ON THE DIELECTRIC RESPONSE FUNCTION AND PHONON SELF ENERGY OF ACOUSTIC PHONONS IN 2D DIRAC CRYSTALS

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ABSTRACT

The unique structure of two-dimensional (2D) Dirac crystals, with electronic bands linear in the proximity of the Brillouin-zone boundary and the Fermi energy, creates anomalous situations where small Fermi-energy perturbations (e.g., by impurities and quasiparticles) are known to critically affect the electron-related lattice properties of the whole system. The Fermi-surface nesting (FSN) conditions determining such effects via electron-phonon interaction, require accurate estimates of the crystal’s response function ($\chi$) as a function of the phonon wavevector $q$ for any values of temperature, as well as realistic hypotheses on the nature of the phonons involved. Numerous analytical estimates of $\chi(q)$ for 2D Dirac crystals beyond the Thomas-Fermi approximation have been so far carried out only in terms of dielectric response function $\chi(q,\omega)$, for photon and optical-phonon perturbations, due to relative ease of incorporating a $q$-independent oscillation frequency ($\omega$) in their calculation. However, models accounting for Dirac-electron interaction with ever-existing acoustic phonons, for which $\omega$ does depend on $q$ and is therefore dispersive, are essential to understand many critical crystal properties, including electrical and thermal transport. The lack of such models has often led to assume that the dielectric response function $\chi(q)$ in these systems can be understood from free-electron behavior, or statically, and from zero-temperature behavior. Here, we show that, different from free-electron systems, $\chi(q)$ calculated from acoustic phonons in 2D Dirac crystals using the Lindhard model, exhibits a cuspidal point at the FSN condition even in the static case and at 0 K. Strong variability of $\frac{\partial \chi}{\partial q}$ persists also at finite temperatures, while $\chi(q)$ may tend to infinity in the dynamic case even where the speed of sound is small, albeit nonnegligible, over the Dirac-electron Fermi velocity. The implications of our findings for electron-acoustic phonon interaction and transport properties such as the phonon line width derived from the phonon self energy will also be discussed.

1 Introduction

Dirac crystals are a broad class of zero band-gap solids in which the electronic band structure is linear in the crystal momentum, $\hbar k$, instead of quadratic, as commonly observed in metals and semiconductors.\cite{1,2,3} This leads to dispersionless electrons with a behavior reminiscent of photons on the Dirac light cone in special relativity.\cite{4} In two-dimensional (2D) Dirac crystals, the best known of which is graphene\cite{5,6,7}, the density of electronic states near the Fermi level also linearly tends to zero, thus enabling additional remarkable properties, including extreme carrier mobility and quantum Hall effects, along with the possibility of topological insulator characteristics.\cite{8,9,10,11,12,13} The experimental discovery of a plethora of new 2D Dirac crystals in recent years such as silicenes\cite{14}, germanenes\cite{15}, Weyl semi-metals\cite{16}, borophene\cite{17} and topological insulators\cite{3,18,19,20} compels more fundamental understanding in this research area.

In undoped Dirac crystals, the valence and conduction bands meet at the Brillouin-zone boundary $K$-point, and at the Fermi energy $E_F$. Thus, the crystal’s Fermi surface degenerates into a single point of the electronic band structure.\cite{1,2}
As far as 2D systems are concerned, such a degeneracy enables to tune the density of electronic states at \( E_F \), as well as the system’s electrical and thermal transport, via external electric fields or tunable doping—an effect that leads to carrier density to increase by orders of magnitude upon small fluctuations of \( E_F \).[21][22] Such Fermi-level shifts are also expected to dramatically alter the strength of interaction between charge carriers and lattice phonons.[23][24] which may have profound effects on the suitability of separation of electron and lattice contributions within the Born-Oppenheimer approximation,[25] for example in thermal transport.[26][27][28][29][30]

A key parameter to understand the effects of strong electron-phonon interactions is the crystal’s dielectric response function, \( \chi \). The dielectric response function differs from the dielectric susceptibility \( \chi(q, \omega) \) in that it must take into account the dispersion relationship \( \omega_q \) of the phonon mode for which it is calculated, and cannot simply be obtained from replacing \( \omega_q \) into \( \chi(q, \omega) \), with which processes violating the conservation of energy or momentum would be inappropriately considered. For a phonon of wavevector \( q \), \( \chi(q) \) is the result from the superposition of all of the inelastic scattering of electrons and holes by such phonon. The customary approach for calculating \( \chi(q) \) relies on the Thomas-Fermi [31][32] or Debye-Huckel [33] approximations, which assumes a long wavelength (i.e. short wavenumber) from the scattered phonon. Such an assumption is specifically designed for metals with large (> \( 10^{22} \text{cm}^{-3} \)) free electron densities in the proximity of \( E_F \), and, therefore, short screening lengths and \( q \) much smaller than the dimensions of the Fermi surface which, as far as Dirac crystals are concerned, can be estimated as \( \sim 2k_F \), twice the magnitude of the Fermi wavevector. For undoped Dirac crystals, with valence and conduction bands meeting at the K-point but not crossing the Fermi level, then \( k_F = 0 \) and the screening length tends to infinity, although \( k_F \) is expected to remain very small also for the small fluctuations of \( E_F \) achievable via external electric fields or doping, leading to free-electron densities of \( 10^{18} \text{cm}^{-3} \), or less. In the 2D case, because 2D Dirac crystals are zero-band gap semiconductors with zero density-of-states at \( E_F \), they are expected to dramatically amplify, in terms of screening length, the effects of any phonon disturbances for which \( q \approx 2k_F \), an effect known as Fermi-surface nesting [34][35][36] (FSN) and potentially leading to Kohn anomalies[37][38][39] at \( T = 0 \text{ K} \). \( q = 2k_F \) and charge density waves.[40]

Based on quantum first-order perturbation theory, the Lindhard model of electron screening enables \( \chi(q) \) to be reliably calculated for any wavenumber of the disturbance, regardless of their size with respect to \( k_F \).[32] For example, Kohn anomalies and FSN conditions for free electron gases of any dimensionality are correctly predicted using a static Lindhard model at 0 K.[41][42]. A disadvantage of the Lindhard model over more simplistic approximations such as Thomas-Fermi, is the requirement of carrying out integrations that often cannot be performed analytically, and may become more cumbersome where: (i) the model is dynamic—i.e. one assumes that phonons not only carry momentum, but also energy \( \hbar \omega_q \); or (ii) non-zero temperature is considered—a necessary requirement to compare \( \chi(q) \) with experiments involving, for example, T-dependent electrical or transport measurements; or (iii) the phonon energy \( \hbar \omega_q \) is wavevector-dependent in a dispersive system—a respect in which it is worthwhile noting that the phonon energy is not only required in dynamic Lindhard-model calculations, but also static ones, as it affects the electron Fermi-Dirac distribution, also at 0 K. Of course, the complexity of the calculation will increase if more than one of the phenomena (i — iii) are considered.

As far as 2D Dirac crystals are concerned, the dynamic Lindhard model has been utilized by Hwang and Das Sarma,[43] and Bahrami and Vasiliopoulos,[44] to calculate the dielectric susceptibility \( \chi(q, \omega_q) \) at any arbitrary energy for surface plasmons in graphene and armchair graphene nanoribbons, respectively, with the implicit assumption of a non-dispersive energy-wavelength relationship. Zhu et al.[45] reviewed and compared different finite-temperature non-dispersive approaches to calculate the dielectric susceptibility and polarizability, including the Lindhard model, with their dispersive numerical estimates utilizing the ab initio calculated electron and phonon band structures for graphene. This makes impossible to extend their results beyond this specific crystal. Iurov et al.[46] have considered \( \chi(q, \omega_q) \) calculated within the Lindhard model for silicene illuminated by circularly polarized light, where disturbances are, therefore, photons—not phonons. Using the Lighthill theorem, Lu[47] has calculated the zero-temperature, static, Lindhard response function for single-layer and bilayer graphene in the presence of an impurity, a work that would require extension to the dynamic and finite-temperature cases, and to dispersive phonons, to be applicable to our problem. Calandra et al.[48] have calculated the electron-phonon coupling in electron doped graphene at the zone center and zone boundary of the crystal using electron-phonon matrix elements extracted from density functional theory simulations however, a direct analytical calculation has not been made and the results can not be extended beyond the specific crystal under study. Lazzeri et al.[33] have derived the dielectric response function in doped graphene as a function of the charge doping for \( q = 0 \) and phonon wave functions where \( q \neq 0 \) has not been considered. Because of the use of a \( q \) independent from the disturbance energy \( \hbar \omega_0 \) in these 3D density-of-states they
are critically important for a host of measurable properties including but not limited to thermal transport \[49, 50, 51\], electric conductivity \[52, 53\], and Brillouin scattering \[54, 55\] particularly at low or room temperatures where the optical phonons are not excited. Such properties are often calculated in 2D Dirac crystals by considering weak electron-phonon interaction and, consequently, short-range charge screening effects at the level of Thomas-Fermi. \[56, 57, 58\] This is unreliable in the very frequent case in which small Fermi-energy fluctuations by doping or impurities produce Fermi level shifts bringing \(k_F\) within the range of acoustic phonon wavenumbers \(q\). This may lead to FSN and anomalous electron-phonon interaction. For example, Ramezanali et al. \[59\] found that the accuracy of specific-heat calculations in graphene can be remarkably improved by introducing a Lindhard-based correction still assuming random-phase approximation and relatively weak electron-phonon coupling, which limits the generality of their approach. Furthermore, by deriving the dielectric response function as a function of \(q\) using the Lindhard model we can improve on the phonon self energy calculation performed in 2D Dirac crystals. The phonon line width derived from the phonon self energy provides a way to gain experimental information about the electron-phonon coupling strength. The calculations for the phonon self energy has been mostly carried out at \(T \rightarrow 0\) \[60\] and \(q = 0\) \[61\] which limits the application of such results.

Objective of our work is to analytically calculate the dielectric response function of 2D Dirac crystals using the Lindhard model. Using scaling laws and introducing reduced phonon and electron wavevectors, respectively \(\psi\) and \(\xi\), as well as a reduced temperature \(\tau\) and reduced speeds of sound \(w_F\)

\[
\xi = \frac{k}{2k_F}, \quad \psi = \frac{q}{2k_F}, \quad \tau = \frac{k_B T}{2\nu_F k_F}, \quad w_F = \frac{c}{\nu_F},
\]

(\text{where } \nu_F = E_F/k_F \text{ is the Fermi velocity}) we show that a universal scaling law for the Lindhard dielectric response of acoustic phonons only depending on the dimensionless quantities in Eq. (1) can be established. Such an expression will be general enough to describe the electron-lattice interaction at any Fermi-level shifts and temperatures even for cases where the small-\(\tau\) Sommerfeld approximation \[32\] customarily used in solid state physics is not valid. Further, using the derived dielectric response function we calculate the phonon line width from the phonon self energy and compare our results with experimental data presented in the literature.

## 2 Methodology

Using the normalized quantities in Eq. (1) the Lindhard dielectric response function \[32\] takes the form:

\[
\chi(q, \omega) = - \frac{e^2}{2\pi^2} \frac{1}{(2k_F)^2} \int_{-\frac{1}{2}}^{\frac{1}{2}} \frac{f_{\xi+\psi/2} - f_{\xi-\psi/2}}{E_{\xi+\psi/2} - E_{\xi-\psi/2} - \hbar\omega} d^2 \xi,
\]

(\text{where } f_{\xi+\psi/2} \text{ are the occupation function of the single particle state following the Fermi-Dirac distribution and } \hbar\omega_{\text{ph}} \text{ is the phonon energy. The integral is over the momentum space of the Fermi sphere and } E_{\xi+\psi/2} \text{ are the energy of the created and annihilated electrons, respectively. To simplify the problem, we do not integrate over the electron spins and we have simplified the problem by multiplying Eq. (2) by a factor of 2. To study the dielectric response function of the electron-phonon interactions in 2D Dirac crystals caused by the increase of their Fermi energy via different experimental methods such as doping \[62, 63\], it is necessary to find the region where these interactions take place inside the reciprocal lattice. As shown in Fig. 1(a) the } \pi-\pi^* \text{ electron energy spacing in a 2D Dirac crystal at the zone center } E_F \[64\] \text{ is too high relative to the energy of acoustical phonons } \[65\] E_{\text{ph}} = \hbar\omega_{\text{ph}} \text{ for any electron-phonon interactions to take place without violating the conservation of energy. The electron energy spacing decreases as we move towards the zone boundary } \mathbf{K} \text{-point of the lattice becoming comparable to the energy of phonons and making the electron-phonon interactions possible. Assuming we have a honeycomb lattice structure as shown in Fig. 1(b) the electron-phonon interactions in the reciprocal lattice shown by the shaded grey region occurs at the two zone boundary points K1 and K2 depicted by the Dirac cones.}
On the dielectric response function and phonon self-energy of acoustic phonons in 2D Dirac crystals

To derive an analytical expression for the Lindhard dielectric response function we must solve the difference between the two Fermi-Dirac distribution functions imposed in the numerator of the integral in Eq.(2) by applying suitable approximations. The most used approximation for simplifying the Fermi-Dirac distribution function is the “single step” function used at $T \approx 0$ K where the Fermi-Dirac distribution has a value of 2 for energies below the Fermi energy, and a value of 0 for energies above. However, at finite temperatures the “single step” function approximation is no longer accurate since the distribution gets smeared out, as some electrons begin to be thermally excited to energy levels above $E_F$. We therefore approximate the Fermi-Dirac distribution with a “double step” function which has three values 2, 1, and 0 and covers the distribution of electrons at different energies more accurately, shown in Fig. 2(a).

Furthermore, while at $T = 0$ K the chemical potential $\mu$ is equal to $E_F$ this is no longer the case at finite temperatures were $\mu$ becomes dependent on both $E_F$ and $T$. Therefore, to find the values of the Fermi-Dirac distribution at different energies using the “double step” function we must find a relation between $\mu$, $E_F$ and $T$.

In condensed matter systems such as metals where we have an abundant number of electrons and the Fermi energy is large, we use the Sommerfeld expansion developed by Arnold Sommerfeld to write the chemical potential as $\mu \approx E_F - (k_B T)^2 / (8 E_F)$. However, Sommerfeld expansion cannot be reliable for 2D Dirac crystals which have a limited concentration of free electrons and a small value of $E_F$. Therefore, to write $\mu$ in terms of $E_F$ and $T$ for 2D Dirac crystals we have to develop a new relation. To this end we define $\Delta E_{\pm}$ to be the range of the singly occupied energy levels in the Dirac cone situated above and below the Fermi energy, respectively, shown in Fig. 2(b). The integrated density of states over $\Delta E_{\pm}$ are equal and are defined as $\Delta g_{\pm}(T)$. By analyzing Fig. 2(b) we can write $\mu$ as a function of $E_F$ and $\Delta E_{\pm}$ in the following manner:

$$\mu = E_F + \Delta E_+ - \Delta E_-.$$

We then write $\Delta E_{\pm}$ in terms of $E_F$ and $T$ in the following two steps. First, as shown in Fig. 2(b) the sum of the singly occupied energy levels in the Dirac cone situated above and below the Fermi energy level is equal to:

$$\Delta E_+ + \Delta E_- = k_B T.$$

Second, we know that the integrated density of states over $\Delta E_+$ and $\Delta E_-$ are equal. This results in the surface area of the two red and blue regions on the Dirac cone in Fig. 2(b) to be equal with one another and results in the following equation:

$$\Delta E_- (2E_F - \Delta E_-) = \Delta E_+ (2E_F + \Delta E_+).$$

By inserting Eq.(4) into Eq.(5) we find a relation between $\Delta E_{\pm}$ and $E_F$ and $T$. We can therefore write the chemical potential as:

$$\mu(E_F, T) = E_F + \frac{\Delta E_+ - \Delta E_-}{2} = \sqrt{E_F^2 - \left(\frac{k_B T}{2}\right)^2}.$$
On the dielectric response function and phonon self-energy of acoustic phonons in 2D Dirac crystals

By analyzing Eq. (6) we observe that at high Fermi energies, it reduces to the Sommerfeld expansion which further validates our result. To find the difference between $f_{\xi+\psi/2}$ and $f_{\xi-\psi/2}$ versus the energy we plot the two on the same graph using the “double step” function approximation and then compute the area under the curve. This is shown in Fig. 2(c), and we have:

$$f_{\xi+\psi/2} - f_{\xi-\psi/2} = \begin{cases} 1 & \sqrt{E_F^2 - \left(\frac{k_BT}{2}\right)^2} - k_BT - \frac{cq}{2} < E_\xi < \sqrt{E_F^2 - \left(\frac{k_BT}{2}\right)^2} - k_BT + \frac{cq}{2} \\ 1 & \sqrt{E_F^2 - \left(\frac{k_BT}{2}\right)^2} + k_BT - \frac{cq}{2} < E_\xi < \sqrt{E_F^2 - \left(\frac{k_BT}{2}\right)^2} + k_BT + \frac{cq}{2} \end{cases}$$ (7)

Where the energy bounds in Eq. (7) for which $f_{\xi+\psi/2} - f_{\xi-\psi/2} = 1$ is shown by the purple shaded region in Fig. 2(c). The difference between the two sets the bounds of integration for calculating the dielectric response function at $T \neq 0$ K. By analyzing Eq. (4) at $T \approx 0$ K we observe that the two purple regions in Fig. 2(c) overlap with one another, and the “double step” function turns into a “single step” function further confirming our results.

Figure 2: (a) “Double step” approximation of the Fermi-Dirac distribution used in this paper to calculate the dielectric response function for $T \neq 0$ K. The “double step” approximation and the Dirac cone of a 2D crystal with an elevated Fermi energy level $E_F$. Areas of the Dirac cone highlighted in red and blue lead to equal number of states at energy ranges $\Delta E_+$ and $\Delta E_-$ above and below $E_F$, respectively. (c) The difference between $f_{\xi+\psi/2}$ and $f_{\xi-\psi/2}$ as a function of energy in a 2D Dirac crystal shown in the two purple squares which set the bounds of integration for calculating the dielectric response function.

By raising the temperature, the Fermi energy of the 2D Dirac crystal shifts leading the bounds of the integration in Eq. (2) for the dielectric response function to also change. While the bounds of the integration for $\xi(\psi, \omega)$ at $T = 0$ K are between $1/2 \pm \psi/2$, using the “double step” function to derive the difference in the Fermi-Dirac distribution for $T \neq 0$ K we have:

$$\chi(\psi, \omega) = -\frac{e^2}{2\pi^2} \int_{\frac{E_F}{k_BT} - \frac{\psi}{2}}^{\frac{E_F}{k_BT} + \frac{\psi}{2}} \frac{d^2\xi}{E_\xi - \psi - \frac{cq}{2}} + \int_{\frac{E_F}{k_BT} + \frac{\psi}{2}}^{\frac{E_F}{k_BT} + \frac{\psi}{2}} \frac{d^2\xi}{E_\xi + \psi - \frac{cq}{2}}$$ (8)

Where we have written the dielectric response function in dimensionless coordinates as $\chi(\psi, \omega) = \chi(q, \omega)/2k_F$. We see that by approximating the Fermi-Dirac distribution with a “double step” function we split the integral in Eq. (2) into two integrals where the bounds of each integral is one of the purple shaded regions depicted in Fig. 2(c).

The extreme carrier mobility in 2D Dirac crystals results in their Fermi velocity to be much larger than the speed of sound, $v_F >> c$. This is confirmed by experiments conducted on various 2D Dirac crystals such as graphene.
On the dielectric response function and phonon self-energy of acoustic phonons in 2D Dirac crystals

Borophene[8], Weyl semimetals[68], and silicene[69] were we see that $c < 0.01 v_F$. Defining $w_F = c/v_F$ we can Taylor expand the dielectric response function around $w_F$ with $w_F \to 0$ in the following manner:

$$\chi_{w_F}(\psi) = \chi_0(\psi) + \frac{\partial \chi_0(\psi)}{\partial w_F} w_F + \frac{1}{2} \frac{\partial^2 \chi_0(\psi)}{\partial w_F^2} w_F^2 + \ldots,$$

(9)

The first addend in Eq.(9) is the static dielectric response of the 2D Dirac crystal with the phonon energy being equal to zero. The next addends are the higher order terms which are the dielectric response at nonzero phonon energy. Due to the convenience in calculation, we derive the static term in the Cartesian coordinate system and derive the dynamic terms in Polar coordinates. In the end, by adding the static term with the dynamic terms we get the dielectric response function of a 2D Dirac crystal.

Figure 3: (a),(b) The shift in the Fermi sphere respectively for $q < 2k_F$ or $\psi < 1$ and $q > 2k_F$ or $\psi > 1$ written in the Cartesian coordinate system. We write the shift in the Fermi sphere in Cartesian coordinates to calculate the static dielectric response function. (c), (d) The shift in the Fermi sphere respectively for $q < 2k_F$ or $\psi < 1$ and $q > 2k_F$ or $\psi > 1$ written in the polar coordinate system. We write the shift in the Fermi sphere in polar coordinates to calculate the 2nd to last addends of the dielectric response function which contain the phonon energy.

3.1 Static dielectric response

The first addend of Eq.(9) expresses the static dielectric response, $\chi_0(\psi)$, function of a 2D Dirac. To derive $\chi_0(\psi)$ of a 2D Dirac crystal we perform the calculations in the Cartesian coordinate system. Therefore, following Eq.(2) $\chi_0(\psi)$ of
a 2D Dirac crystal at T = 0 K is equal to:

\[ \chi_0(\psi) = -\frac{e^2}{\pi^2 v_F} \int_0^{\frac{\pi}{2}} d\xi_x \int_0^{\frac{\pi}{2}} \left[ \frac{1}{1 - (\xi_x^2 + \xi_y^2)^{1/2}} \right] \frac{d\xi_y}{\sqrt{(\xi_x + \psi/2)^2 + \xi_y^2 - \sqrt{(\xi_x - \psi/2)^2 + \xi_y^2}}} \]

\[ + \int_0^{\frac{\pi}{2}} d\xi_x \int_0^{\frac{\pi}{2}} \left[ \frac{1}{1 - (\xi_x^2 + \xi_y^2)^{1/2}} \right] \frac{d\xi_y}{\sqrt{(\xi_x + \psi/2)^2 + \xi_y^2 - \sqrt{(\xi_x - \psi/2)^2 + \xi_y^2}}} \]

\[ = \int_0^{\frac{\pi}{2}} d\xi_x \int_0^{\frac{\pi}{2}} \left[ \frac{1}{1 - (\xi_x^2 + \xi_y^2)^{1/2}} \right] \frac{d\xi_y}{\sqrt{(\xi_x + \psi/2)^2 + \xi_y^2 - \sqrt{(\xi_x - \psi/2)^2 + \xi_y^2}}} \] (10)

Since we are integrating over the two Fermi spheres, we have multiplied \( \chi_0(\psi) \) by a factor of 2. Furthermore, since the bounds along the y-axis change when writing the integral in the Cartesian coordinate system for \( \psi < 1 \), we divide the integral into two, with each integral covering a separate region as shown in Fig. 3(a) by the two blue and green colors. So, the first two integrals in Eq. (10) are for the region \( \psi < 1 \) and the third integral is for the region \( \psi > 1 \). Analyzing each of these two regions separately, for \( \psi < 1 \) we have:

\[ -\left( \frac{\pi^2 v_F}{e^2} \right) \chi_0(\psi) = \frac{1}{\psi} \lim_{\epsilon \to 0} \int_0^{\frac{\pi}{2} - \epsilon} d\xi_x \left[ \frac{1}{1 - (2\xi_x - \psi)^2} \right] \left( 1 + \sqrt{1 + 8\psi\xi_x} \right) + \left( \frac{2\xi_x + \psi}{8\xi_x} \right) \left( \frac{1 - (2\xi_x - \psi)^2}{2\xi_x + \psi} \right) \frac{\text{asinh} \left( \frac{\sqrt{1 - (2\xi_x - \psi)^2}}{2\xi_x + \psi} \right)}{\text{asinh} \left( \frac{\sqrt{1 - (2\xi_x - \psi)^2}}{2\xi_x + \psi} \right)} \]

\[ - \int_0^{\frac{\pi}{2} - \epsilon} d\xi_x \left[ \frac{1}{1 - (2\xi_x + \psi)^2} \right] \left( 1 + \sqrt{1 - 8\psi\xi_x} \right) + \left( \frac{2\xi_x + \psi}{8\xi_x} \right) \left( \frac{1 - (2\xi_x + \psi)^2}{2\xi_x + \psi} \right) \frac{\text{asinh} \left( \frac{\sqrt{1 - (2\xi_x + \psi)^2}}{2\xi_x + \psi} \right)}{\text{asinh} \left( \frac{\sqrt{1 - (2\xi_x + \psi)^2}}{2\xi_x + \psi} \right)} \]

\[ \approx 0.39. \] (11)

where we have integrated over \( \xi_y \). Using a MATLAB routine, we solve Eq. (11) numerically by sums. The designated solid black line in Fig. 3(a) is the integral solution of Eq. (11). To further analyze the integral and come up with an analytical solution we partition the different parts of Eq. (11). The red dashed lines numbered (i) and (ii) are the two positive and two negative terms containing the arc hyperbolic sinus. The sum of these two terms is \( (i) + (ii) = (I_3) \) shown in Fig. 3(a) as a solid red line.

\[ (I_3) = (i) + (ii) = \lim_{\psi \to 0} \int_0^{\frac{\pi}{2} - \epsilon} d\xi_x \left[ \frac{2\xi_x + \psi}{8\xi_x} \text{asinh} \left( \frac{\sqrt{1 - (2\xi_x - \psi)^2}}{2\xi_x + \psi} \right) \right] + \left( \frac{2\xi_x - \psi}{8\xi_x} \text{asinh} \left( \frac{\sqrt{1 - (2\xi_x + \psi)^2}}{2\xi_x + \psi} \right) \right) \]

\[ \approx 0.39. \] (12)

It can be seen in Fig. 4(a) that the designated line \( (I_3) \) is approximately a constant equal to \( (I_3) \approx 0.39 \). This can be proven by Taylor expanding \( (I_3) \) up to the first order about \( \psi = 0 \). We further separate the remaining terms in Eq. (11) in the following manner:

\[ (I_1) = \lim_{\psi \to 0} \left( \int_0^{\frac{\pi}{2} - \epsilon} d\xi_x \left[ \frac{\sqrt{1 - (2\xi_x - \psi)^2}}{16\xi_x} \right] - \int_0^{\frac{\pi}{2} - \epsilon} d\xi_x \left[ \frac{\sqrt{1 - (2\xi_x + \psi)^2}}{16\xi_x} \right] \right) \]

\[ = \frac{\pi \psi + \sqrt{1 - \psi^2} \ln \left( \frac{1 - \psi}{1 + \psi} \right)}{16\psi}, \] (13)
where Eq. (20) is the analytical expression of the static dielectric function of a 2D Dirac crystal in the region of \( \psi > \). By analyzing Fig. 4(a) we observe that (I_2) can be estimated as (I_2) \approx 0.2 + (I_1) / (2 \psi). This can also be proven by Taylor expanding (I_1) and (I_2) up to the second order about the midpoint of the integral bounds which are \((1 + \psi)/4\) and \((1 - \psi)/4\). We can therefore write Eq. (11) as:

\[
- \left( \frac{\pi^2 v_F}{e^2} \right) \chi_0(\psi) = (I_1) + (I_2) + (I_3) = 0.59 + \frac{3(\pi \psi + \sqrt{1 - \psi^2} \ln (\frac{1 - \psi}{1 + \psi}))}{32 \psi},
\]

where Eq. (15) is the analytical expression of the static dielectric response of a 2D Dirac crystal in the region of \( \psi < 1 \). For \( \psi > 1 \) we have:

\[
- \left( \frac{\pi^2 v_F}{e^2} \right) \chi_0(\psi) = \frac{1}{\psi} \left( \int_{1-\psi}^{1+\psi} d\xi \left( \frac{2\xi + \psi^2}{8\xi} \ln \left( \frac{1 - (2\xi - \psi)^2}{2\xi + \psi} \right) + \frac{(2\xi + \psi)^2}{8\xi} \ln \left( \frac{1 - (2\xi - \psi)^2}{2\xi - \psi} \right) \right) \right)
\]

The designated solid black line numbered (I') in Fig. 4(a) is the integral solution of Eq. (16) solved numerically. We again partition the different parts of the integral to come up with an analytical solution. The red dashed lines in Fig. 4(a) numbered (i') and (ii') are the first and second terms containing the arc hyperbolic sin term in Eq. (16). The sum of these two terms is (i') + (ii') = (I'_3), shown in Fig. 4(a) as a solid red line.

\[
(I'_3) = (i') + (ii') = \frac{1}{\psi} \left( \int_{1-\psi}^{1+\psi} d\xi \left( \frac{2\xi + \psi^2}{8\xi} \ln \left( \frac{1 - (2\xi - \psi)^2}{2\xi + \psi} \right) + \frac{(2\xi + \psi)^2}{8\xi} \ln \left( \frac{1 - (2\xi - \psi)^2}{2\xi - \psi} \right) \right) \right)
\]

This can be proven by Taylor expanding (I'_3) up to the first order about the midpoint of the integral bound which is \( \psi/2 \). We further separate the remaining terms in Eq. (16) as following:

\[
(I'_1) = \frac{1}{\psi} \left( \int_{1-\psi}^{1+\psi} d\xi \left( \frac{1 - (2\xi - \psi)^2}{16\xi} \right) \right) = \frac{\pi + \sqrt{1 - \psi^2} \ln \left( \frac{1 - \psi}{1 + \psi} \right)}{16 \psi},
\]

\[
(I'_2) = \frac{1}{\psi} \left( \int_{1-\psi}^{1+\psi} d\xi \left( \frac{1 - (2\xi - \psi)^2}{16\xi} \right) \right) = \frac{\pi + \sqrt{1 - \psi^2} \ln \left( \frac{1 - \psi}{1 + \psi} \right)}{16 \psi}.
\]

Where (I'_1) is shown by a purple solid line while (I'_2) is shown by a blue solid line in Fig. 4(a). By analyzing Fig. 4(a) we observe that (I'_2) can be estimated as (I'_2) \approx [0.4 + (I'_1)] / (2 \psi). This can also be proven by Taylor expanding (I'_1) and (I'_2) up to the first order about their midpoint integral bound which is \( \psi/2 \). We can therefore write Eq. (16) as:

\[
- \left( \frac{\pi^2 v_F}{e^2} \right) \chi_0(\psi) = (I'_1) + (I'_2) + (I'_3) = \frac{1}{\psi} \left( 0.59 + \frac{3(\pi \psi + \sqrt{1 - \psi^2} \ln (\frac{1 - \psi}{1 + \psi}))}{32 \psi} \right).
\]

Where Eq. (20) is the analytical expression of the static dielectric function of a 2D Dirac crystal in the region of \( \psi > 1 \). The comparison between the analytical and numerical solution of the static dielectric response using the Lindhard model is shown in Fig. 4(b) in which the two solutions are in good agreement with one another. By studying both graphs we see their cuspidal points are at \( \psi = 1 \) or \( q = 2k_F \) which is the Fermi wave number. We therefore have the absolute value of the static dielectric response function increase up to \( \psi = 1 \) and then decrease as we go further away.
3.2 Dielectric response at nonzero phonon energy

The second addend of Eq. (9) expresses the dielectric response function for nonzero phonon energy, \( \frac{\partial \chi_0(\psi)}{\partial \omega_F} \cdot w_F \), of a 2D Dirac crystal. To derive \( \frac{\partial \chi_0(\psi)}{\partial \omega_F} \) of a 2D Dirac crystal we perform the calculations in a polar coordinate system.

Therefore, following Eq. (2),

\[ \frac{\partial \chi_0(\psi)}{\partial \omega_F} \cdot w_F \]

we get:

\[ -\left( \frac{\pi^2 v_F}{e^2} \right) \frac{\partial \chi_0(\psi)}{\partial \omega_F} = \lim_{\epsilon \to 0} \left[ \int_{\frac{\pi}{2}}^{\frac{\pi}{2} - \epsilon} d\theta \right. \int_{\frac{\pi}{2}}^{\frac{\pi}{2} + \epsilon} d\theta \left. \frac{\sin \theta}{\sqrt{1 - \psi^2}} \right] \left[ 2 \psi \cos \left( \frac{\pi}{2} - \epsilon \right) \right] + \frac{\psi}{2} \tan \left( \frac{\pi}{2} - \epsilon \right) \ln \left[ \frac{2 \psi \cos \left( \frac{\pi}{2} - \epsilon \right) + \sqrt{4 - 2 \psi^2 + 2 \psi^2 \cos \left( \frac{\pi}{2} - \epsilon \right)}}{-2 \psi \cos \left( \frac{\pi}{2} - \epsilon \right) + \sqrt{4 - 2 \psi^2 + 2 \psi^2 \cos \left( \frac{\pi}{2} - \epsilon \right)}} \right]. \]  

(21)

The first integral is for the region \( \psi < 1 \) and the second integral is for the region \( \psi > 1 \). \( \psi_M \) is the maximum distant we place ourselves from the Fermi sphere to do the calculations for \( \psi > 1 \). Performing the calculations we observe that the second addend of the dielectric response function goes to zero for \( \psi > 3 \) so \( \psi_M \) can be confidently put equal to 3.

To solve the integral in Eq. (21) analytically we use the binomial expansion:

\[ (1 + \alpha)^n = 1 + n\alpha + \frac{n(n-1)}{2} \alpha^2 + ... \]  

(22)

Applying the binomial expansion up to the first order of magnitude to the first addend of Eq. (22) designating the solution for \( \psi < 1 \) we get:

\[ -\left( \frac{\pi^2 v_F}{e^2} \right) \frac{\partial \chi_0(\psi)}{\partial \omega_F} = \lim_{\epsilon \to 0} \left[ \frac{1}{\sqrt{1 - \psi^2}} \right. \left. \frac{\sin \theta}{\sqrt{1 - \psi^2}} \right] \left[ \frac{\sqrt{2 - 2 \psi^2} \sin \left( \frac{\pi}{2} - \epsilon \right)}{\sqrt{2 - \psi^2 + \psi^2 \cos \left( \frac{\pi}{2} - \epsilon \right)}} \right] + \frac{\psi}{2} \tan \left( \frac{\pi}{2} - \epsilon \right) \ln \left[ \frac{2 \psi \cos \left( \frac{\pi}{2} - \epsilon \right) + \sqrt{4 - 2 \psi^2 + 2 \psi^2 \cos \left( \frac{\pi}{2} - \epsilon \right)}}{-2 \psi \cos \left( \frac{\pi}{2} - \epsilon \right) + \sqrt{4 - 2 \psi^2 + 2 \psi^2 \cos \left( \frac{\pi}{2} - \epsilon \right)}} \right]. \]  

(23)

Where Eq. (A.4) is the analytical expression of the first integral in Eq. (21). We have derived the steps to calculate Eq. (A.4) in the appendix for completeness. Applying the binomial expansion up to the first order of magnitude to the second addend of Eq. (21) designating the solution for \( \psi > 1 \) we get:

\[ -\left( \frac{\pi^2 v_F}{e^2} \right) \frac{\partial \chi_0(\psi)}{\partial \omega_F} = \left[ \frac{1}{\sqrt{1 - \psi^2}} \right. \left. \frac{\sin \theta}{\sqrt{1 - \psi^2}} \right] \left[ \frac{\psi_M \sqrt{2 - 2 \psi^2} \cos \left( 2 \arcsin \left( \frac{1}{\psi_M} \right) \right)}{2 \psi^2 - 1} \right] + \frac{\psi_M}{2 \sqrt{\psi_M^2 - 1}} \sin \left[ \frac{2 \psi \sqrt{1 - \frac{1}{\psi_M^2}} - \sqrt{4 - 2 \psi^2 + 2 \psi^2 \cos \left( 2 \arcsin \left( \frac{1}{\psi_M} \right) \right)}}{2 \psi \sqrt{1 - \frac{1}{\psi_M^2}} - \sqrt{4 - 2 \psi^2 + 2 \psi^2 \cos \left( 2 \arcsin \left( \frac{1}{\psi_M} \right) \right)}} \right]. \]  

(24)

Where Eq. (24) is the analytical expression of the second integral in Eq. (21). We solve Eq. (21) numerically and compare it with the analytical results derived in Eq. (A.4) and Eq. (24). The numerical results are shown as the dashed black lines and the analytical results are shown by the red solid line in Fig. 4(c). As is shown in Fig. 4(c) the two results are in good agreement with one another. By analyzing Fig. 4(c) we see that the second order addend of Eq. (9) of the dielectric response function diverges at \( \psi > 1 \) making the study of this point important. Higher order terms of the dielectric
response function present in Eq. (9) can be derived using the same analytical technique. These higher order terms will give us similar plots with a divergence at \( \psi \approx 1 \). However, due to the presence of the term \( \omega_F n \) in the numerator where \( \omega_F \ll 1 \) these higher order terms can be neglected. By knowing the first and second addend of Eq. (9) which are

![Figure 4](image)

Figure 4: (a) The dashed red lines on the left and the red dashed lines on the right are the terms containing the arc hyperbolic sinus terms in Eq. (11) and Eq. (16), respectively. These terms are solved numerically and add up to give the solid red lines on the left and right diagram. The solid blue and purple lines on the left and right diagram are respectively the remaining components of Eq. (11) and Eq. (16) that have also been solved numerically. Adding the solid-colored lines, we get the solid black lines numbered (I) and (I') which are respectively the numerical solutions of Eq. (11) and Eq. (16). (b) Comparing the numerical and analytical solutions for the static dielectric response function of a 2D Dirac crystal at \( T = 0 \) K. We see that there is good agreement between the two solution and we also observe a cuspid near the FSN at \( \psi \approx 1 \). (c) Comparing the numerical and analytical solutions for the second addend of the dielectric response function which contains the phonon energy for a 2D Dirac crystal at \( T = 0 \) K. We see that there is a good agreement between the two solutions and also observe a strong variation near the FSN at \( \psi \approx 1 \).

respectively the static dielectric response function and the dielectric response function at nonzero phonon energy we can write the total dielectric response function in the two regions of \( \psi < 1 \) and \( \psi > 1 \). For the region \( \psi < 1 \) we insert the values derived for \( \chi_0(\psi) \) Eq. (15), and \( \frac{\partial \chi_0(\psi)}{\partial \omega_F} \) Eq. (A.4), into Eq. (9). Therefore, the analytical solution of the total dielectric response function of a 2D Dirac crystal for \( \psi < 1 \) is equal to:

\[
\chi_{\omega_F}(\psi) = - \left( \frac{2E_F e^2}{\pi^2 \omega_F^2} \right) \lim_{\epsilon \to 0} \left[ 0.59 + \frac{3}{32} \left( \pi \psi + \sqrt{1 - \psi^2} \ln \left( \frac{1 - \psi - \epsilon}{1 + \psi + \epsilon} \right) \right) \right] +
\]

\[
\omega_F \cdot \frac{1}{\sqrt{1 - \psi^2}} \tan \left( \frac{\pi}{2} - \epsilon \right) \ln \left[ \frac{\sqrt{2 - 2\psi^2} \sin \left( \frac{\pi}{2} - \epsilon \right)}{\sqrt{2 - \psi^2} \cos \left( \pi - 2\epsilon \right)} \right] +
\]

\[
\frac{\psi}{2} \tan \left( \frac{\pi}{2} - \epsilon \right) \ln \left[ \frac{2\psi \cos \left( \frac{\pi}{2} - \epsilon \right) + \sqrt{4 - 2\psi^2 + 2\psi^2 \cos \left( \pi - 2\epsilon \right)}}{-2\psi \cos \left( \frac{\pi}{2} - \epsilon \right) + \sqrt{4 - 2\psi^2 + 2\psi^2 \cos \left( \pi - 2\epsilon \right)}} \right] \right) \right). \quad (25)
\]
On the dielectric response function and phonon self-energy of acoustic phonons in 2D Dirac crystals

And for the region \( \psi > 1 \) we insert the values derived for \( \chi_0(\psi) \) Eq.(20), and \( \frac{\partial \chi_0(\psi)}{\partial w_F} \) Eq.(24), into Eq.(9). Therefore, the analytical solution of the total dielectric response function of a 2D Dirac crystal for \( \psi > 1 \) is:

\[
\chi_w(\psi) = -\left( \frac{2E_Fe^2}{\pi \psi^2} \right) \left( \frac{0.59}{\psi} + \frac{3[\pi \psi + \sqrt{1-\psi^2} \ln \left( \frac{1-\psi}{1+\psi} \right)]}{32\psi} \right) + w_F \cdot \left( \frac{1}{\sqrt{1-\psi^2}} \right) \operatorname{atanh} \left[ \frac{\sqrt{2-2\psi^2}}{\psi M \sqrt{2-\psi^2+\psi^2 \cos \left( 2 \arcsin \left( \frac{1}{\psi M} \right) \right)}} \right] + \frac{\psi M}{2 \sqrt{1-\psi^2}} \ln \left[ \frac{-2\psi \sqrt{1-\frac{1}{\psi M}} + \sqrt{4-2\psi^2+2\psi^2 \cos \left( 2 \arcsin \left( \frac{1}{\psi M} \right) \right)}}{2\psi \sqrt{1-\frac{1}{\psi M}} + \sqrt{4-2\psi^2+2\psi^2 \cos \left( 2 \arcsin \left( \frac{1}{\psi M} \right) \right)}} \right].
\]

We have therefore derived the analytical expression for the dielectric response function of a 2D Dirac crystal in the two regions of \( \psi < 1 \) and \( \psi > 1 \) at \( T = 0 \) K. We can derive the dielectric response function of a 2D Dirac crystal for \( T \neq 0 \) K by employing Eq.(8) and following the same procedure.

Figure 5: The dielectric response function in the 4 graphs (a-d) for different values of \( \tau = (k_B T/2E_F) \) where the solid red lines are the analytical solution, and the dashed black lines are the numerical solution. The analytical solution is done by assuming the Fermi-Dirac distribution function to be a “double step” function while the numerical solution makes no such approximations. We observe that although the analytical solution always has two cuspidal points the numerical solution only has one cuspidal point for \( \tau \ll 1 \) and as we increase \( \tau \) the single cuspidal point in the numerical solution vanishes. Therefore, the two cuspidal points derived analytically are an artefact of our solution which is caused by using a “double step” function to approximate the Fermi-Dirac distribution.

For deriving the dielectric response function at \( T = 0 \) K we approximate the Fermi-Dirac distribution by a “single step” function. However, to derive the dielectric response function at higher temperatures we employ Eq.(8) where we approximate the Fermi-Dirac distribution with a “double step” function. This results in the dielectric response function to have two integrals with their bounds shown by the two purple shaded regions depicted in Fig. 2(c). Each
of these two integrals can be solved analytically by following the same procedure we used to solve the integral of the dielectric response function at $T = 0$ K. To study the dielectric response function for $T \neq 0$ K we also define the variable $\tau = (k_B T / 2E_F)$ presented in Eq. (1). The static dielectric response function, $\chi_0(\psi)$, of a 2D Dirac crystal derived analytically using the “double step” function for $T \neq 0$ K is shown in Fig. 5(a-d) by the solid red lines. We observe that although $\chi_0(\psi)$ at $T = 0$ K has only one cuspidal point, for $T \neq 0$ K the number of cuspidal points increases to two with each integral giving us a separate cuspid. By analyzing Fig. 5(a-d) we observe that as we increase the temperature for a given Fermi energy the distance between the cuspidal points increases. This is because as we increase $\tau$ the regions covered by the two integrals in Eq. (8) get further apart from each other which results in the cuspidal points of the two integrals to also get further apart from one another. To study the nature of the two cuspidal points we derive $\chi_0(\psi)$ numerically without applying any approximations to the Fermi-Dirac distribution function and compare it with the analytical solution. The numerical solution is shown in Fig. 5(a-d) by the black dashed lines. By analyzing the numerical solution we observe that we only have one cuspidal point for $\psi << 1$ and the cuspidal point starts to vanish as we increase $\tau$. This is not the case for the analytical solution where although as we increase $\tau$ the value of the cuspidal points decrease but they do not vanish. We therefore conclude that the two cuspidal points derived analytically are an artefact of our solution which is caused by using a “double step” function to approximate the Fermi-Dirac distribution. By analyzing Fig. 5(a-d) we observe that the analytical expression using the “double step” function gives us accurate estimations for $\chi_0(\psi) << 1$, and as we increase $\tau$ the analytical solution becomes less accurate, however, it still remains within a good approximation range of the numerical value. This is because although the two cuspid in the analytical solution don’t vanish but their values decrease tending towards the numerical solution.

By deriving the dielectric response function of 2D Dirac crystals using the Lindhard model we are able to calculate the phonon line width of these class of condensed matter systems more accurately. To this end we first write the first order phonon self energy as a function of $\psi$ as follow:

$$\Pi(\psi) = \frac{1}{\sqrt{N}} \sum_{\psi} |M_{\psi}|^2 \frac{f_{\xi_- \psi} - f_{\xi_+ \psi}}{E_{\xi_+ \psi} - E_{\xi_- \psi} - i \hbar \omega},$$

where $|M_{\psi}|$ is the electron-phonon matrix element, and $N$ is the number of points in the summation over $\psi$. The finite line width or inverse lifetime of a phonon mode is connected to the imaginary part of the phonon self-energy and can be written as:

$$\gamma_\psi = -2 Im \Pi(\psi) = \frac{2\pi}{\sqrt{N}} \sum_{\psi} |M_{\psi}|^2 \left( f_{\xi_- \psi} - f_{\xi_+ \psi} \right) \delta \left( \hbar \omega + E_{\xi_- \psi} - E_{\xi_+ \psi} \right).$$

To calculate the phonon line width we write the electron-phonon matrix element $|M_{\psi}|$, as a function of the screening potential in the following manner:

$$|M_{\psi}| = \frac{1}{\Omega} \sum_{\psi} \left( \frac{2k_F \hbar^2}{2mc \pi^2} \right)^{1/2} \phi_s(\psi),$$

where $\Omega$ is the unit cell area of the 2D Dirac crystal, $m$ is the ion mass, and $\phi_s(\psi)$ is the screening potential. The screening potential is a function of the dielectric response function and is equal to:

$$\phi_s(\psi) = \left( \frac{1}{2k_F} \right) \frac{2\pi Q^2}{\psi - 2\pi \chi(\psi)},$$

where $Q$ is the ion charge. By inserting Eq. (29) and Eq. (30) into Eq. (28) we get the phonon line width as a function of $\psi$ in the following manner:

$$\gamma_\psi = \frac{2\pi^3 N \hbar^2 Q^4}{mck_F} \frac{1}{\sqrt{N}} \sum_{\psi} \psi \left( f_{\xi_- \psi} - f_{\xi_+ \psi} \right) \delta \left( c\psi + E_{\xi_- \psi} - E_{\xi_+ \psi} \right).$$

We observe that the role of the dielectric response function in the denominator of Eq. (31) is essential in determining the phonon line width accurately. By knowing $\chi_\psi$, we can write the phonon line width as a function of $\psi$ for acoustic phonons with dispersive energy wavelength relationships. At zero temperature we solve the difference between the Fermi-Dirac distributions using a single step function and inserting the dielectric response function derived from Eq. (8) and Eq. (26). For nonzero temperatures we use the double step function and insert the value of the dielectric response function derived from Eq. (8) for different temperatures. In the next section we analyze the dielectric response function and the phonon line width of 2D Dirac crystals extensively.
4 Discussion

The electron-phonon coupling used to derive the phonon self-energy in our calculation is more sophisticated than the customarily used jellium model[31]. Jellium models disregard the lattice structure and only consider free electrons. Furthermore, the ions in the jellium are approximated into a uniform background of positive charges resulting in a constant electrostatic potential. Such a model is suitable for studying electron-electron and electron-phonon interactions in metals but not in 2D Dirac crystals where the electrostatic potential undergoes strong fluctuations. Specifically, in 2D Dirac crystals the electronic dispersion is linear (i.e. $E = v_F k$ as opposed to $E = \hbar^2 k^2 / 2m$ as in the jellium). In order to consider this, the electrostatic potential is assumed to be Lindhard-screened, as in Eq. (30). This approach, which also consider the specific crystalline structure of 2D Dirac crystals leading to Fermi-level electrons at the Brillouin-zone K-point, has been used by us to derive the phonon line width in our model as in Eq. (31). It is worthwhile noting that the non-uniformity of the electrostatic potential plays a critical role in determining the phonon line width at wavenumbers $q$ approaching Fermi surface nesting conditions, where we anticipate it to increase linearly with the temperature in agreement with the experimental results[72]. This would not be the case if the electron-phonon coupling would have considered at the approximation level of the jellium model.

We will now analyze the dielectric response function for different values $w_F$ and discuss the generality of our results for 2D Dirac crystals. We will further compare the static dielectric response function of a 2D Dirac crystal with that of a Free Fermion gas. As shown in Eq. (9) the dielectric response function of a 2D Dirac crystal is the sum of the static term with zero phonon energy, $w_F = 0$, and higher order terms where the phonon energy is nonzero, $w_F \neq 0$. In Fig. (a) we plot the dielectric response function of a 2D Dirac crystal for $\tau \approx 0$, at different values of $w_F$ as a function of $\psi$. By analyzing Fig. (a) and comparing the red dashed line where $w_F = 0$, with the blue and orange dashed lines where $w_F \neq 0$, we observe that at the two regions $\psi < 1$ and $\psi > 1$, the static term is dominant, however, near the FSN region, $\psi \approx 1$, the higher order terms become more dominant. Therefore, by approximating the Fermi-Dirac distribution by a multi-step function at finite temperatures we observe that the dielectric response function diverges near the FSN at the point $\psi \approx 1$ even for small values of $w_F \neq 0$ where the speed of sound is small, albeit non-negligible, over the Dirac-electron Fermi velocity. It is only when $w_F = 0$ and we assume that we are in a static regime that the strong variation in the dielectric response function vanishes, and we only have a cuspid. Hence, when studying the dielectric response function of 2D Dirac crystals in certain physical settings it is important not to simplify the problem to the static case where the energy of acoustic phonons is put equal to zero. Such physical settings can be the study of the thermal and electrical variations of 2D Dirac crystals caused by electron-phonon interactions[27]. Also, when studying the higher order terms of electron-phonon interactions in 2D Dirac crystals with the employment of a Fermion propagator, [31, 73] which has a time component, we have to consider the energy of the phonons and cannot work in the static regime[27]. By further analyzing Fig. 6(a) we observe that the difference in the dielectric response function of various 2D Dirac crystals with different values of $w_F$ [67, 68, 69, 74], is negligible showing the generality of our solution.

We further compare the static dielectric response function, $\chi_0(\psi)$, of a 2D Dirac crystal with that of a Fermion gas at $T = 0$ K [41]. This is shown in Fig. (b). We observe that $\chi_0(\psi)$ of a 2D Dirac crystals is reminiscent of that of a 1D and a 2D Fermion gas. As can be seen from Fig. (b) $\chi_0(\psi)$ of a 2D Dirac crystal lies between that of a 1D and 2D Fermion gas not diverging near the FSN like the former and not approaching it along a constant line like the latter. Hence, when studying $\chi_0(\psi)$ of a 2D Dirac crystal it is important to distinguish it from a 2D Fermi gas. While $\chi_0(\psi)$ of a 2D Fermi gas approaches the FSN along a constant line for 2D Dirac crystals $\chi_0(\psi)$ increases reaching a maximum at $\psi = 1$. This makes the study of $\chi_0(\psi)$ for 2D Dirac crystals more intricate in the FSN region. By further analyzing Fig. (b) we observe that in the region of $\psi >> 1$, $\chi_0(\psi)$ of the Fermi gas and 2D Dirac crystals are both proportional to $1/\psi$ which is equivalent to the result we get when we use the Thomas-Fermi approach. Therefore, the Thomas-Fermi model for calculating the dielectric response function at long wavelengths is equal for 2D Dirac crystals and Fermi gasses.
Figure 6: (a) The dielectric response function of a 2D Dirac crystal at $T = 0$ K for different values of $w_F$. We observe that the dielectric response function diverges near the FSN at the point $\psi \approx 1$ even for small values of $w_F \neq 0$. The negligible difference in the dielectric response function of various 2D Dirac crystals with different values of $w_F$ shows the generality of our solution for 2D Dirac crystals. (b) Comparing $\chi_0(\psi)$ of a 2D Dirac crystal with that of a 1D and 2D Fermion gas at $T = 0$ K. We observe that $\chi_0(\psi)$ of a 2D Dirac does not follow a constant line like the 2D Fermi gas and it increases reaching a maximum at the FSN point, making the study of 2D Dirac crystals more intricate.

We are able to solve the phonon line width, Eq.(31) numerically for different 2D Dirac crystals by performing the summation over $\psi$. To analyze the correlation between the phonon line width and the phonon wave number we derive $\gamma_\psi$ for different values of $\psi$ with $0.2 < \psi < 1$. Fig. 7(a) shows that there is a linear correlation between $\gamma_\psi$ and $\psi$, with the linear fit having the coefficient of determination $R^2 = 0.99$. We therefore conclude that similar to the linear proportionality between the spectral energy and the fermion wave number, $E \propto k$, there is also a linear correlation between the phonon line width and the phonon wave number, $\gamma_\psi \propto q$, in 2D Dirac crystals. We further compare the phonon line width approaching the FSN condition of 2D Dirac crystals at different temperatures in the static scenario. By studying Fig. 7(b) we observe a linear increase in the phonon line width or a linear decrease in the lifetime of the phonon mode as we increase the temperature. This suggests that at higher temperatures where the lattice vibrations increase the lifetime of the phonon mode decreases. Our results further match the experimental data collected on germanium [72] which further confirms our results.

Figure 7: (a) The phonon line width vs $\psi$ in 2D Dirac crystals. The linear fit has the coefficient of determination $R^2 = 0.99$, indicating a linear correlation between the phonon line width and the phonon wave number. (b) The phonon line width near the FSN of 2D Dirac crystals at different temperatures. The linear fit has the coefficient of determination $R^2 = 0.99$, indicating a linear correlation between the phonon line width and the lattice temperature.

5 Conclusion

In this paper we derive the dielectric response function of 2D crystals from acoustical phonons by using the Lindhard model. We see that, different from free-electron systems, in 2D Dirac crystals the dielectric response function exhibits a cuspidal point near the FSN region in the static case were the phonon energy has been put equal to zero. We further
observe when the phonon energy has not been put equal to zero the dielectric response function of a 2D Dirac crystal varies strongly near the FSN region even when the speed of sound is small, albeit nonnegligible, over the Dirac-electron Fermi velocity. We therefore show that the common approach for calculating the dielectric response function of 2D Dirac crystals by putting the energy of the phonons equal to zero is not accurate. We also show the generality of our solution for different 2D Dirac crystals with different Fermi velocities. We further use our results from calculating the dielectric response function of 2D Dirac crystals to derive their phonon line width. We observe that the phonon line width increases as we move towards the FSN and as we go towards higher temperatures which matches the experimental work done in the literature.

***

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A Appendix: Detailed calculation of the second addend of the dielectric response function

The second addend of the dielectric response function at zero temperature for \( \psi < 1 \) is:

\[
- \left( \frac{\pi^2 v_F}{c^2} \right) \frac{1}{2k_F} \frac{\partial}{\partial w_F} \chi_0(\psi) = \lim_{\epsilon \to 0} \left[ \int_0^{\frac{\pi}{2} - \epsilon} d\theta \int_{-\frac{\pi}{2}}^{\frac{\pi}{2} + \frac{1}{2} \sqrt{\psi^2 - \psi^4 \sin^2 \theta}} d\xi \frac{\xi \psi d\xi}{\psi^2 \cos \theta} \right].
\] (A.1)

To solve the integral analytically we use the binomial expansion. Using the binomial expansion up to the first order the denominator can be written as:

\[
2(\xi^2 + \psi^2)^2 (1 - \frac{1}{2} \frac{\psi^2 \xi^2 \cos \theta^2}{(\xi^2 + \psi^2)^2}) = \frac{\psi^2 \xi^2 \cos \theta^2}{(\xi^2 + \psi^2)^2}.
\] (A.2)

We therefore have:

\[
\lim_{\epsilon \to 0} \left[ \int_0^{\frac{\pi}{2} - \epsilon} d\theta \int_{-\frac{\pi}{2}}^{\frac{\pi}{2} + \frac{1}{2} \sqrt{\psi^2 - \psi^4 \sin^2 \theta}} d\xi \frac{\xi \psi d\xi}{\psi^2 \cos \theta} \right] = \int_0^{\frac{\pi}{2} - \epsilon} d\theta \int_{-\frac{\pi}{2}}^{\frac{\pi}{2} + \frac{1}{2} \sqrt{\psi^2 - \psi^4 \sin^2 \theta}} \frac{\psi^2 \ln \left( \frac{\psi \cos \theta + \sqrt{1 - \psi^2 \sin^2 \theta}}{-\psi \cos \theta + \sqrt{1 - \psi^2 \sin^2 \theta}} \right) + \left( 2 \psi \cos \theta \sqrt{1 - \psi^2 \sin^2 \theta} \right)}{2 \psi \cos \theta^2} \right]
\] (A.3)

Finally integrating Eq. (A.3) over \( \theta \) we have:

\[
\lim_{\epsilon \to 0} \left[ \int_0^{\frac{\pi}{2} - \epsilon} \frac{1}{2 \psi \cos \theta^2} \right] \right] = \lim_{\epsilon \to 0} \left[ \frac{1}{\sqrt{1 - \psi^2}} \ln \left( \frac{\sqrt{2 - 2 \psi^2} \sin \left( \frac{\pi}{2} - \epsilon \right) + 4 - 2 \psi^2 + 2 \psi^2 \cos \left( \pi - \epsilon \right)}{\sqrt{2 - 2 \psi^2 + 2 \psi^2 \cos \left( \pi - \epsilon \right)}} \right)
\] (A.4)

The same derivations can be made for \( \psi > 1 \).

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