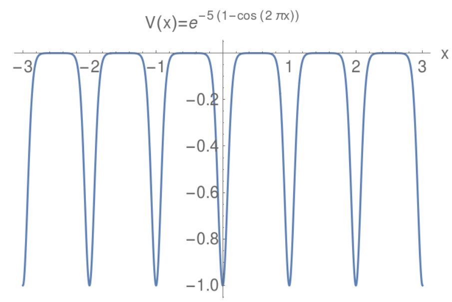

FIG. 1: An example of the Villain potential. The bottom tips can each be each approximated by a Gaussian.

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Problem set - 5

Due: Nov. 16th by 5pm in TA box.

1. Villlain Potential.

   Consider a 2d lattice potential which is given by:

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

   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:

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

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

   (a) What are the reciprocal lattice vectors of the lattice $\vec{k}_1, \vec{k}_2$?

   (b) In 2d momentum space, draw the first 4 Brillouin zones. Actually, I would encourge you to use a computer to draw the Brillouin zones. If you do (optional), try to plot the BZ's of the triangular lattice.

   (c) Write $V(x,y)$ in as an expansion in terms of harmonics of the reciprocal lattice vectors of the lattice:

$$V = \sum_{nm} V_{nm} e^{i(n\vec{k_1}+m\vec{k2})\cdot\vec{r}}. \tag{3}$$

   What are the components V_{nm}?

   (d) What are the band gaps that emerge at the BZ's linked by $n\vec{k}_1 + m\vec{k}_2$?

   (e) 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 δ functions in 1d:

$$V(x) = \sum_n -V_0\delta(x-na). \tag{4}$$

   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.

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

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

(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:

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

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

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

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:

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

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

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

This becomes:

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

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

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

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

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

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 ϵ the binding energy of the state $\psi(x)$.

The Hamiltonian in the ϕ_n basis is the one you found in PS4 variationally:

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

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