Physics 525, Condensed Matter

Homework 5

Due Tuesday, 7th November 2006

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Problem 1: Phonon Spectrum of a Diatomic One-Dimensional Crystal

Consider a one-dimensional, diatomic crystal composed of atoms of mass M_1 and M_2, respectively. We may suppose that the interaction between nearest neighbours is a simple harmonic spring with a universal spring constant K.

a. We are to determine the full phonon spectrum of this system and sketch the dispersions $\omega(q)$.

Let a denote the lattice spacing of the Bravais lattice, and let us label the displacement functions u_1 and u_2 for the atoms with mass M_1 and M_2, respectively. Then the harmonic contribution to the potential is given by

$$U_h = \frac{K}{2}\sum_n \Big\{ \Big(u_1(na) - u_2(na)\Big)^2 + \Big(u_2(na) - u_1((n+1)a)\Big)^2 \Big\}. \tag{1.a.1}$$

This immediately implies the following equations of motion:

$$M_1\ddot{u}_1(na) = -\frac{\partial U_h}{\partial u_1(na)} = -K\Big\{2u_1(na) - u_2(na) - u_2((n-1)a)\Big\}; \tag{1.a.2}$$

$$M_2\ddot{u}_2(na) = -\frac{\partial U_h}{\partial u_2(na)} = -K\Big\{2u_2(na) - u_1(na) - u_1((n+1)a)\Big\}. \tag{1.a.3}$$

We seek phonon solutions to these equations of motion, which have the structure of plane waves:

$$u_1(na) = \alpha e^{i(kna-\omega t)} \qquad \text{and} \qquad u_2(na) = \beta e^{i(kna-\omega t)}. \tag{1.a.4}$$

Inserting these test functions into the equations of motion and simplifying a bit, we find the following (independent of n),

$$M_1\omega^2\alpha = 2K\alpha - K\left(1+e^{-ika}\right)\beta; \tag{1.a.5}$$

$$M_2\omega^2\beta = 2K\beta - K\left(1+e^{ika}\right)\alpha. \tag{1.a.6}$$

This is of course equivalent to the eigenvalue equation

$$\begin{pmatrix} M_1\omega^2 - 2K & K\left(1+e^{-ika}\right) \\ K\left(1+e^{ika}\right) & M_2\omega^2 - 2K \end{pmatrix}\begin{pmatrix} \alpha \\ \beta \end{pmatrix} = 0, \tag{1.a.7}$$

which only has a solution if the determinant of the operator vanishes. Writing out the determinant and solving the quadratic equation for ω^2, we find that this implies

$$\begin{aligned}\omega^2 &= K\frac{(M_1+M_2)}{M_1M_2} \pm \frac{1}{2}\left\{4K^2\frac{(M_1+M_2)^2}{M_1^2M_2^2} - 8\frac{K^2}{M_1M_2}\left(1-\cos(ka)\right)\right\}^{1/2}, \\ &= K\frac{M_1+M_2}{M_1M_2} \pm K\frac{M_1+M_2}{M_1M_2}\left\{1 - 2\frac{M_1M_2}{(M_1+M_2)^2}\left(1-\cos(ka)\right)\right\}^{1/2}; \\ \therefore \omega^2 &= \frac{K}{\mu}\left\{1 \pm \sqrt{1 - 4\frac{\mu}{(M_1+M_2)}\sin^2\left(\frac{ka}{2}\right)}\right\},\end{aligned} \tag{1.a.8}$$

where we have introduced the *reduced mass*: $\mu \equiv \frac{M_1M_2}{M_1+M_2}$.

This phonon dispersion relation is plotted in Figure 1.

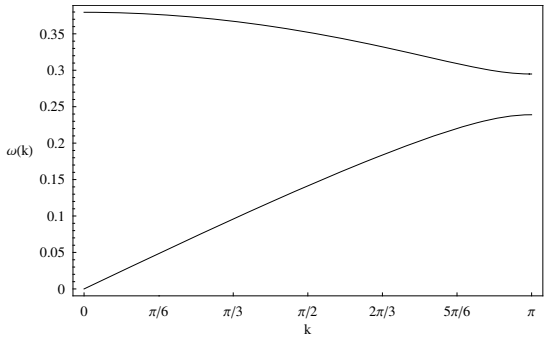


FIGURE 1. The phonon dispersion for a diatomic, one-dimensional crystal. The lower band is represents acoustic mode and the upper band represents optical mode.

b. We are to describe the atomic motion associated with optical and acoustic phonons near the centre and edge of the first Brillouin zone.

Near the centre of the Brillouin zone $k \ll \pi/a$, so we may expand $\sin(ka/2) \approx (ka/2) + \mathcal{O}((ka/2)^3)$. Also Taylor expanding the square-root in equation (1.a.8), we obtain

$$\omega^2 = \frac{K}{\mu}\left\{1 \pm \left(1 - \frac{\mu}{2(M_1+M_2)}(ka)^2 - \dots\right)\right\}; \tag{1.b.9}$$

which implies

$$\omega = \begin{cases} \sqrt{\frac{K}{2(M_1+M_2)}}(ka) + \mathcal{O}(ka)^2 & \text{acoustic} \\ \sqrt{\frac{2K(M_1+M_2)}{M_1 M_2}} + \mathcal{O}(ka)^2 & \text{optical} \end{cases}. \tag{1.b.10}$$

If we plug this back into the eigenvalue equation (1.a.7), we find for the acoustic mode,

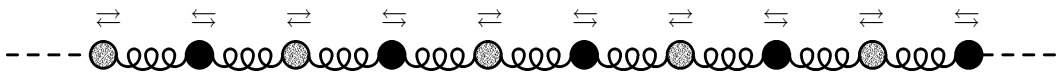
$$\begin{aligned} \frac{\beta}{\alpha} &= \frac{K(2+ika+\mathcal{O}(ka)^2)}{2K^2\left(2-\frac{(ka)^2}{2}+\mathcal{O}(ka)^4\right)}\left(2K - \frac{K}{2}\frac{M_2(ka)^2}{M_1+M_2} + \mathcal{O}(ka)^4\right), \\ &= 1 + \mathcal{O}(ak). \end{aligned}$$

Therefore, the acoustic mode is that for which the two types of atoms are oscillating in phase:

Similarly, looking at the expansion for the optical phonons, we find

$$\begin{aligned} \frac{\beta}{\alpha} &= \frac{K(2-ika+\mathcal{O}(ka)^2)}{2K^2\left(2-\frac{(ka)^2}{2}+\mathcal{O}(ka)^4\right)}\left(2K - 2K\frac{M_1+M_2}{M_2} + \mathcal{O}(ka)^4\right), \\ &= -\frac{M_1}{M_2} + \mathcal{O}(ak). \end{aligned}$$

This implies that the optical phonons near low crystal momentum (modulo the reciprocal lattice) are excitations where the two types of atoms oscillate in opposite phase:



Let us now return to equation (1.a.8), only this time keeping track of M_1 and M_2. Near the edge of the Brillouin zone, $k = \pi/a - \delta$, we may expand $\sin^2(\pi/2 - \delta a/2) =$

$1-(\delta a)^2/4+\mathcal{O}(\delta a)^4$. Using this, we have

$$\begin{aligned}\omega^2 &= \frac{K(M_1+M_2)}{M_1M_2}\left\{1\pm\sqrt{1-4\frac{M_1M_2}{(M_1+M_2)^2}\sin^2\left(\frac{\pi}{2}-\frac{\delta a}{2}\right)}\right\},\\ &= \frac{K(M_1+M_2)}{M_1M_2}\left\{1\pm\sqrt{1-4\frac{M_1M_2}{(M_1+M_2)^2}+\frac{M_1M_2}{(M_1+M_2)^2}(\delta a)^2+\mathcal{O}(\delta a)^4}\right\},\\ &= \frac{K(M_1+M_2)}{M_1M_2}\left\{1\pm\sqrt{\frac{(M_1-M_2)^2}{(M_1+M_2)^2}+\frac{M_1M_2}{(M_1+M_2)^2}(\delta a)^2+\mathcal{O}(\delta a)^4}\right\},\\ &= \frac{K(M_1+M_2)}{M_1M_2}\left\{1\pm\frac{|M_1-M_2|}{M_1+M_2}\sqrt{1+\frac{M_1M_2}{(M_1-M_2)^2}(\delta a)^2+\mathcal{O}(\delta a)^4}\right\}.\end{aligned}$$

Now, without loss of generality we may suppose that $M_1>M_2$, in which case this reduces to

$$\omega=\begin{cases}\sqrt{\frac{K}{M_1}}+\mathcal{O}(ka)^2 & \text{acoustic}\\ \sqrt{\frac{K}{M_2}}+\mathcal{O}(ka)^2 & \text{optical}\end{cases}. \tag{1.b.11}$$

Notice that in this case, the matrix in equation (1.a.7) becomes diagonal, so there is no constraint on β/α. Rather, modes with momenta near the edge of the first Brillouin zone correspond to bulk-modes of lattice of M_1 atoms and the lattice of M_2 atoms oscillating independently of each-other.

c. We are to consider the concrete example of a one-dimensional NaCl lattice, for which it is observed that the highest energy optical phonon is 30 meV. We are to determine the spring constant K in reasonable atomic-physics units, and determine the minimum energy that an incoming neutron must posses to excite all phonons at all crystal momenta.

From our work above we know that the highest energy phonon in the spectrum occurs at zero-crystal momentum, in the optical band[1]. This was derived explicitly in equation (1.b.10). Therefore, we know that

$$E_{ph_{\max}}=\hbar\omega_{\max}=\hbar\sqrt{\frac{2K(M_1+M_2)}{M_1M_2}} \quad\Longrightarrow\quad K=\frac{E_{ph_{\max}}^2M_1M_2}{\hbar^2 2(M_1+M_2)}. \tag{1.c.12}$$

Using the fact that $\omega_{\max}\hbar=30$ meV, and plugging in real numbers (with units!), we see that this gives

$$\therefore K=1.5\text{ eV Å}^{-2}. \tag{1.c.13}$$

When considering a neutron inelastic scattering process, there are two constraints that must be satisfied: first, the difference between the initial and final neutron momenta must be a reciprocal lattice vector; and second, the phonon energy must equal the difference between the initial and final neutron energies. Specifically, these are[2]

$$p_i-p_f=n\hbar\frac{2\pi}{a} \qquad\text{and}\qquad E_{ph}=\frac{(p_i^2-p_f^2)}{2m_n}. \tag{1.c.14}$$

We can combine these two equations by noting $(p_i^2-p_f^2)=(p_i+p_f)(p_i-p_f)=(p_i+p_f)n\hbar\frac{2\pi}{a}$ to arrive at the suggestive pair of equations

$$p_i-p_f=n\frac{h}{a} \qquad\text{and}\qquad p_i+p_f=\frac{2E_{ph}m_na}{nh}; \tag{1.c.15}$$

$$\therefore p_i=\frac{\alpha}{n}+\beta n \qquad\text{where}\quad \alpha=\frac{E_{ph}m_na}{h}\quad\text{and}\quad\beta=\frac{h}{2a}. \tag{1.c.16}$$

We must find the n for which p_i is minimized for the maximum phonon energy of 30 meV. Numerically, β is about an order of magnitude larger than α, so this happens when n is small; in fact, it is minimized at $n=3$, which gives $E_{\text{neutron}}=30.51$ meV.

[1] It may not be obvious that the global maximum occurs at zero crystal momentum in the optical band—for the one-dimensional crystal under consideration—but it turns out to be so.

[2] The lattice spacing for NaCl crystals is known to be $a=5.64$ Å.

Problem 2: Bound States of Phonons Near an Impurity (One-Dimension)

Consider a one-dimensional crystal composed almost entirely of atoms with mass M, but with one impurity atom of mass M'. We may approximate the interactions as nearest-neighbour harmonic potentials with a (universal) spring constant K. We are asked to explore the localized phonon modes that can possibly arise in this situation.

a. Let us determine the range of M' for which localized phonon modes exist.

Our intuition from Quantum Mechanics strongly hints that localized modes exist only if $M' < M$: this is because the potential energy should be lower there, giving rise to a potential well in which phonons could be entrapped. Alternatively, when $M' = M$, we know there are no localized modes because the situation is identical to a one-dimensional crystal; but when $M' < M$ wave amplitudes are locally piqued at M' so we expect localized modes. Enough intuition, let us show that our intuition isn't misguided.

The initial set-up is sufficiently similar to the previous problem (and sufficiently canonical) that we may appear brief. Given the Hooke's law harmonic potential, we can immediately write down the equations of motion for the system:

$$M\ddot{u}_{na} = -K\Big(2u_{na} - u_{(n+1)a} - u_{(n-1)a}\Big) \quad \forall\ n \neq 0 \qquad \text{and} \qquad M'\ddot{u}_0 = -K\Big(2u_0 - u_a - u_{-a}\Big). \tag{2.a.1}$$

Because we are interested in phonon modes which are localized at $n = 0$, we will try the following test functions

$$u_{n>0} = e^{-\lambda a n} e^{i(kan - \omega t)} \equiv \tilde{u}_{n>0} e^{-i\omega t} \qquad \text{and} \qquad u_{n<0} = e^{\lambda a n} e^{i(kan - i\omega t)} \equiv \tilde{u}_{n<0} e^{-i\omega t}, \tag{2.a.2}$$

where $\lambda > 0$; we will use our equations of motion (2.a.1) to determine $\tilde{u}_0$.

Inserting our test functions into the equations of motion, we find that virtually all of the system of equations collapses in redundancy, leaving us with

$$n \geq 2 \qquad M\omega^2 = K\Big(2 - e^{-\lambda a}e^{ika} - e^{\lambda a}e^{-ika}\Big); \tag{2.a.3}$$

$$n = 1 \qquad M\omega^2 = K\Big(2 - e^{-\lambda a}e^{ika} - \tilde{u}_0 e^{\lambda a}e^{-ika}\Big); \tag{2.a.4}$$

$$n = 0 \qquad M'\omega^2 = K\Big(2\tilde{u}_0 - e^{-\lambda a}e^{ika} - e^{-\lambda a}e^{-ika}\Big); \tag{2.a.5}$$

$$n = -1 \qquad M\omega^2 = K\Big(2 - e^{-\lambda a}e^{-ika} - \tilde{u}_0 e^{\lambda a}e^{ika}\Big); \tag{2.a.6}$$

$$n \leq -2 \qquad M\omega^2 = K\Big(2 - e^{-\lambda a}e^{-ika} - e^{\lambda a}e^{ika}\Big). \tag{2.a.7}$$

Subtracting equation (2.a.7) from equation (2.a.3) we see that

$$e^{-\lambda a}\left(e^{-ika} - e^{ika}\right) + e^{\lambda a}\left(e^{ika} - e^{-ika}\right) = 4i\sin(ka)\sinh(\lambda a) = 0.$$

This implies that either $\lambda = 0$—which would run contrary to our analysis: we are interested in the case when $\lambda > 0$—or that $ka = m\pi$ for some $m \in \mathbb{Z}$. Actually, we have no need to keep this level of generality: it is $e^{\pm ika}$ that appears throughout our equations of motion, and this leaves only two possibilities: $e^{i2\pi} = e^{-i2\pi} = 1$ or $e^{i\pi} = e^{-i\pi} = -1$; labelling these possibilities as $\pm$, respectively, equation (2.a.3) becomes

$$M\omega^2 = 2K\Big(1 \mp \cosh(\lambda a)\Big). \tag{2.a.8}$$

Now, $\cosh(\lambda a) > 1$ if $\lambda > 1$. Because this would lead to negative ω^2 for the '$-$' case above—corresponding to $ka = 2m\pi$—we must exclude this as a possibility, leaving only $e^{ika} = e^{-ika} = -1$. Which allows us to conclude[3]

$$\therefore \omega = 2\sqrt{\frac{K}{M}}\cosh\left(\frac{\lambda a}{2}\right). \tag{2.a.9}$$

Inserting our expression for ω^2 into equation (2.a.4) we see that

$$\begin{aligned} 2(1 + \cosh(\lambda a)) &= 2 + e^{-\lambda a} + \tilde{u}_0 e^{\lambda a}; \\ \implies e^{-\lambda a} + e^{\lambda a} &= e^{-\lambda a} + \tilde{u}_0 e^{\lambda a}, \end{aligned}$$

[3]We made use of the hyperbolic identity $1 + \cosh(\xi) = 2\cosh^2(\xi/2)$.

which of course implies that $\tilde{u}_0 = 1$. It is not hard to see that the only independent equation left for us to consider is (2.a.5). Let us see what this equation implies about M'/M.

$$\begin{aligned} M'\omega^2 &= K\Big(2 + e^{-\lambda a} + e^{-\lambda a}\Big), \\ \implies 4K\frac{M'}{M}\cosh^2\left(\frac{\lambda a}{2}\right) &= 2K\Big(1 + e^{-\lambda a}\Big), \\ \implies \frac{M'}{M} &= \frac{1 + e^{-\lambda a}}{2\cosh^2\left(\frac{\lambda a}{2}\right)}, \\ &= e^{-\lambda a/2}\frac{2\cosh\left(\frac{\lambda a}{2}\right)}{2\cosh^2\left(\frac{\lambda a}{2}\right)}, \\ \therefore \frac{M'}{M} &= \frac{e^{-\lambda a/2}}{\cosh\left(\frac{\lambda a}{2}\right)}. \end{aligned} \tag{2.a.10}$$

Now, because the expression on the right hand side of (2.a.10) is strongly bounded above by 1—and is equal to one iff $\lambda = 0$—we may conclude that localized phonon modes exist only if

$$\frac{M'}{M} < 1. \tag{2.a.11}$$

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b. We are to give explicit solutions for the frequency and displacement patterns of this localized mode and describe what happens as $M' \to M$.

Perhaps the first thing we should do is revisit equation (2.a.10) and give λ as a function of $\eta \equiv \frac{M'}{M}$. A little bit of manipulation shows that

$$\eta = \frac{2}{e^{\lambda a} + 1}, \tag{2.b.12}$$

which of course implies that

$$e^{\lambda a} = \frac{2 - \eta}{\eta} = \frac{2M - M'}{M'}. \tag{2.b.13}$$

This equation allows us to tidy up much of our previous work. For example, equation (2.a.9) can be combined with (2.a.10) using our work above,

$$\therefore \omega = 2\sqrt{\frac{KM}{M'\left(2M - M'\right)}}. \tag{2.b.14}$$

We can put everything together and now give all the functions u_n at once:

$$u_{na} = \left(\frac{M'}{2M - M'}\right)^{|n|} e^{i(kan - \omega t)}. \tag{2.b.15}$$

Now, looking at these plane waves (2.b.15) and the dispersion relation (2.b.14), we see that when $M' \to M$ the 'suppression' term in (2.b.15) becomes 1, and the dispersion relation matches onto the solution for normal phonons in one-dimension—i.e. there are no localized modes when $M' = M$.

Problem 3: Wigner Crystals in Various Dimensions

At low temperatures and densities, electrons in an ideal semiconductor 'crystallize' into what is known as a Wigner crystal. This can be modelled as a crystal of electrons in a uniform background of stationary, neutralizing positive charges, where only the electrons are able to move. The long-range Coulomb repulsion between the electrons can affect the long-wavelength longitudinal acoustic phonons. We are to determine the parametric low-q behaviour of this mode (called a 'plasmon') in one-, two-, and three-dimensional Wigner crystals.

In order to determine the dispersion of plasmons, we will use the harmonic approximation for the Coulomb interaction potential[4]; for dimensions higher than one, we will have need to recall recall some elementary multi-dimensional calculus—namely, the generalization of Taylor's theorem to higher dimensions,

$$f(\vec{r}-\vec{a}) = f(\vec{r}) + \vec{a}\cdot\vec{\nabla}f(\vec{r}) + \frac{1}{2}\left(\vec{a}\cdot\vec{\nabla}\right)f(\vec{r}) + \dots\ , \tag{3.a.1}$$

for any scalar function $f(\vec{r})$. Because the scalar function we are interested in is radial, it will be helpful to recall the expression for the gradient in polar and spherical coordinates in two- and three-dimensions respectively.

In one-dimension the situation is rather more elementary—there are at least no angles to worry us. Let us suppose that at zero temperature, the electrons are spaced a distance 1 apart (in appropriate units)[5]—so that the electrons are located at $r = n$ for $n \in \mathbb{Z}$. Then the equilibrium Coulomb-potential energy at the point $r = 0$ is simply

$$\varphi_{eq}(0) = -e^2 \sum_{r\neq 0} \frac{1}{|r|} = -2e^2 \sum_{r>0}^{N} \frac{1}{r}. \tag{3.a.2}$$

It is this potential that we will Taylor-expand for the plasmon perturbations.

Now, let us label the displacement from equilibrium of electron n from the point r as u_n. Then the actual potential energy at the site of the electron labeled 0—which is now located at u_0—is given by

$$\varphi(u_0) = -e^2 \sum_{r\neq 0} \left\{ \frac{1}{|r|} - (u_r - u_0)\frac{1}{r^2} + \frac{1}{2}(u_r-u_0)^2 \frac{1}{|r|^3} - \dots \right\}. \tag{3.a.3}$$

Assuming that the values $u_r = 0$ are equilibrium, then the first term in (3.a.3) is a constant and the second term vanishes. It is the third term—the 'harmonic' term—that we are interested in:

$$\varphi_h(u_0) = -\frac{e^2}{2} \sum_{r=1}^{\infty} \frac{1}{r^3} \left\{ (u_r - u_0)^2 + (u_{-r} - u_0)^2 \right\}. \tag{3.a.4}$$

The equations of motion are relatively simple; for u_0, they give

$$m\ddot{u}_0 = -\frac{\partial \varphi_h(u_0)}{\partial u_0} = e \sum_{r=1}^{\infty} \frac{1}{r^3} \Big\{ 2u_0 - (u_r + u_{-r}) \Big\}. \tag{3.a.5}$$

We are looking for plasmon solutions. These are

$$u_r = e^{i(kr-\omega t)}$$

where q is the momentum. Putting this into the equations of motion, we have

$$\frac{m}{e^2}\omega^2 = 2\sum_{r=1}^{\infty} \frac{1}{r^3}(1-\cos(kr)) \qquad \Longrightarrow \qquad \omega^2 \propto \sum_{r=1}^{\infty} \frac{1}{r^3} \sin^2\left(\frac{kr}{2}\right). \tag{3.a.6}$$

[4]This is actually a bit more subtle than it may seem at first: the leading order Coulomb interaction potential is a 'strong' effect. By taking the harmonic approximation, we are implicitly assuming that the leading Coulomb term (which is highly divergent in all dimensions—at least for infinite crystals) is completely neutralized by the positive charges; or, put another way, we ignore the machinery by which the electron system finds itself in an equilibrium distribution. Then, only the electron Coulomb interaction energy is considered as the sub-leading part of the potential. We will find that this is fine in each dimension under consideration—because it will dominate $\omega \sim cq$ in the limit of $q \to 0$—but this was by no means obvious.

[5]Because we are only interested in the parametric q-dependence of ω, there is no reason to bother about units.

In the limit where $k \to 0$, this sum is well-approximated as an integral,

$$\omega^2 \sim \int_1^\infty dr\ \frac{\sin^2\left(\frac{kr}{2}\right)}{r^3}. \tag{3.a.7}$$

Now, there are two obvious regions of interest: first, if $r \lesssim 2/k$, then $\sin^2(kr/2)$ can be well-approximated by its leading Taylor expansion. When $r \gg 2/k$, the integrand is rapidly oscillating and can be well-approximated by the average value of $\sin^2(x)$ which is $\frac{1}{2}$. That is

$$\omega^2 \sim \int_1^{2/k} dr\ \frac{1}{r^3}\sin^2\left(\frac{kr}{2}\right) + \int_{2/k}^\infty dr\ \frac{1}{r^3}\sin^2\left(\frac{kr}{2}\right), \tag{3.a.8}$$

$$\sim \int_1^{2/k} dr\ \frac{k^2}{4r} + \int_{2/k}^\infty dr\ \frac{1}{2r^3}, \tag{3.a.9}$$

$$= \frac{1}{4}k^2\log\left(\frac{2}{k}\right) - \frac{1}{16}k^2. \tag{3.a.10}$$

Now, the leading term (divergently) dominates as $k \to 0$ (and the other terms will not dominate other $\omega \sim ck$ phonons anyway), so we see that in one-dimension, Wigner-crystal plasmons have a low-momentum dispersion

$$\therefore \omega \underset{k\to 0}{\sim} k\sqrt{-\log(k)}. \tag{3.a.11}$$

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To generalize the work above requires keeping track of coordinate systems, indices, &tc. In two dimensions, we would like to use polar coordinates for the potential (because the Coulomb potential is radial), but label the points by their Cartesian coordinates. Specifically, let us denote the equilibrium locations of the electrons as In two-dimensions, we will use polar coordinates (ρ, θ) to expand the potential. Doing this, we find that[6]

$$\begin{aligned}\varphi_h(u_{\vec{0}}) = &-\frac{e^2}{2}\sum_{r_x,r_y=1}^\infty \frac{1}{\rho^3}\left\{\left(u_{r_x+r_y}-u_{\vec{0}}\right)_\rho^2 + \left(u_{r_x-r_y}-u_{\vec{0}}\right)_\rho^2 + \left(u_{-r_x+r_y}-u_{\vec{0}}\right)_\rho^2 + \left(u_{-r_x-r_y}-u_{\vec{0}}\right)_\rho^2\right\}\\ &-\frac{e^2}{2}\sum_{r_x=1}^\infty \frac{1}{r_x^3}\left\{\left(u_{r_x+0\hat{y}}-u_{\vec{0}}\right)_x^2 + \left(u_{-r_x+0\hat{y}}-u_{\vec{0}}\right)_x^2\right\} - \frac{e^2}{2}\sum_{r_y=1}^\infty \frac{1}{r_y^3}\left\{\left(u_{0\hat{x}+r_y}-u_{\vec{0}}\right)_y^2 + \left(u_{0\hat{x}-r_y}-u_{\vec{0}}\right)_y^2\right\},\end{aligned} \tag{3.b.1}$$

where $\rho = (r_x^2 + r_y^2)^{1/2}$. The last two terms in this expression grow only linearly with N, the number of electrons in one direction, whereas the first term grows like N^2; i.e. both terms in the second line of equation (3.b.1) are of measure zero in two-dimensions[7]. Therefore, it is consistent to simply ignore these contributions when taking the large-N-limit—when we will replace the sums in equation (3.b.1) by integrals over the plane.

As before, we are interested in plasmons which are longitudinal plane-waves,

$$\vec{u}_{r_x+r_y} = \hat{x}e^{i(kr_x-\omega t)}, \tag{3.b.2}$$

where we have used the longitudinality of the wave, $\vec{k} = k\hat{x}$. Inserting this test function into equation (3.b.1) we obtain the equations of motion

$$m\omega^2 = 4e^2\sum_{r_x,r_y=1}^\infty \frac{1}{\rho^3}\Big\{1-\cos\left(kr_x\right)\Big\} \to 8e^2\int_0^{\pi/2}d\theta\int_1^\infty \frac{d\rho}{\rho^2}\sin^2\left(\frac{kr_x}{2}\right). \tag{3.b.3}$$

[6]The displacement functions u are of course vector quantities. The subscript 'ρ' appearing in the expression is to indicate that it is only the ρ-component of the vector-difference that is considered. This comes about because $\vec{a}\cdot\vec{\nabla} = a_\rho\frac{\partial}{\partial r} + \frac{a_\theta}{\rho}\frac{\partial}{\partial\theta}$ and the second term's contribution vanishes when acting on a radial function.

[7]This could be a point of confusion—if it were not for the fact that the sums along the x- and y-axes gavie no contribution (are of measure zero in two-dimensions) then we would of course find the one-dimensional result for this one-dimensional subsystem of the crystal. It can be checked explicitly that this term is subleading in N—but the skeptical reader should also bear in mind that k is bounded below by $1/N$.

Noting that $r_x = \rho \sin\theta$ in polar coordinates and approximating $\sin^2(x)$ by its Taylor expansion for small argument and by its average (which is $1/2$) for large argument, we see that parametrically,

$$\begin{aligned}\omega^2 &\sim \int_0^{\pi/2} d\theta \int_1^\infty \frac{d\rho}{\rho^2} \sin^2\left(\frac{k\rho\cos\theta}{2}\right), \\ &\sim \int_0^{\pi/2} d\theta \left\{ \int_1^{2/(k\cos\theta)} d\rho \; k^2\cos^2(\theta) + \frac{1}{2}\int_{2/(k\cos\theta)}^\infty d\rho \; \frac{1}{\rho^2} \right\}, \\ &\propto \int_0^{\pi/2} d\theta \left\{ 3k\cos\theta - k^2\cos^2\theta \right\}, \\ &= 3k - \frac{\pi}{4}k^2.\end{aligned}$$

The linear term obviously dominates in the limit of $k \to 0$, in which we are interested. Therefore, we see that in two-dimensions the plasmon dispersion is parameterically given by

$$\therefore \omega \underset{k\to 0}{\sim} \sqrt{k}. \tag{3.b.4}$$

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Lastly, let us turn out attention to the case in three-dimesnions. Like in the two-dimensional case, we must be mindful of coordinates. We will again chose to label the equilibrium positions[8] by their Cartesian coordinates $\vec{r} = r_x\hat{x} + r_y\hat{y} + r_z\hat{z}$, but we will express the potential in spherical coordinates (ρ, θ, φ). In the limit of large N, the leading contribution to the potential at $u_{\vec{0}}$[9]

$$\begin{aligned}\varphi(u_{\vec{0}}) = -\frac{e^2}{2}\sum_{r_x,r_y,r_z=1}^{N} \frac{1}{\rho^3}\Big\{&\left(u_{r_x+r_y+r_z} - u_{\vec{0}}\right)^2 + \left(u_{r_x+r_y-r_z} - u_{\vec{0}}\right)^2 + \left(u_{r_x-r_y+r_z} - u_{\vec{0}}\right)^2 + \left(u_{-r_x+r_y+r_z} - u_{\vec{0}}\right)^2 \\ &+ \left(u_{r_x-r_y-r_z} - u_{\vec{0}}\right)^2 + \left(u_{-r_x+r_y-r_z} - u_{\vec{0}}\right)^2 + \left(u_{-r_x-r_y+r_z} - u_{\vec{0}}\right)^2 + \left(u_{-r_x-r_y-r_z} - u_{\vec{0}}\right)^2\Big\}.\end{aligned} \tag{3.c.1}$$

The cpontributions that we are ignoring here are those from electrons in the planes normal to each of the coordinate axes. As argued before, these contribute nothing—'are regions of measure zero'—in three-dimensions.

Taking a longitudinal plasmon aligned in the z-direction as our test function,

$$\vec{u}_{r_x+r_y+r_z} = \hat{z}e^{i(kr_z-\omega t)} \qquad \text{where} \qquad \vec{k} = k\hat{z}, \tag{3.c.2}$$

we find the equations of motion to be

$$m\omega^2 = 8e^2 \sum_{r_x,r_y,r_z=1}^{N} \frac{1}{\rho^3}\Big\{1 - \cos\left(kr_z\right)\Big\} \to 16e^2 \int_0^{\pi/2} d\varphi \int_1^N d\rho \int_0^1 d\cos\theta \; \frac{1}{\rho}\sin^2\left(\frac{k\rho\cos\theta}{2}\right). \tag{3.c.3}$$

Notice that we've chosen to keep the range of the ρ integration explicit. This will come in handy later. Now, instead of doing the ρ integration first, notice that that we can exactly evaluate the angular integrals and greatly simplify the situation.

[8] We assume here, as before, a cubical lattice. This assumption is probably not accurate physically, but there are reasons to suspect that the parametric dispersions for small crystal momentum should be independent of the type of lattice.

[9] As before, the displacement $u_{\vec{r}}$ is obviously a vectorial quantity. However, for the sake of convenience—and using the foresight that we will consider plane waves for which $u_{\vec{r}}$ only has a component in the radial-direction—we will not write the vector label over $u_{\vec{r}}$. Lastly, the 'ρ' subscripts that appeared in equation (3.b.1) will be implicit in the expressions to follow.

Specifically,

$$\begin{aligned}
\omega^2 &= \frac{16e^2}{m}\int_0^{\pi/2}d\varphi\int_1^N d\rho\int_0^1 d\cos\theta\ \frac{1}{\rho}\sin^2\left(\frac{k\rho\cos\theta}{2}\right),\\
&= \frac{8\pi e^2}{m}\int_1^N d\rho\int_0^{k\rho/2} d\xi\ \frac{2}{k\rho^2}\sin^2(\xi)\,,\\
&= \frac{8\pi e^2}{m}\int_1^N d\rho\ \frac{1}{k\rho^2}\ \Big(\xi-\sin(\xi)\cos(\xi)\Big)\Big|_0^{k\rho/2},\\
&= \frac{4\pi e^2}{m}\int_1^N d\rho\ \frac{1}{k\rho^2}\Big(k\rho-\sin(k\rho)\Big),\\
&= \frac{4\pi e^2}{m}\int_k^{Nk}\frac{d\alpha}{\alpha^2}\Big(\alpha-\sin(\alpha)\Big);
\end{aligned}$$

Here, attention to detail has paid off: the minimum (non-vanishing) crystal momentum is $k = 1/N$ so that in the limit of low crystal momentum and infinite Wigner crystal, $kN \to 1$. This means that for the entire range of integration, $\alpha \leq 1$ and we can effectively approximate the integrand by Taylor-expanding $\sin(\alpha)$. This gives

$$\begin{aligned}
\omega^2 &= \frac{2\pi e^2}{3m}\int_k^1 d\alpha\ \Big(\alpha-\frac{\alpha^3}{20}+\frac{\alpha^5}{840}-\dots\Big),\\
&= \frac{4\pi e^2}{m}\left(\sum_{n=1}^{\infty}\frac{(-1)^{n+1}}{(2n+1)!}\frac{1-k^{2n}}{2n}\right),
\end{aligned}$$

Having come this far, we would have really like to have a closed-form expression for the constant part, but we haven't found one. To better than one part in a thousand, the constant term is

$$\omega^2 \approx \frac{983\pi e^2}{7\cdot 3^3\cdot 2^4 m} + k^2\frac{\pi e^2}{3m} + \mathcal{O}(k^4). \tag{3.c.4}$$

To an accuracy of about 2%, the constant term is just $\frac{e^2}{m}$. At any rate, the important point is that as $k \to 0$, $\omega \to$ constant. That is

$$\therefore\ \omega \underset{k\to 0}{\sim} \frac{e}{\sqrt{m}}. \tag{3.c.5}$$

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