Estudiantes

Real Sociedad Española de Física

R.S.E.F.

Preliminares PLANCKS

PLANCKS 2021

Preliminares de PLANCKS 2021
Fase Española

One-dimensional crystal lattices

María Varela del Arco
Universidad Complutense de Madrid

This problem deals with several different properties of one dimensional (1D) crystal lattices, a paradigm in Solid State Physics.

1) When a monochromatic x-ray beam of wave number k is used to probe a one dimensional chain of N identical atoms, of lattice distance a, a diffraction pattern is obtained. Find the intensity of the diffracted radiation. Show that the width of the maxima is inversely proportional to N. (0.5 points)

2) Consider a 1D crystal lattice in equilibrium made of two species of alternating ions of charges $+e$ and $-e$, separated a distance R. Aside from the Coulomb interaction, consider a short range repulsive interaction potential of the form A/R^n, with $A > 0$ and $n > 1$, that only acts between nearest neighbors since n is large. Show that the potential energy of a single ion due to the Coulomb interaction with the rest of ions in the lattice can be written as

$$V(R) = -\frac{\alpha e^2}{4\pi\varepsilon_0}\frac{1}{R}$$

where α is a numerical constant that you are only asked to show how to calculate it explicitly, (you would need to use numerical tables that you don't have at hand to give its numerical value). (0.5 points)

3) Give the total potential energy of that lattice when composed of a large number N of ions of each species, and find the work per unit length needed to compress the chain in such a way that the separation between nearest neighbours is $R_0(1-\delta)$, being R_0 the equilibrium separation and $\delta <<< 1$. (1 point)

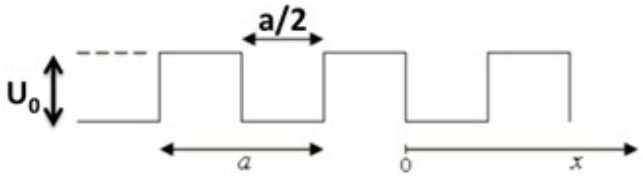
4) The equation describing the atomic displacements (respect to their equilibrium position) of a 1D monoatomic chain can be written as:

$$M\ddot{u}_n = K\left(u_{n+1} + u_{n-1} - 2u_n\right)$$

Where M represents the atomic mass and K is the interaction constant between neighbors. If a is the equilibrium separation between atoms, would $u_n(t) = A\cos(kan - \omega t)$ constitute a solution for the above equations? Under what conditions? (0.5 points)

5) Consider now the alternating chain made of two atoms, of masses M_1 and M_2 respectively (being $M_1 > M_2$), with the same values of a and K as before. Is the harmonic approximation for the displacements $u_n^{(j)} = A_j \exp i(kan - \omega t)$ still good in this case?. Find the values of the allowed frequencies and amplitudes in the limit of the first Brillouin zone. (1 point)

6) A simple model of an electron in 1D lattice is given by a periodic square potential of the form given in the figure:



Find the Fourier series coefficients of this potential when the wells exhibit a width equal to $a/2$ and a barrier height U_0. (1 point)

7) Write, for the square potential of 6), the energy width of the first couple of forbidden energy band gaps given by the nearly free electron approach. (0.5 points)

8) In general, for a fixed lattice distance , the barrier width b may be arbitrarily small. In the limiting case where $b \to 0$ and $U_0 \to \infty$ but $b \cdot U_0$ is finite, the barriers can be described by Dirac deltas:

$$U(x) = \sum_{n=-\infty}^{\infty} V(x - na) \text{ being } V(x) = \lambda\delta(x)$$

Where a is the lattice parameter and λ represents the potential coupling constant. Write the value of the band gaps predicted by the nearly free electron model in this case. (0.5 points)

9) Consider a 1D chain made up of all the same type of atom, but in such a way that the spacing between atoms alternates as long-short-long- as follows: $\cdots - A = A - A = A - A = A - \ldots$ (where $=$ means short bond and $-$ represents the long bond). In a tight binding model, the shorter bonds will have a hopping matrix element $t_{short} = t(1 + \varepsilon)$, whereas the longest bonds have hopping matrix element $t_{long} = t(1 - \varepsilon)$. Calculate the tight-binding energy spectrum of this chain (being the onsite energy, ε, the same on every atom). (2 points)

10) Consider a 1D chain of atoms where one of the atoms in the chain (atom $n = 0$) is an impurity such that it has an atomic orbital energy which differs by Δ from all the other atomic orbital energies. In this case, the tight binding Hamiltonian can be written as:

$$H_{n,m} = \varepsilon_0\delta_{n,m} - t(\delta_{n+1,m} + \delta_{n-1,m}) + \Delta\delta_{n,m}\delta_{n,0}.$$

Use the ansatz: $\varphi_n = Ae^{-qa|n|}$ with q real and positive and a the lattice constant, to find the value of q and show that for $t > 0$ there is a localized eigenstate for any negative Δ. Finally, determine the energy of this eigenstate. (2.5 points)

SOLUTIONS

1) The amplitude of the dispersed wave will be: $\sum_{mnp} e^{-i\Delta\vec{k}\cdot\vec{r}_{mnp}}$, being $\vec{r}_{mnp}$ the atomic positions. For a one dimensional chain we can simply write $\Delta\vec{k}\cdot\vec{r}_{mnp} = m\,\Delta k\cdot a$, where $r = ma$ are the atomic positions and Δk momentum components along the chain.

Then:

$$A = \sum_{m=0}^{N-1} e^{-im\Delta k\cdot a} = \frac{1-e^{-iN\Delta k\cdot a}}{1-e^{-i\Delta k\cdot a}} \quad \Rightarrow \quad |A|^2 = \frac{\sin^2(\frac{N}{2}\Delta k\cdot a)}{\sin^2(\frac{1}{2}\Delta k\cdot a)}$$

The diffraction maxima appear when $\Delta k\cdot a = 2\pi h$, being h an integer number. Since the diffraction pattern is periodic, we can take the zeroth order ($h=0$) and look at the interval between the first couple of maxima $\Delta k\cdot a$ in between $[0, 2\pi] \quad \longrightarrow$ within such interval $|A|^2$ goes to zero when $(N/2)\Delta k\cdot a = \pi$. Therefore, the separation between the maximum and the zero is $2\pi/N$, which indeed goes like $1/N$.

2) The energy of one ion due to its two nearest neighbors is $-2e^2/4\pi\varepsilon_0 R$. The next pair of nearest neigbors are at a distance $2R$ and repel it with a potential energy $2e^2/4\pi\varepsilon_0 2R$. Continuing this reasoning we get the electrostatic potential energy of the ion in the lattice:

$$U(R) = -\frac{2e^2}{4\pi\varepsilon_0 R}\,(1-\frac{1}{2}+\frac{1}{3}-\frac{1}{4}+\cdots)$$

hence, $\alpha = 2(1-\frac{1}{2}+\frac{1}{3}-\frac{1}{4}+\cdots)$. If you had the numerical tables at hand $\alpha = 2\ln 2 = 1.386$.

3) The total potential energy will be:

$$U_{TOT}(R) = -\frac{e^2 N\alpha}{4\pi\varepsilon_0 R} + \frac{2NA}{R^n},$$

where we took into account that the repulsive interaction only acts between nearest neighbors, and also avoided the double counting of the interactions. The equilibrium distance will be at its minimum

$$\frac{A}{R_0^n} = \frac{e^2\alpha}{8\pi\varepsilon R_0 n}\cdot \quad \text{Then } U_{TOT}(R_0) = -\frac{e^2 N\alpha}{4\pi\varepsilon_0 R_0}(1-\frac{1}{n}).$$

Now, the work needed to compress the chain will be:

$$W = U_{TOT}(R) - U_{TOT}(R_0) = -\frac{e^2 N\alpha}{4\pi\varepsilon_0 R_0}\left(\frac{R_0}{R}-1\right) + \frac{2NA}{R_0^n}\left(\frac{R_0^n}{R^n}-1\right).$$

Substituting the separation $R = R_0(1-\delta)$ given in the text and the value for A/R_0^n given above, we get

$$W = -\frac{N\alpha}{4\pi\varepsilon_0 R_0}\left(1-\frac{1}{1-\delta}+\frac{1}{n(1-\delta)^n}-\frac{1}{n}\right).$$

Approximating to second order in δ

$$\frac{W}{2NR_0} = -\frac{e^2\alpha}{8\pi\varepsilon_0 R_0^2}\frac{(n-1)}{2}\delta^2,$$

where we have divided by the lenght of the chain, $2NR_0$, to give the work per unit lenght.

4) Substituting the proposed solution into the displacements equation:

$$\omega^2 = \frac{K}{M}\left[2 - \frac{\cos\{(n+1)ka-\omega t\}+\cos\{(n-1)ka-\omega t\}}{\cos(ka-\omega t)}\right] = \frac{2K}{M}(1-\cos ka) = \frac{4K}{M}\sin^2 ka/2.$$

Hence, the proposed solution would work as long as the following dispersion relation holds:

$$\omega(k) = 2\sqrt{\frac{K}{M}}\left|\sin\left(\frac{ka}{2}\right)\right|.$$

5) We can write the motion equations for $u_n^{(j)}$, that represents the displacement from the equilibrium position of an atom of type j (being $j=1,2$), which sits in the n-th unit cell, as:

$$\begin{aligned} M_1\ddot{u}_n^{(1)} &= K\left(u_n^{(2)} + u_{n-1}^{(2)} - 2u_n^{((1)}\right) \\ M_2\ddot{u}_n^{(2)} &= K\left(u_{n+1}^{(1)} + u_n^{(1)} - 2u_n^{(2)}\right) \end{aligned} \tag{1}$$

These equations can be solved if we use a solution of the form $u_n^{(j)} = A_j e^{i(kan-\omega t)}$ for $j=1,2$, which gives:

$$\begin{aligned} (M_1\omega^2 - 2K)A_1 + K(1+e^{-ika})A_2 &= 0 \\ K(1+e^{ika})A_1 + (M_2\omega^2 - 2K)A_2 &= 0 \end{aligned}$$

Hence, $\omega^2 = K\left(\frac{1}{M_1}+\frac{1}{M_2}\right) \pm \left[K^2\left(\frac{1}{M_1}+\frac{1}{M_2}\right)^2 - \frac{4K^2}{M_1M_2}\sin^2\left(\frac{ka}{2}\right)\right]^2$.

At the edge of the Brillouin zone $ka=\pi$, and therefore $\omega^2 = K\left(\frac{1}{M_1}+\frac{1}{M_2}\right) \pm \left(\frac{1}{M_1}-\frac{1}{M_2}\right)$, and since $M_1 > M_2$, $\omega_+ = \sqrt{\frac{2K}{M_2}}$; $\omega_- = \sqrt{\frac{2K}{M_1}}$.

6) We choose the origin $x=0$ in the linear chain in the middle of a region where the potential is zero, so this periodic potential admits a Fourier series

$$U(x) = \frac{1}{a}\int_0^a dx e^{-i\pi n(\frac{x}{a})}U(x) = \frac{U_0}{2\pi n}\int_{a/4}^{3a/4} dz e^{-iz} = \frac{iU_0}{2\pi n}\left[e^{-i3\pi n/2} - e^{i\pi n/2}\right].$$

Now, using that

$$\sin\frac{3\pi n}{2} - \sin\pi\frac{n}{2} = \begin{cases} (-1)^{l+1}\,2\,\delta_{n,2l+1} & \text{for } l=0,1,2... \\ 0 & \text{for } n=2l \;\; l=0,1,2,... \end{cases}$$

and that $\cos\frac{3\pi n}{2} - \cos\pi\frac{n}{2} = 0 \;\; \forall n$, we get

$$U_n = \frac{U_0}{\pi n}(-1)^{l+1}\,\delta_{n,2l+1} \quad \text{for} \quad l = 0, 1, 2...$$

7) The first two band gaps in the nearly free electron model will be:

$$\begin{aligned} E_{G1} &= 2|U_1| = \frac{2U_0}{\pi} \\ E_{G2} &= 2|U_3| = \frac{2U_0}{3\pi} = \frac{1}{3}E_{G1}. \end{aligned}$$

8) Within this model a Dirac delta function is associated with every node of the 1D lattice. If we write the Fourier series:

$$U(x) = \sum_G U_G e^{iGx}, \quad \text{being} \quad U_G = \frac{1}{a}\int_{-a/2}^{a/2} e^{-iGx}U(x)dx = \frac{\lambda}{a},$$

we obtain $E_G = 2\,|U_G| = 2|\lambda|/a$ for the nearly free electron model.

9) Let's consider the unit cell ($A = A-$) as made of two sites: A (left site) and B (right site). Without loss of generality we can set the onsite energy $\varepsilon_0 = 0$ for simplicity and assume t is a real number. Then, the tight binding Schrödinger equation can be written as:

$$\begin{aligned} E\varphi_n^A &= -t(1+\varepsilon)\varphi_n^B - t(1-\varepsilon)\varphi_{n-1}^B \\ E\varphi_n^B &= -t(1+\varepsilon)\varphi_n^A - t(1-\varepsilon)\varphi_{n+1}^A \end{aligned}$$

With the usual ansatz $\varphi_{n+1}^I = e^{ika}\varphi_n^I$, for $I = A$ or B and a the lattice distance

$$\begin{aligned} EA &= -t(1+\varepsilon)B - t(1-\varepsilon)Be^{-ika} \\ EB &= -t(1+\varepsilon)A - t(1-\varepsilon)Ae^{ika} \end{aligned}$$

The solutions for this eigenvalue problem are of the type

$$E(k) = \pm\left|2t\left[\cos\left(\frac{ka}{2}\right) + i\varepsilon\,\sin\left(\frac{ka}{2}\right)\right]\right| = \pm|2t|\sqrt{\varepsilon^2 + (1-\varepsilon^2)cos^2\left(\frac{ka}{2}\right)}$$

10) Consider first the case without the impurity. If we use exponentially decaying or growing solutions:
$\varphi_n = Ae^{\pm qa|n|} \Rightarrow E = \varepsilon_0 - 2t\,\cosh(qa)$.

Note that for q real $(\varepsilon_0 - E)/2t = \cosh(qa) > 1$, in other words, for these solutions give energies below the bottom of the band.

Now, we can patch together two of these evanescent waves at the impurity. Examining the Schrodinger equation at position zero, we have:

$$E\phi_0 = (\varepsilon_0 + \Delta)\phi_0 - t(\phi_1 + \phi_{-1}) \Rightarrow E - \varepsilon_0 - \Delta = 2te^{-qa}$$

Using the value of E obtaned above we get $\Delta = -2\sinh(qa)$. Since Δ is negative, there is a solution for any value of Δ<0 with

$$q = \frac{1}{a}\,\sinh^{-1}(|\Delta|/2t)$$

Then, for the bound state energy

$$E = \varepsilon_0 - 2t\sqrt{\left(\frac{\Delta}{2t}\right)^2 + 1} \ .$$

Note that for $\Delta = 0$ this gives the energy at the bottom of the band.