that it could be neglected.

- (a) Show that the chemical potential obeys the following equation:

$$\rho_0 T \ln(1 + e^{\mu\beta}) = N_D \frac{1}{e^{(\delta+\mu)\beta} + 1} \quad (14)$$

with  $\mu$  measured from the bottom of the conduction band.

- (b) Find an approximate expression for  $\mu$  when the temperature is small -  $T \ll \delta$ .  
 (c) Find an approximate expression for  $\mu$  when the temperature is large -  $T \gg \delta$ .  
 (d) Provide a qualitative plot of the chemical potential and the number of carrier as a function of  $T$ . If you'd like to solve the problem numerically, reasonable parameters are:  $\rho_0 \sim 10^{28} \frac{1}{m^3 eV}$  and  $N_D \sim 10^{23} \frac{1}{m^3}$ , and  $\delta \sim 0.05 eV$ .  
 (e) What is the number of carriers as a function of  $T$  for the two limits?  
 Hint:  $e^{\mu\beta} \ll 1$  in all circumstances.