Mini Project Report

Jinyuan Wu

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Problem 1 Consider a one dimensional infinite chain with the lattice constant Λ on the z direction consisting of metallic balls, each of which have radius a and is made of a metal with permittivity

$$\epsilon_{\mathrm{r}} = 1 - \frac{\omega_{\mathrm{p}}^2}{\omega(\omega + \mathrm{i}\gamma)}. \tag{1}$$

When $a \to 0$, the polarizability of a single ball is

$$\alpha(\omega) = 4\pi\epsilon_0 a^3 \frac{\epsilon_{\mathrm{r}}(\omega) - 1}{\epsilon_{\mathrm{r}}(\omega) + 2}, \tag{2}$$

We use Mathematica to plot the real and the imaginary part of $\alpha(\omega)$ and recalculate them with K-K relations

$$\operatorname{Re}\alpha(\omega) = -\frac{1}{\pi} \mathrm{P} \int_{-\infty}^{\infty} \frac{\operatorname{Im}\alpha(\nu)}{\omega - \nu} \mathrm{d}\nu, \quad \operatorname{Im}\alpha(\omega) = \frac{1}{\pi} \mathrm{P} \int_{-\infty}^{\infty} \frac{\operatorname{Re}\alpha(\nu)}{\omega - \nu} \mathrm{d}\nu \tag{3}$$

in Figure 1. It can be found that K-K relations do hold for α.

Note: Numerical details of K-K relations

The prime value integral is implemented using the replacement

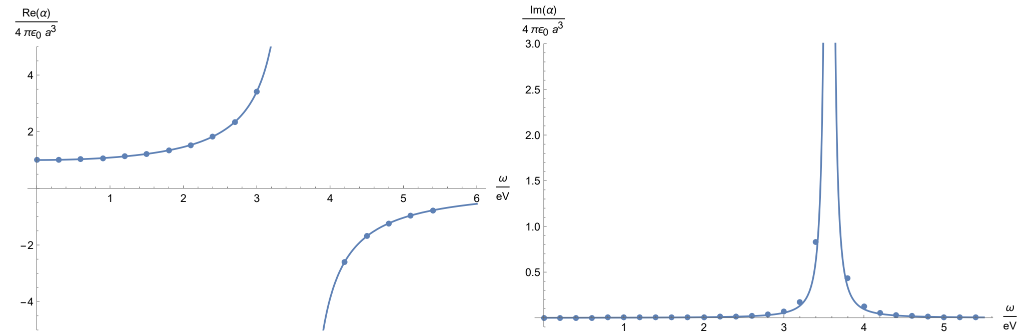
$$\mathrm{P} \int_{-\infty}^{\infty} \longrightarrow \int_{-\infty}^{\omega - o} + \int_{\omega + o}^{\infty},$$

where $o \sim 0.01$ is a small number. If o is too large, the peak of $\operatorname{Im}\alpha$ calculated by the K-K relation will be broader than the exact value (see Figure 1, where the scattered points are slightly "out" of the exact peak). If o is too small, there are severe convergence problems.

Qualitatively, the behavior of $\alpha(\omega)$ is just like the behavior of the response of a driven damped oscillator, where the imaginary part diverges when $\epsilon_{\mathrm{r}}(\omega) + 2 = 0$, or considering that γ is small, when

$$\omega = \sqrt{\frac{1}{3}} \omega_{\mathrm{p}} = 3.56\,\mathrm{eV}. \tag{4}$$

This frequency is the frequency of the local surface plasmon polariton of a single ball. When the driving frequency is larger than $\omega_{\mathrm{p}}/\sqrt{3}$, the real part of α is positive, which means the system is able to "keep in track with" the driving field. When $\omega > \omega_{\mathrm{p}}$, $\operatorname{Re}\alpha < 0$, which means that the system is too slow to response "in time" to the driving field and therefore has an opposite phase to the driving field.



(a) (b)

Figure 1: The real and the imaginary part of $\alpha(\omega)$. The lines are plotted by definition, and the scattered points are obtained by K-K relations. (a) The real part. (b) The imaginary part.

Problem 2 We need to solve

$$\boldsymbol{p}_m = \alpha(\boldsymbol{E}_{\text{ext}}(\boldsymbol{r}_m) + \omega^2\mu_0 \sum_{n\neq m} \overleftrightarrow{\boldsymbol{G}}(\boldsymbol{r}_m - \boldsymbol{r}_n)\cdot \boldsymbol{p}_n), \tag{5}$$

and when there is no external field, by the Bloch condition

$$\boldsymbol{p}_m = \boldsymbol{u}\mathrm{e}^{\mathrm{i}kz_m}, \tag{6}$$

we have

$$\boldsymbol{u}\mathrm{e}^{\mathrm{i}kz_m} = \alpha\omega^2\mu_0 \sum_{n\neq m} \overleftrightarrow{\boldsymbol{G}}(\boldsymbol{r}_m - \boldsymbol{r}_n)\cdot \boldsymbol{u}\mathrm{e}^{\mathrm{i}kz_n},$$

$$\left(\overleftrightarrow{\boldsymbol{I}} - \alpha\omega^2\mu_0 \sum_{n\neq m} \overleftrightarrow{\boldsymbol{G}}(\boldsymbol{r}_m - \boldsymbol{r}_n)\mathrm{e}^{\mathrm{i}kz_n}\mathrm{e}^{-\mathrm{i}kz_m}\right)\boldsymbol{u} = 0,$$

and we have

$$\overleftrightarrow{\boldsymbol{M}} = \alpha^{-1}\overleftrightarrow{\boldsymbol{I}} - \omega^2\mu_0 \sum_{n\neq m} \overleftrightarrow{\boldsymbol{G}}(\boldsymbol{r}_m - \boldsymbol{r}_n)\mathrm{e}^{\mathrm{i}k(z_n - z_m)}, \quad \overleftrightarrow{\boldsymbol{M}}\boldsymbol{u} = 0, \tag{7}$$

and we need to evaluate

$$\overleftrightarrow{\boldsymbol{W}} = \omega^2\mu_0 \sum_{n\neq m} \overleftrightarrow{\boldsymbol{G}}(\boldsymbol{r}_m - \boldsymbol{r}_n)\mathrm{e}^{\mathrm{i}k(z_n - z_m)}. \tag{8}$$

The dyadic Green function is

$$\overleftrightarrow{\boldsymbol{G}}(\boldsymbol{R}) = \frac{k_0}{4\pi}\frac{\mathrm{e}^{\mathrm{i}k_0 R}}{k_0 R}\left(\overleftrightarrow{\boldsymbol{I}}\left(1 - \frac{4\pi R}{3k_0^2}\delta(\boldsymbol{R}) - \frac{1}{k_0^2R^2} + \frac{\mathrm{i}}{k_0 R}\right) + \frac{\boldsymbol{R}\boldsymbol{R}}{R^2}\left(\frac{3}{k_0^2R^2} - 1 - \frac{3\mathrm{i}}{k_0 R}\right)\right). \tag{9}$$

Since $\boldsymbol{R} = \boldsymbol{r}_m - \boldsymbol{r}_n \neq 0$, the δ-function term vanishes. Since $\boldsymbol{r}_m - \boldsymbol{r}_n$ is along the z axis, We have

$$\frac{\boldsymbol{R}\boldsymbol{R}}{R^2} = \boldsymbol{e}_z\boldsymbol{e}_z, \quad R = |z_m - z_n|\,.$$

Therefore, by the definition (8), we have

$$\begin{aligned}
\overleftrightarrow{\boldsymbol{W}} &= \omega^2\mu_0 \sum_{m\neq n} \mathrm{e}^{\mathrm{i}k(z_n - z_m)}\frac{k_0}{4\pi}\mathrm{e}^{\mathrm{i}k_0 R}\left(\overleftrightarrow{\boldsymbol{I}}\left(\frac{1}{k_0R} + \frac{\mathrm{i}}{k_0^2R^2} - \frac{1}{k_0^3R^3}\right)\right. \\
&\quad \left. + \boldsymbol{e}_z\boldsymbol{e}_z\left(-\frac{1}{k_0R} - \frac{3\mathrm{i}}{k_0^2R^2} + \frac{3}{k_0^3R^3}\right)\right) \\
&= \omega^2\mu_0\frac{k_0}{4\pi}\left(\sum_{z_m<z_n} + \sum_{z_m>z_n}\right)\mathrm{e}^{\mathrm{i}k_0R - \mathrm{i}k(z_m - z_n)}\left(\overleftrightarrow{\boldsymbol{I}}\left(\frac{1}{k_0R} + \frac{\mathrm{i}}{k_0^2R^2} - \frac{1}{k_0^3R^3}\right)\right. \\
&\quad \left. + \boldsymbol{e}_z\boldsymbol{e}_z\left(-\frac{1}{k_0R} - \frac{3\mathrm{i}}{k_0^2R^2} + \frac{3}{k_0^3R^3}\right)\right) \\
&= \omega^2\mu_0\frac{k_0}{4\pi}\left(\sum_{l=1}^{\infty}\mathrm{e}^{\mathrm{i}(k_0-k)\Lambda l} + \sum_{l=1}^{\infty}\mathrm{e}^{\mathrm{i}(k_0+k)\Lambda l}\right)\left(\overleftrightarrow{\boldsymbol{I}}\left(\frac{1}{k_0\Lambda l} + \frac{\mathrm{i}}{k_0^2\Lambda^2l^2} - \frac{1}{k_0^3\Lambda^3l^3}\right)\right. \\
&\quad \left. + \boldsymbol{e}_z\boldsymbol{e}_z\left(-\frac{1}{k_0\Lambda l} - \frac{3\mathrm{i}}{k_0^2\Lambda^2l^2} + \frac{3}{k_0^3\Lambda^3l^3}\right)\right).
\end{aligned}$$

Using formulae from Wikipedia, we have

$$\left(\sum_{l=1}^{\infty}\mathrm{e}^{\mathrm{i}(k_0-k)\Lambda l} + \sum_{l=1}^{\infty}\mathrm{e}^{\mathrm{i}(k_0+k)\Lambda l}\right)\frac{1}{l^s} = \mathrm{Li}_s(\mathrm{e}^{\mathrm{i}(k_0-k)\Lambda}) + \mathrm{Li}_s(\mathrm{e}^{\mathrm{i}(k_0+k)\Lambda}),$$

So finally we have

$$\overleftrightarrow{\boldsymbol{W}} = \frac{\omega^2\mu_0 k_0}{4\pi}\Bigg(\frac{1}{k_0\Lambda}(\overleftrightarrow{\boldsymbol{I}} - \boldsymbol{e}_e\boldsymbol{e}_z)(\mathrm{Li}_1(\mathrm{e}^{\mathrm{i}(k_0-k)\Lambda}) + \mathrm{Li}_1(\mathrm{e}^{\mathrm{i}(k_0+k)\Lambda})) \\ + \frac{\mathrm{i}}{k_0^2\Lambda^2}(\overleftrightarrow{\boldsymbol{I}} - 3\boldsymbol{e}_z\boldsymbol{e}_z)(\mathrm{Li}_2(\mathrm{e}^{\mathrm{i}(k_0-k)\Lambda}) + \mathrm{Li}_2(\mathrm{e}^{\mathrm{i}(k_0+k)\Lambda})) \\ - \frac{1}{k_0^3\Lambda^3}(\overleftrightarrow{\boldsymbol{I}} - 3\boldsymbol{e}_z\boldsymbol{e}_z)(\mathrm{Li}_3(\mathrm{e}^{\mathrm{i}(k_0-k)\Lambda}) + \mathrm{Li}_3(\mathrm{e}^{\mathrm{i}(k_0+k)\Lambda})).\Bigg) \tag{10}$$

Problem 3 When the system is in a single mode, we have $\boldsymbol{p}_m = \alpha_{\text{eff}}\boldsymbol{E}_{\text{eig}}$, and from (5) we have

$$\alpha^{-1}\boldsymbol{p}_m = \alpha_{\text{eig}}^{-1}\boldsymbol{p}_m + \omega^2\mu_0\sum_{n\neq m}\overleftrightarrow{\boldsymbol{G}}(\boldsymbol{r}_m - \boldsymbol{r}_n)\cdot\boldsymbol{p}_n,$$

and we find it is equivalent to

$$\overleftrightarrow{\boldsymbol{M}}\cdot\boldsymbol{u} = \frac{1}{\alpha_{\text{eff}}}\boldsymbol{u} = \lambda\boldsymbol{u}. \tag{11}$$

The eigenvalues are inverse effective polarizabilities. (11) is equivalent to

$$\alpha^{-1}\boldsymbol{u} - \overleftrightarrow{\boldsymbol{W}}\cdot\boldsymbol{u} = \alpha_{\text{eig}}^{-1}\boldsymbol{u},$$

and we known that $\overleftrightarrow{\boldsymbol{W}}$ is diagonal in the $\boldsymbol{e}_x, \boldsymbol{e}_y, \boldsymbol{e}_z$ basis, so the eigenvectors - which are polarization directions - are just $\boldsymbol{e}_x, \boldsymbol{e}_y, \boldsymbol{e}_z$, and it is straightforward to find that the polarizabilities on the x and y directions are the same:

$$\alpha_{\text{eig},xy}^{-1} = \alpha^{-1} - \frac{\omega^2\mu_0 k_0}{4\pi}\Bigg(\frac{1}{k_0\Lambda}(\mathrm{Li}_1(\mathrm{e}^{\mathrm{i}(k_0-k)\Lambda}) + \mathrm{Li}_1(\mathrm{e}^{\mathrm{i}(k_0+k)\Lambda})) \\ + \frac{\mathrm{i}}{k_0^2\Lambda^2}(\mathrm{Li}_2(\mathrm{e}^{\mathrm{i}(k_0-k)\Lambda}) + \mathrm{Li}_2(\mathrm{e}^{\mathrm{i}(k_0+k)\Lambda})) - \frac{1}{k_0^3\Lambda^3}(\mathrm{Li}_3(\mathrm{e}^{\mathrm{i}(k_0-k)\Lambda}) + \mathrm{Li}_3(\mathrm{e}^{\mathrm{i}(k_0+k)\Lambda}))\Bigg), \tag{12}$$

and the polarizability on the z direction is

$$\alpha_{\text{eig},z}^{-1} = \alpha^{-1} - \frac{\omega^2\mu_0 k_0}{4\pi}\Bigg(-\frac{2\mathrm{i}}{k_0^2\Lambda^2}(\mathrm{Li}_2(\mathrm{e}^{\mathrm{i}(k_0-k)\Lambda}) + \mathrm{Li}_2(\mathrm{e}^{\mathrm{i}(k_0+k)\Lambda})) \\ + \frac{2}{k_0^3\Lambda^3}(\mathrm{Li}_3(\mathrm{e}^{\mathrm{i}(k_0-k)\Lambda}) + \mathrm{Li}_3(\mathrm{e}^{\mathrm{i}(k_0+k)\Lambda}))\Bigg). \tag{13}$$

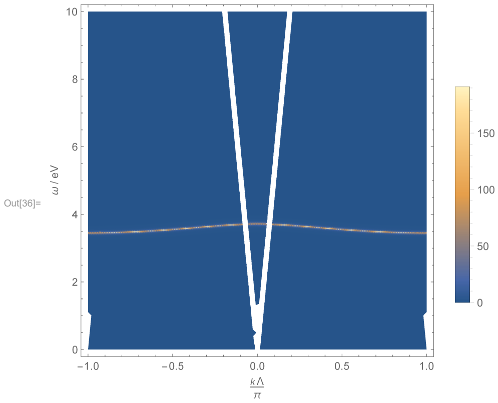
Plotting (12) and (13) on the complex plane, we get Figure 2. It can be found that between 3 eV and 4 eV, $\mathrm{Im}\,\alpha$ is considerably large, indicating that there are bands of eigenmodes in this frequency range. This frequency range is close to $\omega_{\mathrm{p}}/\sqrt{3}$, which means these eigenmodes are modified (since there is a periodic lattice, and dipoles interact with each other) local surface plasmon polariton modes. The behaviors of the x- and y-polarized modes are the same, which is expected because of the rotational symmetry around the z axis.

We also see two V-shaped blank regions in the plots, which means there are singularities along two $\omega = ak$ lines. These singularity lines come from the fact that $\mathrm{Li}_s\,z$ is actually a multi-valued function, and its principal branch has a branch cut $1 < z < \infty$. When k_0 is close to k, $\mathrm{e}^{\mathrm{i}(k_0-k)\Lambda}$ is close to 1. In Figure 4 we plot the points where $k_0 = k$ onto Figure 2, and it can be seen that these points determine the position of the V-shaped blank regions.

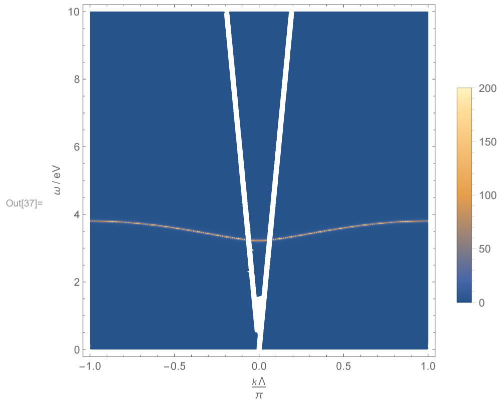
We find that there is no $1/k_0\Lambda$ term in (13), because it is a longitude mode (the polarization direction is the same as the direction of the wave vector), while the $\sim 1/r$ term in the electric field generated by an oscillating dipole corresponds to the far-field electromagnetic wave behavior, which is definitely not a longitude mode.

Problem 4 In the $c \to \infty$ limit, $k_0 \to 0$, so all $1/(k_0\Lambda)^s$ terms in (10) diverges, and only the most divergent terms where $s = 3$ are important, i.e. we only keep the near field terms in $\overleftrightarrow{\boldsymbol{G}}$, and we have

$$\overleftrightarrow{\boldsymbol{W}} = \omega^2\frac{\mu_0 k_0}{4\pi}\left(\frac{3\boldsymbol{e}_z\boldsymbol{e}_z - \overleftrightarrow{\boldsymbol{I}}}{k_0^3\Lambda^3}\right)(\mathrm{Li}_3(\mathrm{e}^{\mathrm{i}k\Lambda}) + \mathrm{Li}_3(\mathrm{e}^{-\mathrm{i}k\Lambda})).$$



(a) α_{xy}



(b) α_z

Figure 2: $\alpha_{xy}(\omega)$ and $\alpha_z(\omega)$ on the complex plane.

In the $\gamma \to 0$ limit, we have

$$\frac{1}{\alpha} = \frac{1}{4\pi\epsilon_0 a^3}\frac{\epsilon_{\rm r}+2}{\epsilon_{\rm r}-1} = \frac{1}{4\pi\epsilon_0 a^3}\frac{\omega_{\rm p}^2 - 3\omega^2}{\omega_{\rm p}^2}.$$

So $\overleftrightarrow{\boldsymbol{W}} \cdot \boldsymbol{u} = \boldsymbol{u}/\alpha$ can be written as

$$\frac{1}{\alpha} = \frac{1}{4\pi\epsilon_0 a^3}\frac{\omega_{\rm p}^2 - 3\omega^2}{\omega_{\rm p}^2}\boldsymbol{u} = \underbrace{\omega^2\frac{\mu_0}{4\pi}\frac{1}{k_0^2}}_{=\frac{\mu_0 c^2}{4\pi}=\frac{1}{4\pi\epsilon_0}}\left(\frac{3\boldsymbol{e}_z\boldsymbol{e}_z - \overleftrightarrow{\boldsymbol{I}}}{\Lambda^3}\right)(\mathrm{Li}_3(\mathrm{e}^{\mathrm{i}k\Lambda}) + \mathrm{Li}_3(\mathrm{e}^{-\mathrm{i}k\Lambda}))\boldsymbol{u},$$

and finally

$$\overleftrightarrow{\boldsymbol{H}} \cdot \boldsymbol{u} = \frac{\omega^2}{\omega_{\rm p}^2}\boldsymbol{u}, \tag{14}$$

where

$$\overleftrightarrow{\boldsymbol{H}} = \frac{1}{3}\left(1 - \frac{a^3}{\Lambda^3}(3\boldsymbol{e}_z\boldsymbol{e}_z - \overleftrightarrow{\boldsymbol{I}})(\mathrm{Li}_3(\mathrm{e}^{\mathrm{i}k\Lambda}) + \mathrm{Li}_3(\mathrm{e}^{-\mathrm{i}k\Lambda}))\right). \tag{15}$$

By definition we know that $(\mathrm{Li}_3(\mathrm{e}^{\mathrm{i}k\Lambda}) + \mathrm{Li}_3(\mathrm{e}^{-\mathrm{i}k\Lambda}))$ is a real number, so (15) is a Hermitian matrix, and therefore qualifies as a Hamiltonian. Again, we find that $\overleftrightarrow{\boldsymbol{H}}$'s eigenvectors are $\boldsymbol{e}_x$, $\boldsymbol{e}_y$ and $\boldsymbol{e}_z$ (the same as Problem 3), and the eigenvalues are

$$\frac{\omega_{xy}^2}{\omega_{\rm p}^2} = \frac{1}{3}\left(1 + \frac{a^3}{\Lambda^3}(\mathrm{Li}_3(\mathrm{e}^{\mathrm{i}k\Lambda}) + \mathrm{Li}_3(\mathrm{e}^{-\mathrm{i}k\Lambda}))\right), \tag{16}$$

and

$$\frac{\omega_z^2}{\omega_{\rm p}^2} = \frac{1}{3}\left(1 - \frac{2a^3}{\Lambda^3}(\mathrm{Li}_3(\mathrm{e}^{\mathrm{i}k\Lambda}) + \mathrm{Li}_3(\mathrm{e}^{-\mathrm{i}k\Lambda}))\right). \tag{17}$$

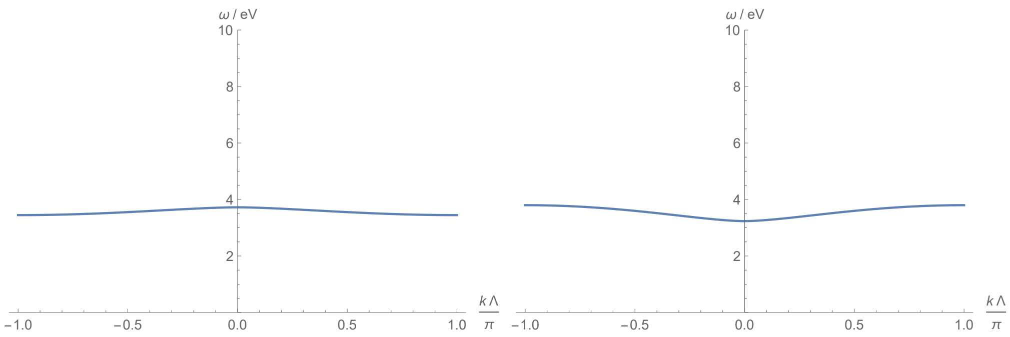
These dispersion relations are plotted as Figure 3.

Plotting the dispersion relations and the singularity points into Figure 2, we get Figure 4. It can be seen that α is significantly large at the dispersion relation curves, as is expected. The features of the dispersion relations have been discussed in Problem 3. The reason why the quasi-stationary approximation works well here is because for the quasi-stationary approximation to work we need

$$\hbar\omega \ll \frac{2\pi c\hbar}{\Lambda} = 16.5\,\mathrm{eV},$$

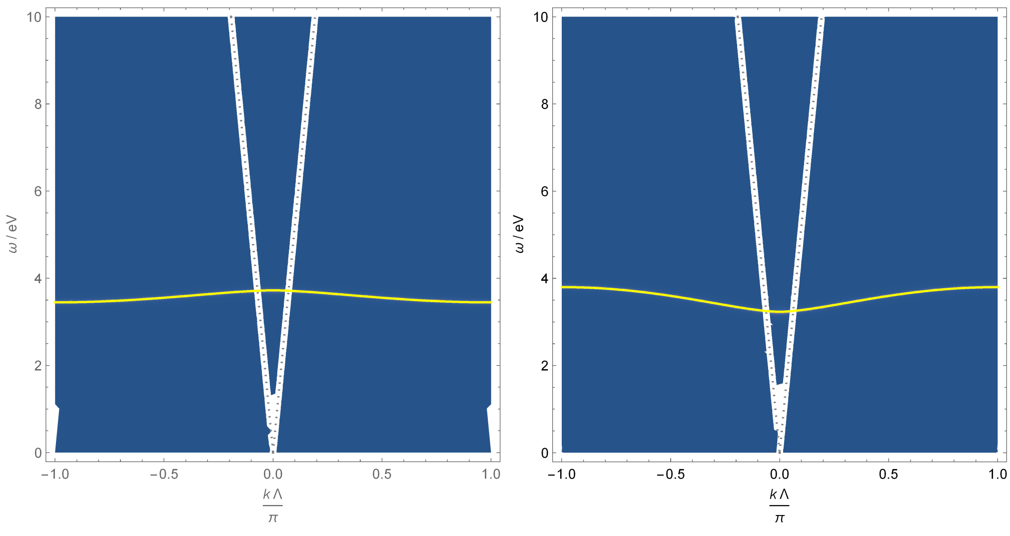
and for ω around $\omega_{\rm p}/\sqrt{3}$ this is not a bad approximation.

The fact that all collective modes can be obtained using the quasi-stationary approximation also explains the shape of the dispersion relations. We can just regard the electric field generated



(a) ω_{xy} (b) ω_z

Figure 3: Dispersion relations (16) and (17).



(a) α_{xy} (b) α_z

Figure 4: Im α on the complex plane, with the dispersion relations (the yellow line) obtained from the quasi-stationary approximation and the singularity points (the gray dotted lines) annotated.

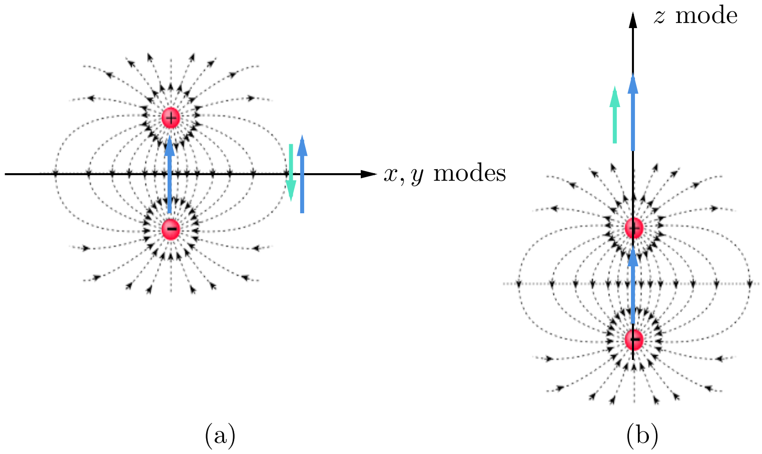


Figure 5: The interaction between dipoles: a dipole (blue arrow) induces another dipole (green arrow) in balls nearby. (a) The case of x- or y-polarized mode. (b) The case of z-polarized mode.

by a single dipole as the electric field of a (quasi)-static dipole. For the x- or y-polarized mode, a dipole induces another dipole in the balls nearby that has the opposite direction with itself (see Figure 5(a)), while for a z-polarized mode, a dipole induces another dipole in the balls nearby that has the same direction with itself (see Figure 5(b)). In other words, in x- and y-polarized modes, a dipole *suppresses* dipoles nearby, while in the z-polarized modes, a dipole *enhances* dipoles nearby. For a 1D oscillator chain

$$\ddot{x}_n = -\omega_0^2 + K(x_{n+1} + x_{n-1} - 2x_n),$$

where $K > 0$ means an oscillator lifts the neighbors, while $K < 0$ means an oscillator suppresses the neighbors, the periodic solution is

$$x_n = A\mathrm{e}^{\mathrm{i}k\Lambda n - \mathrm{i}\omega t}, \quad \omega^2 = \omega_0^2 + 2K(1 - \cos(k\Lambda)), \tag{18}$$

so if $K > 0$, ω increases when k increases, and when $K < 0$ it is exactly the opposite. This explains why for x- and y-polarized modes, as k goes up, ω decreases, while for z-polarized modes, as k goes up, ω increases.