Solid state physics 2020 Minitest 2 (120 minutes) $_{12 \text{ March } 2020}$

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
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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.

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

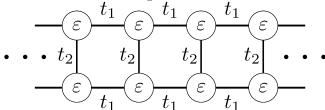
We consider two atoms with equal masses m that interact via the potential U(r) described above, where r is the interatomic distance between the two atoms.

(10 points) Expand U(r) around the equilibrium position up to the second order and find an expr for the spring constant κ in terms of ϵ and r_0 .							
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(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).
(d)	(10 points) Calculate the frequency of the vibrational mode and find the ground state energy of the molecule.
(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.

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 LCAC 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 dispersion yet, that is the next question).
(b)	(5 points) Compute the dispersion relation.

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

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