Analytic:

[1.] Compute the energy bands of a 2D square lattice which has different hoppings \( t_x \) and \( t_y \) in the \( \hat{x} \) and \( \hat{y} \) directions. That is,

\[
H = -t_x \sum_1 \left( c_{1+\hat{x}}^\dagger c_1 + c_1^\dagger c_{1+\hat{x}} \right) - t_y \sum_1 \left( c_{1+\hat{y}}^\dagger c_1 + c_1^\dagger c_{1+\hat{y}} \right).
\]

Actually, this Hamiltonian might more appropriately be viewed as that of a rectangular lattice, where the different separations in the \( \hat{x} \) and \( \hat{y} \) directions lead to different hoppings.

[2.] I am considering asking one of the students in my group to start some simulations of a square lattice tight-binding Hamiltonian with the usual near-neighbor hopping \( t \) between site \( l \) and sites \( l + \hat{x} \) and \( l + \hat{y} \), but also a hopping \( t' \) which connects sites \( l \) with sites \( l + 2\hat{x} + \hat{y} \) and \( l + \hat{x} + 2\hat{y} \). What is \( \epsilon(k) \) for this model? (Note: I am really thinking of giving this project to a student. It could have, I think, some quite interesting features!)

[3.] Finish the calculation of the energy bands of the tight-binding Hamiltonian appropriate to \( \text{CuO}_2 \) sheets of cuprate superconductors:

\[
H = -t \sum_1 \left( d_1^\dagger p_1^{(x)} + p_1^{(x)} \right) + d_1 \left( p_1^{(y)} + p_1^{(y)} \right) + d_1^{\dagger} \left( p_1^{(x)} + p_1^{(x)} \right) + d_1^{\dagger} \left( p_1^{(y)} + p_1^{(y)} \right) + \epsilon_p \sum_{1} \left( p_1^{(x)} p_1^{(x)} + p_1^{(y)} p_1^{(y)} \right)
\]

Remember that the \((x), (y)\) superscripts on the \( p \) operators distinguish the oxygen orbitals lying between copper atoms separated in the \( \hat{x}, \hat{y} \) directions. In class, we made a lot of progress on this problem: We went to momentum space, did the sum over \( l \) got the \( \delta_{k,k'} \), which collapsed the two momenta sums to one. Since we have a three site basis, we were left with a three-by-three matrix. You need to get that matrix correctly, and then diagonalize it. A clue that you are on the right track is that you should find you get one band which is completely flat (energy is independent of momentum).

What happens in the limit \( \epsilon_p >> t \)? (To answer, expand the square root appropriately.) You should get an energy band which looks like that of a square lattice with an effective hopping \( t_{\text{eff}} = t^2/\epsilon_p \). The physical justification of this form is that an electron gets from one copper to the next by two hoppings \( t \) but also must pass through the high energy intermediate state of sitting briefly on the intervening oxygen. If you think about it, the form is reminiscent of second order perturbation theory. This is in fact the rigorous justification for it.

[4.] (Optional) Compute the energy bands of a honeycomb lattice.
Numeric:

I will be available in the computer lab, room 106, Wednesday noon - 2:00 pm to help anyone who needs assistance with these problems.

[5.] Compute the density of states my student will find associated with the geometry of Problem 2. (This should be a simple modification of your code from a previous assignment.)

[6.] (Optional) Compute the density of states for the honeycomb lattice. (See problem [4].) Show that $N(\omega = 0) = 0$, but that there is no gap: $N(\omega)$ vanishes linearly on both sides of $\omega = 0$. This is the origin of many of the fascinating properties of graphene.