Solid state physics 2020 Minitest 2 (120 minutes)

12 March 2020

These are example solutions for your reference under the following conditions.

- If these solutions contain mistakes (and they may), the physical correctness has priority over them in grading.
- You may not distribute or repost this document.

1. (50 points) **Exponential interatomic potential**

In the lecture you have encountered the Lennard-Jones potential, which is used a lot to model the interaction between atoms. Consider instead the following potential approximating covalent bonding energy.

$$U(r) = -\epsilon \frac{r}{r_0} e^{-\frac{r}{r_0}}$$

We consider two atoms with equal masses m that interact via the potential $U(r)$ described above, where r is the interatomic distance between the two atoms.

(a) (10 points) Sketch the potential profile. Find the equilibrium distance r between the two atoms interacting via the potential $U(r)$, as well as the depth of the potential well.

Solution:

$$\frac{dU}{dr} = (-\frac{\epsilon}{r_0} + \frac{\epsilon r}{r_0^2}) e^{-r/r_0}$$

Minimum at $dU/dr = 0$. hence we obtain:

$$r_{\min} = r_0$$

$$U(r_{\min}) = -\epsilon e^{-1}$$

(b) (10 points) Expand U(r) around the equilibrium position up to the second order and find an expression for the spring constant κ in terms of ϵ and r_0.

Solution:

$$U(r) \approx -\epsilon e^{-1} + \frac{\epsilon}{2 e r_0^2} (r - r_0)^2$$

Hence κ is given by:

$$\kappa = \frac{\epsilon}{e r_0^2}$$

(c) (10 points) Write down the equation of motion of the two atoms near the equilibrium position, considering only the harmonic part of the potential obtained in (b).

Solution:

$$F(r_i) = m\ddot{r}_i = -\frac{\partial U(r_i)}{\partial r_i}$$

$$\begin{aligned} m\ddot{r}_1 &= F(r_1) - F(r_2) \\ &= -\kappa\,(r_1 - r_0) + \kappa\,(r_2 - r_0) \\ &= -\kappa\,(r_1 - r_2) \\ &= -\frac{\epsilon}{e r_0^2}\,(r_1 - r_2)\,. \end{aligned}$$

We can follow the same procedure for the second particle, which yields:

$$m\ddot{r}_2 = -\frac{\epsilon}{e r_0^2}\,(r_2 - r_1)$$

(d) (10 points) Calculate the frequency of the vibrational mode and find the ground state energy of the molecule.

Solution: We know that the solutions to r_1 and r_2 have the following form:

$$r_1(t) = r_{0,1}e^{i\omega t}, \quad r_2(t) = r_{0,2}e^{i\omega t}.$$

By plugging this into the equations of motion obtained in (c) yields the following system of equations:

$$\begin{cases} m\omega^2 r_{0,1} = \frac{\epsilon e^{-1}}{r_0^2}\,(r_{0,1} - r_{0,2}) \\ m\omega^2 r_{0,2} = \frac{\epsilon e^{-1}}{r_0^2}\,(r_{0,2} - r_{0,1}) \end{cases}$$

Solving the set of equations results in the following frequency of the vibrational mode

$$\omega = \sqrt{\frac{2\epsilon e^{-1}}{m r_0^2}}$$

The ground state of the molecule is given by

$$E_0 = -\epsilon + \hbar\omega/2 = -\epsilon + \hbar\sqrt{\frac{\epsilon e^{-1}}{2m r_0^2}}$$

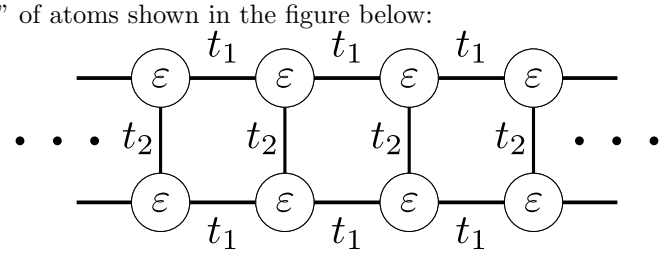
(e) (10 points) Determine for what values of ϵ, r_0, and m can the anharmonicity of the potential be neglected if the particles are in the ground state. *Hint: consider the condition that the ground state energy is close to the bottom of the potential.*

Solution: The anharmonic part of the potential can be neglected if $\hbar\omega \ll \epsilon$, substituting $\omega = \sqrt{\frac{2\epsilon e^{-1}}{m r_0^2}}$ yields:

$$\hbar\sqrt{\frac{2\epsilon e^{-1}}{m r_0^2}} \ll \epsilon \Rightarrow m r_0^2 \epsilon \gg \hbar^2$$

2. (50 points) **Ladder arrangement of atoms**

We consider a "ladder" of atoms shown in the figure below:



The arrangement is infinite in the x-direction, the onsite potential is ε, and the hoppings t_1 and t_2 being as shown in the figure.

(a) (20 points) Use the wave function $|\Psi\rangle = \sum_n (\phi_n |n,1\rangle + \psi_n |n,2\rangle)$, with $|n,1\rangle$ and $|n,2\rangle$ the wave functions of the orbitals of the top and bottom rows of atoms respectively. Write down the LCAO Schrödinger equations assuming that the orbitals on different atoms are orthogonal: $\langle n,l|m,p\rangle = \delta_{n,m}\delta_{l,p}$. Use the plane wave Ansatz to obtain the eigenvalue problem that gives the dispersion relation (do not compute the disperion yet, that is the next question).

Solution: The Schrödinger equation is given by $E|\Psi\rangle = H|\Psi\rangle$. Computing the dot products with $\langle n,1|$ (the states of the upper part of the ladder) and $\langle n,2|$ (the states of the lower part of the ladder) yields:

$$\begin{aligned} E\phi_n =& \varepsilon\phi_n + t_1\phi_{n-1} + t_1\phi_{n+1} + t_2\psi_n \\ E\psi_n =& \varepsilon\psi_n + t_1\psi_{n-1} + t_1\psi_{n+1} + t_2\phi_n \end{aligned}$$

Substituting the Ansatz $\begin{pmatrix}\phi_n\\ \psi_n\end{pmatrix} = \begin{pmatrix}\phi_0\\ \psi_0\end{pmatrix} e^{iEt/\hbar - ikx_n}$ gives:

$$E\begin{pmatrix}\phi_0\\ \psi_0\end{pmatrix} = \begin{pmatrix}\varepsilon + 2t_1\cos(ka) & t_2\\ t_2 & \varepsilon + 2t_1\cos(ka)\end{pmatrix}\begin{pmatrix}\phi_0\\ \psi_0\end{pmatrix}$$

(b) (5 points) Compute the dispersion relation.

Solution: Computing the eigenvalues yields:

$$\begin{aligned} (\varepsilon + 2t_1\cos(ka) - E)^2 - t_2^2 =& 0 \\ E = \varepsilon + 2t_1\cos(ka) \pm& t_2 \end{aligned}$$

(c) (5 points) Explain how this disperion relation with $t_1 \neq 0$ and $t_2 = 0$ relates to that of a simpler model.

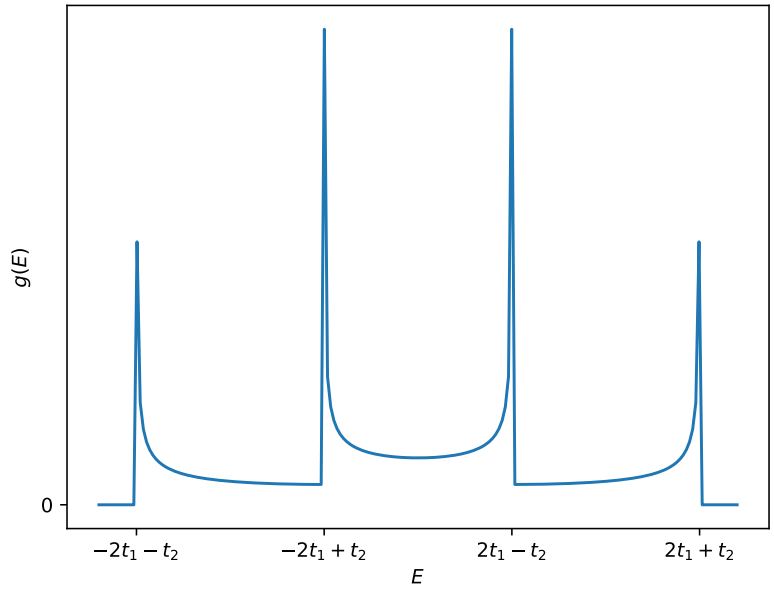
Solution: If $t_2 = 0$ we should get two copies of the dispersion of a monotomic chain, which we do since $E = \varepsilon + 2t_1 \cos(ka) \pm t_2 \rightarrow E = \varepsilon + 2t_1 \cos(ka)$.

(d) (5 points) Explain how this disperion relation with $t_1 = 0$ and $t_2 \neq 0$ relates to that of a simpler model.

Solution: If $t_1 = 0$ we should get the "dispersion" of a two atom system, which we obtain since we get: $E = \varepsilon + 2t_1 \cos(ka) \pm t_2 \rightarrow E = \varepsilon \pm t_2$ which are exactly the energies of the two atom system.

(e) (15 points) In the general case $t_1 \neq 0$ and $t_2 \neq 0$ sketch the dispersion relation and sketch the density of states. In your sketches remember to label the axes and relevant parameter values.

Solution: For $2t_1 > t_2$ the answer should be as shown below. Otherwise a gap between the bands should be visible.



3. **Extra answer space**