Problem set 5 (due on Dec 2. at 3:30pm)

Provide individual solutions for problems 1 and 3. Problem 2 is a group problem. The groups are posted on Canvas, and they will be different for each problem set. The solutions should be uploaded through Canvas before the deadline.

1. Polarons in the anti-adiabatic limit: Consider the Holstein model for a 1D chain:

\[ \mathcal{H}_H = -t \sum_{n,\sigma} (c_{n\sigma}^\dagger c_{n+1,\sigma} + \text{h.c.}) + \Omega \sum_n b_n^\dagger b_n + g_H \sum_{n,\sigma} c_{n\sigma}^\dagger c_{n\sigma} (b_n + b_n^\dagger) \]

in the anti-adiabatic limit where \( \Omega \gg t, g \). Here we can use perturbation theory to infer the behavior of the corresponding polarons. We will choose \( \mathcal{H}_0 = \Omega \sum_n b_n^\dagger b_n \) and the sum of the other two terms will be the small perturbation \( \hat{V} \).

(a) Assume that there is a single electron on the chain. What are the eigenfunctions of the ground-state manifold of \( \mathcal{H}_0 \)? What is the corresponding energy \( E_0 \)?

(b) Now do perturbation theory to second order, and find the corresponding Hamiltonians:

\[ \hat{h}_{\text{eff}} = \mathcal{H}_0 + \hat{P}_0 \hat{V} \hat{P}_0 + \hat{P}_0 \hat{V} \frac{1 - \hat{P}_0}{E_0 - \mathcal{H}_0} \hat{V} \hat{P}_0 \]

where \( \hat{P}_0 \) is the projector on the lowest-energy manifold from (a). \textbf{Hint:} show that \( \hat{h}_{\text{eff}} c_{n\sigma}^\dagger |0\rangle = ac_{n\sigma}^\dagger |0\rangle - b \left( c_{n+1\sigma}^\dagger |0\rangle + c_{n-1\sigma}^\dagger |0\rangle \right) = a |n\sigma\rangle - b (|n+1,\sigma\rangle + |n-1,\sigma\rangle) \), where \( a \) and \( b \) are some energies that you have to identify. Then use \( \hat{h}_{\text{eff}} = \sum_{n,m,\sigma} (m\sigma|\hat{h}_{\text{eff}}|n\sigma) c_{m\sigma}^\dagger c_{n\sigma} \).

(c) Diagonalize \( \hat{h}_{\text{eff}} \) and find the polaron formation energy \( E_P \) and its effective mass \( m^* \).

\textbf{For fun:} repeat for the Peierls model:

\[ \mathcal{H}_P = -t \sum_{n,\sigma} (c_{n\sigma}^\dagger c_{n+1,\sigma} + \text{h.c.}) + \Omega \sum_n b_n^\dagger b_n + g_P \sum_{n,\sigma} (c_{n\sigma}^\dagger c_{n+1,\sigma} + \text{h.c.}) (b_{n+1} + b_{n+1}^\dagger - b_n - b_n^\dagger) \]

in the anti-adiabatic limit where \( \Omega \gg t, g \). This will give you some idea as to why Peierls polarons can be much lighter than Holstein ones.

2. Polyacetylene, the Su-Schrieffer-Heeger (SSH) model and the Peierls distortion. Polyacetylene (CH)_n is a polymer with a backbone made of C with H sidebonds. Given that all C are identical, one would expect the structure to look like in the top panel of the figure below, with constant distance \( a \) between any two consecutive C atoms. The zig-zaggy structure is because 3 of the 4 valence electrons of each C occupy in-plane \( sp^2 \) orbitals, oriented at 120° from each other (same as in graphene), and form covalent bonds with corresponding orbitals from the 2 neighbor C and the H. These covalent bonds stabilize the backbone. This leaves a single electron per C (the 4th valence electron, which is in a \( p_z \) orbital). We would like understand what happens to these \( p_z \) valence electrons.
a) If the structure is as depicted in the top panel, write the simplest non-interacting Hamiltonian $H_{el}$ describing these $p_z$ electrons.

b) Diagonalize it, plot the corresponding band structure, and explain if this system is a metal or an insulator.
c) Now let us consider the role of lattice distortions. For simplicity, we will treat these as being classical variables, not quantum ones. We allow each CH pair to be displaced out of its equilibrium by a distance $u_n$, as shown by the lower panel, with $|u_n| \ll a$. Justify why the total Hamiltonian can be written as: $\mathcal{H} = H_{el} + H_{latt} + H_{el-latt}$ where $H_{latt} = \sum_n \left[ \frac{p_n^2}{2M} + \frac{M\Omega^2}{2}(u_{n+1} - u_n)^2 \right]$ and $H_{el-latt} = \alpha \sum_{n,\sigma} (u_{n+1} - u_n) \left( c_{n,\sigma}^\dagger c_{n+1,\sigma} + h.c. \right)$.

d) Now consider a so-called Peierls distortion, with $u_n = (-1)^n u$ where $u$ is a constant – this ”dimerizes” the lattice, i.e. divides the bonds into alternating shorter and longer ones. Find the equation that gives the value of $u$, and argue that it has a finite solution (do not do the integral). **Hint:** the best $u$ is the one that minimizes the total GS energy. Is the state with $u \neq 0$ a metal or an insulator?

e) Which is the true ground-state, the undistorted chain ($u = 0$) or this dimerized one that you found at (d)? Explain why this makes sense.

f) Now consider the same system with $N = 6$ and PBC – this molecule is called benzene. Does benzene dimerize? Use as typical values $t = 2.5eV$, $\alpha = 4eV/\AA$, $M\Omega^2 = K = 21eV/\AA^2$.

3. Draw a “concept map” for the material covered in this course. For an example of a concept map, see https://notatextbook.files.wordpress.com/2014/04/physics-concept-map.png

Basically, start by writing down things like “model Hamiltonian”, “metals”, “phonons”, ”screening” and any other main concepts we discussed, and try to make a map showing how they are related to one another. This should be a good exercise to help you organize for yourselves the material covered in this class. All reasonable efforts will get full grades. The best maps will get bonus points, and I’ll post them online for all to see.