

Session 3 - Individual problem solving session.

1. **Li-H chain (again).** Consider the infinite chain of the simple molecule we have defined in the previous class (with Li 2s and H 1s states only) where atoms are evenly spaced with distance R .
 - a) What is the periodicity of the Hamiltonian?
 - b) Using Bloch theorem, write the generic form of the eigenfunctions of this Hamiltonian.
 - c) Sketch the band structure of this system.
 - d) If we replaced all Li atoms with H, while keeping everything else the same in this system, how would the band structure change? Comment on the difference of this band structure with respect to the one of the H-chain we obtained in class (i.e. when we consider a single H as the repeating unit).

2. **Peierls Distortion in H chain** In the previous problem you have defined the band structure of an equally spaced H chain. Now let us introduce a slight dimerization, i.e. H atoms are allowed to pair up with a deformation such that they are either $R + \epsilon$ or $R - \epsilon$ apart from their formerly nearest neighbors.
 - a) Assuming the hopping to change linearly with the deformation, sketch the band structure of this deformed system.
 - b) Show that the evenly spaced system is energetically unstable against such deformations.
 - c) Show how the band structure changes as the inter-dimer distance goes to infinity.
 - d) [Optional] Some phonon modes in metals are very special, they cost very little energy to excite at certain wavevectors, sometimes as little as zero energy! This is known as Kohn anomaly. To see that what you have observed in the dimerized chain is also a Kohn anomaly i) show that the undistorted H-chain is a metal ii) show which phonon mode at which wavevector has reduced excitation energy iii) does this wavevector coincide with any special length scale of your system?

3. **Variational Principle Example.** Consider a simple Hamiltonian for a single electron bound to a nucleus with atomic number Z (Hydrogen-like atoms).
 - a) Consider a trial wavefunction $\Psi(\mathbf{r}) \propto \exp(-\alpha r/a_0)$ where α is a variational parameter and $a_0 = \frac{\hbar^2}{me^2}$ is the Bohr radius. Derive the minimum energy according to variational principle. How does it compare to real ground state energy?
 - b) Now consider an additional electron in the system, where the electrons interact via Coulomb interaction (Helium-like atom). This time consider a trial wavefunction of the form $\Psi(\mathbf{r}_1, \mathbf{r}_2) \propto \exp(-\alpha r_1/a_0) \exp(-\alpha r_2/a_0)$. Is this a proper wavefunction for a fermionic system? Comment on its symmetry.
 - c) Derive the variational estimate for the ground state of the system described above (see the hints for a few integrals that may be useful). How does the minimizing value of the variational parameter change with respect to the previous case? Could you estimate the direction of the change before doing the calculation?
 - d) On the basis of your calculation would you expect the negative Hydrogen ion to be stable ?
 - e) Considering Z as a real valued parameter, what is the minimum value of Z for which the 2-electron system is stable? If you were to include electronic correlation in your calculation do you expect this critical value to become larger or smaller?

hint: $\int_0^\infty \exp(-x)x^n dx = n!$, $\int \frac{\exp(-2(r_1+r_2))}{|\mathbf{r}_1-\mathbf{r}_2|} d\mathbf{r}_1 d\mathbf{r}_2 = \frac{5}{8}\pi^2$