Supplementary material for

Anomalous Plasmons in Two-Dimensional Dirac Nodal-Line Lieb Lattice

Chao Ding, Han Gao, Wenhui Geng, Mingwen Zhao*

School of Physics & State Key Laboratory of Crystal Materials, Shandong University,

Jinan 250100, Shandong, China
S1. INTRA-BAND POLARIZATION FUNCTION

In this section, we will systematically derive the intra-band polarization function and its long-wavelength limit under the random-phase approximation (RPA) approach.

The intra-band polarization function of band $E_{k,n}$ is \[1, 2\]

$$
\Pi_n(q, \omega) = \frac{g_s}{V} \sum_k \frac{f(E_{k,n}) - f(E_{k+q,n})}{E_{k,n} - E_{k+q,n} + \hbar \omega + i\eta} \left| \langle k, n | q, k, n \rangle \right|^2 .
$$

(1)

We assume $\left| \langle k, q, n | k, n \rangle \right|^2 \approx 1$ in our discussion. Because of $E_{k,n} = E_{k+G,n}$ ($G$ is an arbitrary reciprocal lattice vector.), a standard replacement $k \rightarrow k - q$ can be performed in the term containing $f(E_{k+q,n})$. This gives

$$
\Pi_n(q, \omega) = \frac{g_s}{V} \sum_k \left( \frac{f(E_{k,n})}{E_{k,n} - E_{k+q,n} + \hbar \omega + i\eta} - \frac{f(E_{k,n})}{E_{k+q,n} - E_{k,n} + \hbar \omega + i\eta} \right) .
$$

(2)

Assuming that $E_{k,n} = E_{-k,n}$,

$$
\Pi_n(q, \omega) = \frac{g_s}{V} \sum_k \left( \frac{f(E_{k,n})}{E_{k,n} - E_{k+q,n} + \hbar \omega + i\eta} - \frac{f(E_{k,n})}{E_{k+q,n} - E_{k,n} + \hbar \omega + i\eta} \right) .
$$

(3)

Eq. (3) can also be written as an integral, this gives

$$
\Pi_n(q, \omega) = \frac{g_s}{(2\pi)^2} \int \left( \frac{f(E_{k,n})}{E_{k,n} - E_{k+q,n} + \hbar \omega + i\eta} - \frac{f(E_{k,n})}{E_{k+q,n} - E_{k,n} + \hbar \omega + i\eta} \right) d^2 k .
$$

(4)

Now, let $\eta \rightarrow 0$, we obtain

$$
\Pi_n(q, \omega) = \frac{g_s}{(2\pi)^2} \int f(E_{k,n}) \frac{2(E_{k+q,n} - E_{k,n})}{\hbar^2 \omega^2 - (E_{k+q,n} - E_{k,n})^2} d^2 k .
$$

(5)

In the long-wavelength limit, where $\hbar \omega \gg \left| E_{k+q,n} - E_{k,n} \right|$, 

$$
\Pi_n(q, \omega) = \frac{1}{\pi \hbar^2 \omega^2} \int f(E_{k,n}) (E_{k+q,n} - E_{k,n}) d^2 k .
$$

(6)

S2. DETAILS OF THE ELECTRON-HOLE MODEL
We supposed that the two-dimensional (2D) DNL is formed from two crossing bands described by parabolic dispersion relations as follows:

\[
E_{k,1} = \frac{\hbar^2}{2m_1^*} k^2, \quad E_{k,2} = -\frac{\hbar^2}{2m_2^*} k^2 + E_0, \tag{7}
\]

with \( m_1^* > 0, m_2^* > 0 \) and \( E_0 > 0 \). Assuming that electron wavefunctions of the two bands are orthogonal, the inter-band transition of electrons is prohibited. We therefore only considered the intra-band contribution to the polarization functions.

Under long-wavelength limit, the polarization function of band \( E_{k,1} \) is

\[
\Pi_1(q, \omega) = \frac{1}{\pi^2 \hbar^2 \omega^2} \int_{E_{k,1} < E_f} (E_{k+q,1} - E_{k,1}) \delta^2(k) \, d^2k. \tag{8}
\]

Due to the region where \( E_{k,1} < E_f \) has the symmetry of space inversion,

\[
\Pi_1(q, \omega) = \frac{1}{2\pi^2 \hbar^2 \omega^2} \int_{E_{k,1} < E_f} (E_{k+q,1} + E_{k-q,1} - E_{k,1} - E_{-k,1}) \delta^2(k) \, d^2k. \tag{9}
\]

Considering that \( E_{k,1} = E_{-k,1} \), Eq. (9) can also be written as

\[
\Pi_1(q, \omega) = \frac{1}{2\pi^2 \hbar^2 \omega^2} \int_{E_{k,1} < E_f} (E_{k+q,1} + E_{k-q,1} - 2E_{k,1}) \delta^2(k) \, d^2k. \tag{10}
\]

Considering the Taylor's expansion to the second order,

\[
E_{k+q,1} - E_{k,1} \approx \nabla_k E_{k,1} \cdot q + \frac{1}{2} (q \cdot \nabla_k)^2 E_{k,1}. \tag{11}
\]

Combining Eq. (7), Eq. (10) and Eq. (11), we finally obtain

\[
\Pi_1(q, \omega) = \frac{g_s}{4\pi \omega^2} \frac{q^2}{m_1^*} k_{1f}^2, \tag{12}
\]

where \( k_{1f} \) is the Fermi wave vector of band \( E_{k,1} \). The polarization function can also be written as \( \Pi_1(q, \omega) = \frac{n_1 q^2}{m_1^* \omega} \), where \( n_1 = \frac{g_s}{4\pi} k_{1f}^2 \) is the carrier density of band \( E_{k,1} \).

It is exactly the polarization function of the 2D electron gas [3].
The polarization function of band $E_{k,2}$ can be derived in a similar way. Under long-wavelength limit,

$$
\Pi_2(q, \omega) = \frac{1}{\pi^2 \hbar^2 \omega^2} \int_{E_{k,2}} (E_{k+q,2} - E_{k,2}) d^2k.
$$

(13)

Assuming that band $E_{k,2}$ is periodic of reciprocal lattice vector, we obtain

$$
\int_{\Omega'} (E_{k+q,2} - E_{k,2}) d^2k = 0, \text{ where } \Omega' \text{ is the Brillouin zone. Hence,}
$$

$$
\Pi_2(q, \omega) = -\frac{1}{2\pi^2 \hbar^2 \omega^2} \int_{E_{k,2} > E_f} (E_{k+q,2} + E_{k-q,2} - 2E_{k,2}) d^2k
$$

(14)

Combining Eq. (7) and Eq. (14), and performing a second order Taylor’s expansion similar to Eq. (11), we can obtain

$$
\Pi_2(q, \omega) = \frac{g_s}{4\pi \omega} \frac{q^2}{m_2^2} k_{2f}^2,
$$

(15)

where $k_{2f}$ is the Fermi wave vector of band $E_{k,2}$. Then, we obtain the polarization function of this system

$$
\Pi(q, \omega) = \Pi_1(q, \omega) + \Pi_2(q, \omega) = \frac{g_s}{4\pi \omega} \left( \frac{k_{1f}^2}{m_1^2} + \frac{k_{2f}^2}{m_2^2} \right) q^2.
$$

(16)

Considering that $\frac{\hbar^2}{2m_1} k_{1f}^2 = -\frac{\hbar^2}{2m_2} k_{2f}^2 + E_0 = E_f$, we finally obtain

$$
\Pi(q, \omega) = \frac{g_s}{2\pi \omega} \frac{E_0}{\hbar^2} q^2.
$$

(17)

The dispersion of plasmon mode of this system can be written as

$$
\hbar \omega = \sqrt{\frac{g_s e^2 E_0}{\varepsilon_r} \sqrt{q}}.
$$

(18)
S3. DETAILS OF THE TIGHT-BINDING MODEL FOR 2D PLASMONS IN LIEB LATTICE

We first derive the intra-band polarization function of $E_{k,1}$.

The dispersion of band $E_{k,1}$ is

$$E_{k,1} = -2t(c\cos k_x + \cos k_y).$$  (19)

Under long-wavelength limit, the polarization function $\Pi_1(q,\omega)$ is

$$\Pi_1(q,\omega) = \frac{1}{\pi^2 H^2 \omega^2} \int_{\Omega} (E_{k+q,1} - E_{k,1}) d^2k,$$  (20)

where $\Omega_1$: $\cos(k_x) + \cos(k_y) > \mu(\mu = \frac{E_f}{2t})$, is the region where $E_{k,1} < E_f$, as shown by shaded areas in Fig. 2(c). Assuming the whole Brillouin zone is $\Omega$, and $\Omega'$ is the region shown by white in Fig. 2(c), hence

$$\int_{\Omega} (E_{k+q,1} - E_{k,1}) d^2k = \int_{\Omega} (E_{k+q,1} - E_{k,1}) d^2k - \int_{\Omega'} (E_{k+q,1} - E_{k,1}) d^2k.$$  (21)

Considering that the band $E_{k,1}$ is periodic of reciprocal lattice vector, we can obtain

$$\int_{\Omega} (E_{k+q,1} - E_{k,1}) d^2k = 0,$$  hence

$$\int_{\Omega'} (E_{k+q,1} - E_{k,1}) d^2k = -\int_{\Omega} (E_{k+q,1} - E_{k,1}) d^2k.$$  (22)

The region $\Omega'$ is bounded by $\cos(k_x) + \cos(k_y) = \mu$, which contains

$$k_{x1} = \arccos(\mu + 1),$$
$$k_{x2} = 2\pi - \arccos(\mu + 1),$$
$$k_{y1} = \arccos(\mu - \cos k_x),$$
$$k_{y2} = 2\pi - \arccos(\mu - \cos k_x),$$  (23)

with $\mu < 0$. Substituting Eq. (19) into Eq. (20) and using the relationship of Eq. (22), we get
\[
\Pi_1(q, \omega) = -\frac{2t}{\pi^2 \hbar^2 \omega^2} \left( \int_{\Omega_k} [(1 - \cos q_x) \cos k_x + (1 - \cos q_y) \cos k_y] d^2k \right) \\
+ \int_{\Omega_k} (\sin k_x \sin q_x + \sin k_y \sin q_y) d^2k.
\] (24)

To calculate Eq. (24), the following calculation was performed:

\[
\int_{\Omega_k} \cos k_x d^2k = \int_{\Omega_k}^k \cos k_x dk_x = -4\pi \sqrt{-\mu^2 - 2\mu - 2F_1(\mu)},
\]

\[
\int_{\Omega_k} \cos k_y d^2k = \int_{\Omega_k} \cos k_y dk_y = \cos \theta d^2k,
\]

\[
\int_{\Omega_k} \sin k_x d^2k = \int_{\Omega_k} \sin k_y d^2k = 0,
\]

where \( F_1(x) \) is a function defined as

\[
F_1(x) = \int_{\arccos(x+1)}^{2\pi \arccos(x+1)} \cos \theta \arccos(x - \cos \theta) d\theta.
\] (26)

Substituting Eq. (25) into Eq. (24), we finally obtain

\[
\Pi_1(q, \omega) = \frac{1}{\pi^2 \hbar^2 \omega^2} \alpha (2 - \cos q_x - \cos q_y),
\] (27)

with \( \alpha = 8\pi t \sqrt{-\mu^2 - 2\mu + 4tF_1(\mu)} \).

The intra-band polarization function of \( E_{k,2} \) can be derived in a similar way.

The dispersion of band \( E_{k,2} \) is

\[
E_{k,2} = \Delta - 4t' \sin \frac{k_x}{2} \sin \frac{k_y}{2}.
\] (28)

And the polarization function \( \Pi_2(q, \omega) \) under long-wavelength limit is

\[
\Pi_2(q, \omega) = \frac{1}{\pi^2 \hbar^2 \omega^2} \int_{\Omega_2} (E_{k+q,2} - E_{k,2}) d^2k,
\] (29)

where \( \Omega_2: \sin \left( \frac{k_x}{2} \right) \sin \left( \frac{k_y}{2} \right) > \nu \left( \frac{\Delta - E_{k,2}}{4t'} \right) \), is the region where \( E_{k,2} < E_f \), as shown by shaded areas in Fig. 2(d). The region \( \Omega_2 \) is bounded by
Substituting Eq. (28) into Eq. (29), then we get

\[
\Pi_2(q, \omega) = \frac{-4t'}{\pi^2 \hbar^2 \omega^2} \left( \int_{\Omega_2} (\cos \frac{q_x}{2} \cos \frac{q_y}{2} - 1) \sin \frac{k_x}{2} \sin \frac{k_y}{2} d^2k \right.
\]

\[
+ \int_{\Omega_2} \sin \frac{k_x}{2} \cos \frac{k_y}{2} \cos \frac{q_x}{2} \sin \frac{q_y}{2} d^2k
\]

\[
+ \int_{\Omega_2} \cos \frac{k_x}{2} \sin \frac{k_y}{2} \sin \frac{q_x}{2} \cos \frac{q_y}{2} d^2k
\]

\[
+ \int_{\Omega_2} \cos \frac{k_x}{2} \cos \frac{k_y}{2} \sin \frac{q_x}{2} \sin \frac{q_y}{2} d^2k) \right)
\]

To calculate Eq. (31), the following calculation was performed:

\[
\int_{\Omega_2} \sin \frac{k_x}{2} \sin \frac{k_y}{2} d^2k = \int_{\Omega_2} \frac{k_x}{2} dk_x \int_{\Omega_2} \sin \frac{k_y}{2} dk_y = 16F_2(\nu),
\]

\[
\int_{\Omega_2} \sin \frac{k_x}{2} \cos \frac{k_y}{2} d^2k = \int_{\Omega_2} \cos \frac{k_x}{2} \sin \frac{k_y}{2} d^2k = 0,
\]

\[
\int_{\Omega_2} \cos \frac{k_x}{2} \cos \frac{k_y}{2} d^2k = 0,
\]

where \( F_2(x) \) is a function defined as

\[
F_2(x) = \int_{0}^{\frac{\pi}{2}} \frac{\sqrt{1 - x^2 - \sin^2 \eta} d\eta}{\sqrt{1 - x^2 - \sin^2 \eta}}.
\]

Substituting Eq. (32) into Eq. (31), we finally obtain

\[
\Pi_2(q, \omega) = \frac{1}{\pi^2 \hbar^2 \omega^2} \beta (1 - \cos \frac{q_x}{2} \cos \frac{q_y}{2}),
\]

with \( \beta = 64t'F_2(\nu) \).

Then the polarization function of this system can be written as
\[ \Pi(q, \omega) = \Pi_1(q, \omega) + \Pi_2(q, \omega) \]
\[ = \frac{1}{\pi \hbar^2 \omega^3} \left[ \alpha (2 - \cos q_x - \cos q_y) + \beta (1 - \cos \frac{q_x}{2} \cos \frac{q_y}{2}) \right]. \] 

(35)

The plasmon dispersion identified as the roots of \( \varepsilon(q, \omega) = 0 \) is

\[ \hbar \omega = \sqrt[\varepsilon(q, \pi)]{\alpha \left( 2 - \cos q_x + \cos q_y \right) + \beta \left( 1 - \cos \frac{q_x}{2} \cos \frac{q_y}{2} \right)}. \]

(36)

Making the substitution \( \cos x \to 1 - \frac{1}{2} x^2 \), Eq. (36) can be reduced to:

\[ \hbar \omega \approx \gamma \sqrt{q}. \]

(37)

with \( \gamma = \sqrt[\varepsilon(q, \pi)]{\frac{2e^2}{4\pi t \sqrt{\mu^2 - 2\mu + 2tF_1(\mu) + 8t'F_2(\nu)}}}. \)

S4. SOME COMPUTATIONAL DETAILS OF TIGHT-BINDING MODEL

The parameters we use to calculate in Sec. III (B) are \( t = 0.5eV, t' = 2.7eV, \Delta = 10.84eV, \varepsilon_r = 1.5 \quad a = 3.278 \, \text{Å} \quad \eta = 0.05eV \). The tight-binding parameters come from fitting the bands of our TB model to Be\(_2\)C monolayer, as shown in Fig. S1. \( \varepsilon_r \), that we use to calculate is derived from fitting the plasmon dispersion of the more complicated TB model constructed by WANNIER90 [4] to the results of GPAW [5]. \( a \) is the lattice constant of Be\(_2\)C monolayer.

S5. ELECTRONIC BAND STRUCTURES OF DIFFERENT DOPPING LEVELS

The electronic band structures of pristine, hole-doped and electron-doped Be\(_2\)C monolayer are shown in Fig. S2.
Figure S1. Band structure obtained from TB model and density-functional theory calculations of Be$_2$C monolayer.

Figure S2. The electronic band structures of (a) pristine, (b) hole-doped and (c) electron-doped Be$_2$C monolayer, respectively.


