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Phonons in Yukawa lattices and liquids

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Abstract

The understanding of the theoretical structure of phonon dispersion in Yukawa lattices and the relationship between these perfect lattice phonons on the one hand, and the excitations in the disordered and liquid states on the other, is an important issue in analysing experimental and simulation results on plasma crystals. As the first step in this programme, we have numerically calculated the full phonon spectrum for 2D triangular Yukawa lattices, for a wide range of $\bar{\kappa}$ (screening parameter) values and along different propagation angles. Earlier calculations of the excitation spectra of the 2D and 3D Yukawa liquids were based on the quasilocalized charge approximation (QLCA), whose implicit premise is that the spectrum of an average distribution (governed by the isotropic liquid pair correlation function) is a good representation of the actual spectrum. To see the implications of this model more clearly, we compare the high Γ (near crystallization) QLCA phonon spectra with the angle-averaged phonon spectra of the lattice phonons.

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(Some figures in this article are in colour only in the electronic version)

1. Introduction

A 2D Yukawa system is a good representation of structures forming in dusty plasma and colloidal experiments [1, 2]. The potential is $\phi(r) = (q^2/r)\,\mathrm{e}^{-\kappa r}$ and its Fourier transform $\phi(\mathbf{k}) = 2\pi q^2(k^2+\kappa^2)^{-\frac{1}{2}}$ (q is the particle charge, κ is the inverse screening length). In the strong coupling regime, the system is either in the liquid or in the crystalline solid (hexagonal

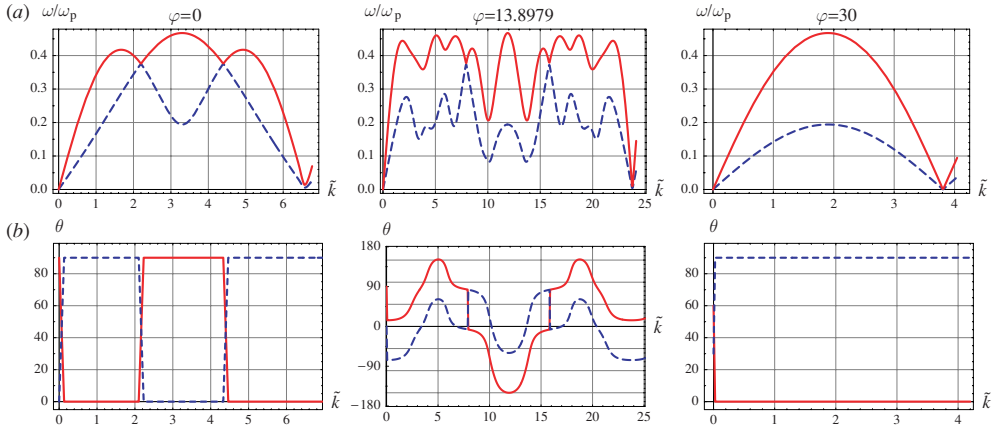

Figure 1. (*a*) Representative dispersion curves and (*b*) polarization angles θ, for $\bar{\kappa} = 3.81$ (corresponding to $\tilde{\kappa} = 2$). The periodicity for $\varphi = 13.8979^\circ$ is $\bar{k} = 23.7891$, in agreement with (3). The plasma frequency is $\omega_p^2 = \frac{2\pi n q^2}{m a_{\rm ws}}$.

lattice) phase. The phase boundary has recently been calculated [3]. We address the problem of collective modes in the lattice versus collective modes in the liquid state. In the lattice, we calculate the dispersion relations, the polarizations, the frequency spectra and the angle-averaged dispersion, which are compared with the dispersion relations in the liquid state for the longitudinal and transverse modes, as calculated in the QLCA approximation and confirmed by MD simulations [4]. In the case of lattice calculations, the distance, wave number and the screening parameter are normalized by the lattice constant a: $\bar{r} = r/a$, $\bar{k} = ka$, $\bar{\kappa} = \kappa a$, while in the liquid phase calculations the Wigner–Seitz radius $a_{\rm ws}$ is used: $\tilde{r} = r/a_{\rm ws}$, $\tilde{k} = ka_{\rm ws}$ and $\tilde{\kappa} = \kappa a_{\rm ws}$.

2. Lattice phonons

The phonon dispersion relation for a lattice is [5, 6]

$$\|\omega^2(k,\varphi) - D_{\mu\nu}(\mathbf{k})\| = 0 \tag{1}$$

where

$$D_{\mu\nu}(\mathbf{k}) = -\frac{q^2}{ma^3}\sum_i M_{\mu\nu}(\bar{\mathbf{r}}_i)(\mathrm{e}^{\mathrm{i}\bar{\mathbf{k}}\cdot\bar{\mathbf{r}}_i} - 1) \qquad M_{\mu\nu}(\mathbf{r}) = \frac{\mathrm{e}^{-\bar{\kappa}\bar{r}}}{\bar{r}^5}\{3\bar{r}_\mu\bar{r}_\nu A(\bar{\kappa}\bar{r}) - \delta_{\mu\nu}\bar{r}^2 B(\bar{\kappa}\bar{r})\}. \tag{2}$$

$A(x) = x^2/3 + x + 1$, $B(x) = x + 1$ and the summation is over the lattice points of a triangular lattice. While it is sufficient to consider $\mathbf{k}$ values within the 1st Brillouin zone to obtain full information on the frequency spectrum, it is instructive to follow the dispersion for high values of $\mathbf{k}$ and study the angle dependence of the periodicity of the $\omega(\mathbf{k})$ curves. Simple periodicity of $\omega(\mathbf{k})$ in k prevails only in the principal directions of the lattice (figure 1). In a general direction φ (see figure 2), the period in $\bar{k}$ is given by

$$\bar{k} = (4\pi/\sqrt{3})(m/2 + n)/\cos\left(\frac{\pi}{6} - \varphi\right) = (4\pi/\sqrt{3})\sqrt{m^2 + mn + n^2} \tag{3}$$

such that m and n exist as the minimum integers satisfying the relation $\tan\left(\frac{\pi}{6} - \varphi\right) = \frac{m\sqrt{3}}{m+2n}$. Moreover, 'longitudinal' and 'transverse' polarizations occur only in the principal directions,

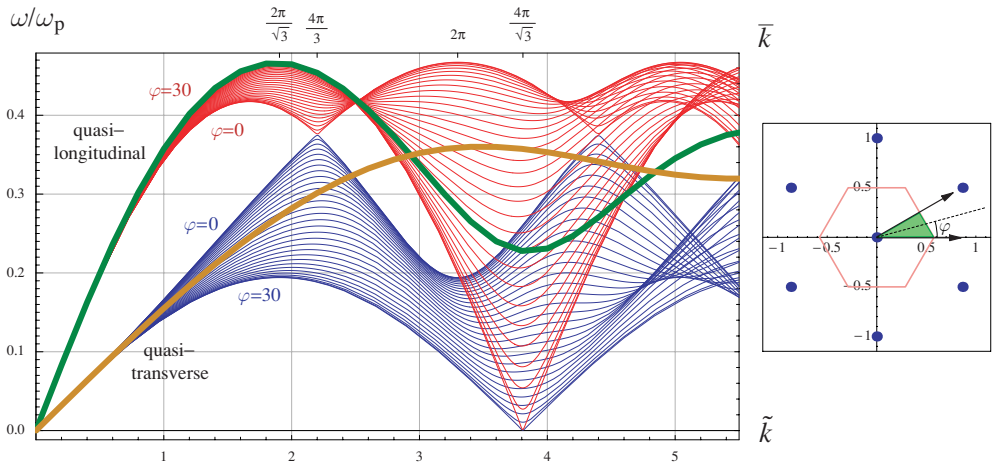

Figure 2. Bands of the two phonon modes for $\varphi = 1$–30°, for $\tilde{\kappa} = 2$, shown together with the longitudinal and transverse QLCA dispersion curves for $\Gamma = 360$ (thick lines). Also shown is the reciprocal hexagonal lattice, its principal directions, the 1st Brillouin zone and its irreducible part. The wavevectors in the second picture are in units of $4\pi/(\sqrt{3}a)$.

while, in general, the polarizations are mixed and the polarization angle θ (the angle with respect to **k**) is a sensitive function of k and φ (figure 1(*b*)). A complete family of dispersion curves is shown in figure 2.

We have calculated the frequency spectrum $g(\omega)$ by numerical integration over the angles: $g(\omega)$ is the quantity that can be most directly compared with molecular dynamics (MD) simulations. The *angularly* resolved frequency spectra are

$$g(\omega, \varphi) = \frac{k}{\frac{\mathrm{d}\omega}{\mathrm{d}k}(k, \varphi)|_{k=k(\omega,\varphi)}} \tag{4}$$

with **k** taken within the irreducible part of the first Brillouin zone, while the full frequency spectrum is obtained by angular integration

$$g(\omega) = \int g(\omega, \varphi)\, \mathrm{d}\varphi. \tag{5}$$

The calculated frequency spectra have been confirmed by MD simulations of a solid, finite temperature system of 990 particles. The histogram of frequencies was determined from the Fourier analysis of an exceedingly long time series of the coordinates of a single test particle (figure 3). We have also verified that the frequency spectra satisfy the important sum rule established by Bakshi [7]

$$\int \omega^2 g(\omega)\, \mathrm{d}\omega = \omega^2_{\mathrm{Einstein}} \tag{6}$$

where $\omega_{\mathrm{Einstein}}$ is the characteristic Einstein frequency of the system, defined as the oscillation frequency of a single particle in the frozen environment of all the others [4, 8].

3. Collective modes in the liquid

The collective modes in the liquid state can be calculated in the QLCA approximation whose validity has been verified by MD simulations. The dispersion relation is [4]

$$\left\| \omega^2(k, \varphi) - \Omega_0^2(k) \frac{k_\mu k_\nu}{k^2} - D_{\mu\nu}(\mathbf{k}) \right\| = 0 \tag{7}$$

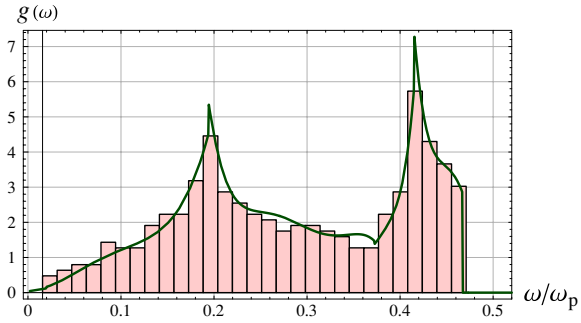

Figure 3. Calculated frequency spectrum (solid line) and MD simulation (histogram) for $\tilde{\kappa} = 2$.

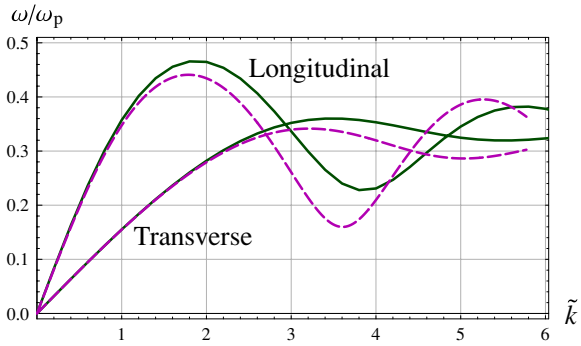

Figure 4. QLCA (solid line) for $\Gamma = 360$ and angularly averaged lattice curves (dashed) for $\tilde{\kappa} = 2$.

where

$$D_{\mu\nu}(\mathbf{k}) = -\omega_p^2 \int M_{\mu\nu}(\tilde{\mathbf{r}})(\mathrm{e}^{\mathrm{i}\tilde{\mathbf{k}}\cdot\tilde{\mathbf{r}}} - 1)h(\tilde{r})\,\mathrm{d}\tilde{r} \qquad \Omega_0^2(k) = \omega_p^2 \frac{\tilde{k}^2}{\sqrt{\tilde{k}^2 + \tilde{\kappa}^2}} \tag{8}$$

$n = 1/\left(\pi a_{\mathrm{ws}}^2\right)$ is the particle number density, $h(r)$ is the pair correlation function and $\omega_p^2 = \frac{2q^2}{ma_{\mathrm{ws}}^3}$. A comparison between the lattice dispersions calculated here and the QLCA dispersions calculated in [4] for $\Gamma = 360$ is shown in figure 2. The lattice and phonon spectra are markedly different: the dispersion in the liquid is isotropic and splits into well-defined longitudinal and transverse polarizations; in contrast, the *angularly averaged* lattice dispersions and the QLCA dispersions show a remarkable similarity (figure 4). The former have been calculated from (1), (2) by decomposing the polarization vectors into their longitudinal and transverse components and by integrating $M_{\mu\nu}$ over all angles to produce angularly averaged kernels. This process results into the following results:

$$\begin{aligned}
\omega_L^2(k) &= \frac{\tilde{k}^3}{2}\sum_{r_i}\frac{\mathrm{e}^{-y}}{x^3}\left[1 + y + y^2 - (4 + 4y + 2y^2)J_0(x) + (6 + 6y + 2y^2)\frac{J_1(x)}{x}\right] \\
\omega_T^2(k) &= \frac{\tilde{k}^3}{2}\sum_{r_i}\frac{\mathrm{e}^{-y}}{x^3}\left[1 + y + y^2 + (2 + 2y)J_0(x) - (6 + 6y + 2y^2)\frac{J_1(x)}{x}\right]
\end{aligned} \tag{9}$$

where $x = kr$ and $y = \kappa r$, while ω_L and ω_T are in units of ω_p.

Thus, we have shown that the phonon spectrum of the crystal lattice is substantially different from that of the strongly coupled isotropic liquid. This is well demonstrated by figure 2. The difference is primarily due to the anisotropy of the lattice. On the other hand, the dispersion resulting from angular averaging over the lattice positions closely emulates the dispersion of the liquid state. The similarity can be understood by realizing that the local structure of the strongly coupled liquid is similar to that of the crystal lattice, but with an orientation that changes randomly from point to point.

Acknowledgments

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