Theory of Plasmons for Two-Dimensional Materials in the Random Phase Approximation

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Abstract: A theory is derived for plasmons in two-dimensional (2D) materials by using three-dimensional (3D) plasmon theory, which was reported previously in the random phase approximation under high frequency conditions. When the 3D local electron density is expressed by the 2D local electron density n_{2D} multiplied by the delta function in the thickness direction, a self-consistent integral equation for the scalar potential is derived using only n_{2D} and the 2D Coulomb potential. The integral equation consists of the edge and planar plasmon terms which give their resonant frequencies. These frequencies are analytically calculated for uniform 2D atomic layers and nanodisks with step function-like electron densities at their edges. The light emission intensities from the nanodisks are also calculated. These frequencies are compared with those for the 2D and 3D Weyl fermions, i.e., massless Dirac fermions.

Keywords: plasmon; 2D material; Schrödinger fermion; Weyl fermion

1. Introduction

Surface plasmons can couple with photons to produce collective excitations, called surface plasmon polaritons and localized surface plasmons [1–7]. They can concentrate optical waves into regions that are much smaller than their wavelengths and can also greatly enhance their local electric fields at surface plasmon excitation energies. These effects make it possible to use them to fabricate nanoscale photonic devices and to greatly enhance detection sensitivities for optical measurements. A new field, called graphene plasmonics, has recently developed, where the electron density in graphene can be varied over a wide range by gating it to tune the plasmon resonance frequency [8–10]. The electrons (fermions) in graphene satisfy the two-dimensional (2D) Weyl equation, i.e., the massless Dirac equation.

Semiconducting and metal 2D materials such as transition metal dichalcogenides (TMDCs) have recently been noticed for their atomically thin electronics and photonics [11–13]. The electrons (fermions) in these materials satisfy the Schrödinger equation, unlike those in graphene. Plasmons in these 2D materials are also interesting because the electron density can be varied over a wide range by gating it to tune the plasmon resonance frequency.

The author has developed theories of three-dimensional (3D) localized plasmons in the random phase approximation (RPA) under high frequency conditions, where the coupling between the bulk and surface plasmons is properly considered in metal nanostructures [14–16]. In these theories, the local electron density in metal nanostructures plays an essential role in the plasmon excitations. They cannot be applied to the electron-hole pair excitation frequency region but are tractable for application to various configurations and large system sizes.

In this study, a theory of plasmons for 2D materials is derived from the 3D localized plasmon theories in the RPA under high frequency conditions. The calculated plasmon frequencies are also compared with those for the 2D and 3D Weyl fermions.

2. Theory of Two-Dimensional Plasmons

2.1. Derivation of 2D Plasmon Theory from the 3D One

Considering an effective potential $\varphi_{eff}(\mathbf{r}, \omega)$ and an external scalar potential $\varphi_{ext}(\mathbf{r}, \omega)$ within the 3D electrons in metal nanostructures at frequency ω, previous studies [14–16] have shown that they satisfy the following integral equation in the RPA under high frequency conditions, i.e., plasmon excitation condition for the quasi-static case in Gaussian units:

$$\varphi_{eff}(\mathbf{r}, \omega) = \varphi_{ext}(\mathbf{r}, \omega) + \frac{1}{m_e\omega^2} \int d\mathbf{r}_1 n(\mathbf{r}_1) \nabla_1 \frac{e^2}{|\mathbf{r}-\mathbf{r}_1|} \cdot \nabla_1 \varphi_{eff}(\mathbf{r}_1, \omega),$$
$$n(\mathbf{r}_1) = D\sum_n |\psi_n(\mathbf{r}_1)|^2 \theta(E_F - E_n), \tag{1}$$

where $e^2/|\mathbf{r} - \mathbf{r}_1|$ is the 3D Coulomb potential between the electrons, $\psi_n(\mathbf{r}_1)$ is the normalized single-electron wave functions in the metal nanostructures, which satisfy the Schrödinger equation, D is the number of degeneracy (spin and valley), θ is the step function, and E_F and E_n are the Fermi energy and the single electron energy, respectively. $n(\mathbf{r}_1)$ is the local electron density in the metal nanostructure, m_e and $-e$ are the electron mass and charge, and ∇_1 represents the gradient with respect to $\mathbf{r}_1$. The derivation of Equation (1) is described in Appendix A.

When the 3D electron density $n(\mathbf{r}_1)$ is expressed by $n(\mathbf{r}_1) \approx n_{2D}(\mathbf{X}_1)\delta(z_1)$, $\mathbf{r}_1 = (\mathbf{X}_1, z_1)$ where $n_{2D}(\mathbf{X}_1)$ is the 2D local electron density and $\delta(z_1)$ is the delta function for the coordinate z_1, the following equation is derived by using the property $\partial \varphi_{eff}(\mathbf{r}_1, \omega)/\partial z_1 = 0$ at $z_1 = 0$ due to the mirror symmetry in the z_1 direction:

$$\varphi_{eff}(\mathbf{X}, \mathbf{z}; \omega) = \varphi_{ext}(\mathbf{X}, \mathbf{z}; \omega) + \frac{e^2}{m_e\omega^2} \int d\mathbf{X}_1 n_{2D}(\mathbf{X}_1) \nabla_{\mathbf{X}_1} \frac{1}{|\mathbf{X}+\mathbf{z}-\mathbf{X}_1|} \cdot \nabla_{\mathbf{X}_1} \varphi_{eff}(\mathbf{X}_1, 0; \omega). \tag{2}$$

Putting $z = 0$ and integrating Equation (2) by parts gives the following 2D integral equation:

$$\begin{aligned} \varphi_{eff}(\mathbf{X}, \omega) &= \varphi_{ext}(\mathbf{X}, \omega) - \frac{e^2}{m_e\omega^2} \int d\mathbf{X}_1 \, \varphi_{eff}(\mathbf{X}_1, \omega) \nabla_{\mathbf{X}_1} n_{2D}(\mathbf{X}_1) \cdot \nabla_{\mathbf{X}_1} \frac{1}{|\mathbf{X}-\mathbf{X}_1|} \\ &\quad - \frac{e^2}{m_e\omega^2} \int d\mathbf{X}_1 \, \varphi_{eff}(\mathbf{X}_1, \omega) n_{2D}(\mathbf{X}_1) \nabla^2_{\mathbf{X}_1} \frac{1}{|\mathbf{X}-\mathbf{X}_1|}. \end{aligned} \tag{3}$$

The Laplacian of the 3D Coulomb potential gives the 3D delta function. The Laplacian of the 2D Coulomb potential, however, does not give the 2D delta function that is derived by the Laplacian of $\ln|\mathbf{X} - \mathbf{X}_1|$. Since the value of $1/|\mathbf{X} - \mathbf{X}_1|$ is larger than that of $|\ln|\mathbf{X} - \mathbf{X}_1||$ at $\mathbf{X} \approx \mathbf{X}_1$, the following approximate equation for the third term of the right side of Equation (3) can be used:

$$\begin{aligned} \varphi_{eff}(\mathbf{X}, \omega) &\approx \varphi_{ext}(\mathbf{X}, \omega) - \frac{e^2}{m_e\omega^2} \int d\mathbf{X}_1 \, \varphi_{eff}(\mathbf{X}_1, \omega) \nabla_{\mathbf{X}_1} n_{2D}(\mathbf{X}_1) \cdot \nabla_{\mathbf{X}_1} \frac{1}{|\mathbf{X}-\mathbf{X}_1|} \\ &\quad - \frac{e^2 n_{2D}(\mathbf{X})}{m_e\omega^2} \int_{\substack{\text{2D material} \\ \text{area}}} d\mathbf{X}_1 \, \varphi_{eff}(\mathbf{X}_1, \omega) \nabla^2_{\mathbf{X}_1} \frac{1}{|\mathbf{X}-\mathbf{X}_1|}. \end{aligned} \tag{4}$$

The third term becomes exact for the uniform 2D materials, i.e., $n_{2D}(\mathbf{X}_1) = n_{2D}$ (const.) and also for 3D case. The second term in Equation (4) corresponds to the edge plasmon, which includes the gradient of the 2D local electron density and the third term corresponds to the planar plasmon, which includes the 2D local electron density. This approximation physically indicates that the scalar potential of the planar plasmon is shielded by the induced charge of the edge plasmon, which is similar to the fact that the scalar potential of the 3D bulk plasmon is shielded by the induced charge of the surface plasmon as indicated previously [14–16].

2.2. Planar and Edge Plasmons

2.2.1. Planar Plasmon

A uniform 2D atomic layer is firstly considered where $\nabla_{\mathbf{X_1}} n_{2D}(\mathbf{X_1}) = 0$, indicating that the second term in Equation (4) disappears. The use of following 2D Fourier transformations:

$$\varphi_{eff}(\mathbf{X}, \omega) = \frac{1}{(2\pi)^2} \int d\mathbf{k}\, \varphi_{eff}(\mathbf{k}, \omega) \exp(i\mathbf{k} \cdot \mathbf{X}), \quad \frac{1}{|\mathbf{X} - \mathbf{X_1}|} = \frac{1}{(2\pi)^2} \int d\mathbf{k} \frac{2\pi}{k} \exp[i\mathbf{k} \cdot (\mathbf{X} - \mathbf{X_1})],$$

(5)

and their substitution into Equation (4) give

$$\varphi_{eff}(\mathbf{k}, \omega)\left(1 - \frac{2\pi e^2 n_{2D}}{m_e \omega^2} k\right) = \varphi_{ext}(\mathbf{k}, \omega).$$

(6)

The pole of Equation (6) gives the planar plasmon frequency:

$$\omega_{pl} = \sqrt{\frac{2\pi e^2 n_{2D} k}{m_e}} \propto (n_{2D})^{1/2} \sqrt{k},$$

(7)

where k is the 2D wave number of the planar plasmon. The planar plasmon frequency coincides with that previously derived for 2D electron systems in the metal-insulator-semiconductors at the wave number $k \to 0$ [17].

Stacked multi-atomic layers are next considered, where the local electron density is given by $n(\mathbf{r}_1) = n_{2D} \sum_{z_n} \delta(z_1 - z_n)$. By using Bloch's theorem with equal spacing l in the z direction

$$\varphi_{eff}(\mathbf{X}_1, \mathbf{z}_n; \omega) = \exp[iq_z(z_n - z_s)]\varphi_{eff}(\mathbf{X}_1, \mathbf{z}_s; \omega),$$

$$\frac{1}{|\mathbf{X} - \mathbf{X}_1 + \mathbf{z}_s - \mathbf{z}_n|} = \frac{1}{(2\pi)^2} \int d\mathbf{k} \frac{2\pi}{k} \exp[i\mathbf{k} \cdot (\mathbf{X} - \mathbf{X}_1) - k|z_s - z_n|], \quad |z_s - z_n| = |s - n|l,$$

(8)

and Equation (2), the following equation is derived:

$$\varphi_{eff}(\mathbf{k}, \mathbf{z}_s; \omega)\left\{1 - \frac{2\pi e^2 n_{2D}}{m_e \omega^2} k\left[1 + \frac{2e^{-kl}\left(\cos q_z l - e^{-kl}\right)}{1 - 2e^{-kl}\cos q_z l + e^{-2kl}}\right]\right\} = \varphi_{ext}(\mathbf{k}, \mathbf{z}_s; \omega),$$

(9)

where q_z is the wave number in the z direction. The pole of Equation (9) gives the following planar plasmon frequency for small wave number limits where $q_z = 0$, which corresponds to the case for the uniform external potential in the z direction and subsequent $k \to 0$ limits are considered:

$$\omega_{pl} = \sqrt{\frac{4\pi e^2 n_{2D}}{m_e l}}.$$

(10)

This coincides with the bulk plasmon frequency for the averaged 3D electron density n_{2D}/l. This kind of relationship has previously been reported for the intercalated graphite [18] and the semiconductor superlattices [19].

2.2.2. Edge Plasmon

When a nanodisk with radius a is considered at $X \geq a$ where $n_{2D}(\mathbf{X}) = 0$, indicating that the third term disappears in Equation (4), the following equation is derived from Equation (4):

$$\varphi_{eff}(\mathbf{X}, \omega) = \varphi_{ext}(\mathbf{X}, \omega) - \frac{e^2}{m_e \omega^2} \int d\mathbf{X}_1 \varphi_{eff}(\mathbf{X}_1, \omega) \nabla_{\mathbf{X_1}} n_{2D}(\mathbf{X}_1) \cdot \nabla_{\mathbf{X_1}} \frac{1}{|\mathbf{X} - \mathbf{X}_1|}.$$

(11)

Using expansions for the scalar potential and the 2D Coulomb potential by $\exp(im\phi)$ (see Appendix B):

$$\varphi_{eff}(\mathbf{X}, \omega) = \sum_{m=-\infty}^{\infty} \varphi_{eff}^m(X, \omega) \exp(im\phi),$$

$$\frac{1}{|\mathbf{X}-\mathbf{X}_1|} = \sum_{m=-\infty}^{\infty} \exp[im(\phi - \phi_1)] \int_0^{\infty} dk J_m(kX) J_m(kX_1), \tag{12}$$

and step-function-like electron density $n_{2D}(\mathbf{X}_1) = n_{2D}\,\theta(a - X_1)$ whose derivative with respect to X_1 is $-n_{2D}\delta(X_1 - a)$, the following equation is given using Equation (11) at $X = a$ and integration by parts for $dJ_m(s)/ds$ by:

$$\varphi_{eff}^m(a, \omega)\left\{1 - \frac{\pi e^2 n_{2D}}{m_e \omega^2 a} \int_0^{\infty} ds(\alpha s - 1)[J_m(s)]^2 \exp(-\alpha s)\right\} = \varphi_{ext}^m(a, \omega), \tag{13}$$

where $J_m(s)$ is the Bessel function of the first kind and α is the small positive value to remove the divergence. The pole of Equation (13) gives the following edge plasmon frequency:

$$(\omega_{ed}^m)^2 = \frac{\pi e^2 n_{2D}}{m_e a} \int_0^{\infty} ds(\alpha s - 1)[J_m(s)]^2 \exp(-\alpha s) \propto n_{2D}/a. \tag{14}$$

For the pure 2D case, i.e., $\alpha = 0$, the square of the edge plasmon frequency becomes negatively divergent (logarithmic-like), giving no physically reasonable results. It has been, however, confirmed by numerical calculations, using $Q_{\frac{1}{2}}(s)$ in Equation (B1) for $m = 1$, that this has a positive value when the α is larger than about 0.15. The 3D property for the Coulomb potential is needed to get physically reasonable results in this formula. The step-function-like density at the edge may be too extreme for the 2D case, unlike for the 3D case [14]. The 2D electron density profile near the edge should be more carefully considered as indicated in the previous studies [20,21], where the electron density near the edge is supposed to gradually vary. This should be investigated in future studies.

2.3. Light Emission from Edge Plasmon in Nanodisk

The previous studies [15,16] have shown that the 3D induced charge density by the plasmon excitation is given by

$$\rho(\mathbf{r}, \omega) = -\frac{e^2}{m_e \omega^2} \nabla \cdot \left[n(\mathbf{r}) \nabla \varphi_{eff}(\mathbf{r}, \omega)\right]. \tag{15}$$

Using the induced charge density, the 3D electric dipole moment is given by

$$\mathbf{p}_{3D}(\omega) = \int \mathbf{r} \rho(\mathbf{r}, \omega) d\mathbf{r} = \frac{-e^2}{m_e \omega^2} \int d\mathbf{r} \varphi_{eff}(\mathbf{r}, \omega) \nabla n(\mathbf{r}). \tag{16}$$

When the 3D electron density $n(\mathbf{r})$ is expressed by $n(\mathbf{r}) \approx n_{2D}(\mathbf{X})\delta(z)$, the 2D electric dipole moment is given using the odd function property of $\varphi_{eff}(\mathbf{r}, \omega)\nabla n(\mathbf{r})$ in the z direction by

$$\mathbf{p}_{2D}(\omega) = \frac{-e^2}{m_e \omega^2} \int d\mathbf{X}\, \varphi_{eff}(\mathbf{X}, \omega) \nabla_{\mathbf{X}}\, n_{2D}(\mathbf{X}). \tag{17}$$

Using expansions of the scalar potential by $\exp(im\phi)$ and the step-function-like electron density, the 2D electric dipole moment is derived:

$$\mathbf{p}_{2D}(\omega) = \mathbf{e}_x \frac{2\pi e^2 n_{2D} a}{m_e \omega^2} \text{Re}\left[\varphi_{eff}^1(a, \omega)\right], \tag{18}$$

where $\mathbf{e}_x$ is the unit vector in the $\mathbf{x}$ direction, i.e., an external electric field E_x direction, Re means real part and $\varphi_{eff}^1(a, \omega)$ is given by Equation (13) at $m = 1$. It is found that only the scalar potential of $m = 1$ at the nanodisk edge $X = a$ contributes to the dipole moment. Using Equation (13) and the

external scalar potential $\varphi_{ext}^1(a, \omega) = -E_x a/4\pi$, the second order derivative of the dipole moment with respect to time is given by

$$\ddot{\mathbf{p}}_{2D}(\omega) = -\omega^2 \, \mathbf{p}_{2D}(\omega) = \mathbf{e}_x \frac{e^2 n_{2D} \, a^2 E_x}{2 \, m_e} \frac{\omega^2}{\omega^2 - \left(\omega_{ed}^1\right)^2} \, . \tag{19}$$

Then, the photon number with energy $\hbar\omega$ per solid angle Ω [15,16] is given by

$$I_{ph}(\Omega, \omega) = \frac{1}{4\pi^2 c^3 \hbar \omega} \left| \mathbf{e}_r \times \ddot{\mathbf{p}}_{2D}(\omega) \right|^2 = \frac{e^4 n_{2D}^2 \, a^4 E_x^2 \sin^2 \theta}{16\pi^2 m_e^2 c^3 \hbar} \frac{\left(\omega^3 + \omega \Gamma^2\right)}{\left[\omega^2 - \left(\omega_{ed}^1\right)^2\right]^2 + \omega^2 \Gamma^2}, \tag{20}$$

where $\mathbf{e}_r$ is the unit vector in the $\mathbf{r}$ direction, i.e., detection direction, θ is the angle between $\mathbf{e}_r$ and $\mathbf{e}_x$, and Γ is the plasmon damping frequency. To consider the plasmon damping correctly, ω^2 is replaced by $\omega(\omega + i\Gamma)$ in Equation (19) [22]. Equations (14) and (20) indicate that the resonant light emission frequency can be widely tuned by changing the 2D electron density due to gating and the radius of the nanodisk, as indicated for the graphene [8–10].

2.4. Plasmons in Uniform 2D and 3D Weyl Fermions

The electrons in a single layer graphene satisfy the 2D Weyl equation, i.e., massless Dirac equation [23]. The electrons in the uniform Weyl semimetals such as $Y_2Ir_2O_7$, satisfy the following 3D Weyl equation [24]:

$$\gamma \begin{pmatrix} \hat{k}_z & \hat{k}_x - i\hat{k}_y \\ \hat{k}_x + i\hat{k}_y & -\hat{k}_z \end{pmatrix} \psi_{\mathbf{k}}(\mathbf{r}) = E_{\mathbf{k}} \, \psi_{\mathbf{k}}(\mathbf{r}),$$

$$\therefore \hat{k}_x = \frac{1}{i}\frac{\partial}{\partial x}, \, \hat{k}_y = \frac{1}{i}\frac{\partial}{\partial y}, \, \hat{k}_z = \frac{1}{i}\frac{\partial}{\partial z}. \tag{21}$$

The wave functions and single fermion energies satisfying Equation (21) are given by

$$\psi_{\mathbf{k},s}(\mathbf{r}) = \frac{1}{\sqrt{2k(k+sk_z)}} \begin{pmatrix} k_z + sk \\ k_x + ik_y \end{pmatrix} \exp(i\mathbf{k} \cdot \mathbf{r}),$$

$$\psi_{\mathbf{k},s}^*(\mathbf{r}) = \frac{1}{\sqrt{2k(k+sk_z)}} \begin{pmatrix} k_z + sk, & k_x - ik_y \end{pmatrix} \exp(-i\mathbf{k} \cdot \mathbf{r}), \tag{22}$$

$$\psi_{\mathbf{k},s}^*(\mathbf{r})\psi_{\mathbf{k},s}(\mathbf{r}) = 1, E_{\mathbf{k}} = s\gamma\sqrt{k_x^2 + k_y^2 + k_z^2} = s\gamma k, \quad \gamma = \hbar v_F, \quad s = +1, -1,$$

where v_F is the Fermi velocity and $s = +1, -1$ correspond to the conduction and valence bands, respectively, in the Dirac cones.

Using Equations (A2) and (A5) in Appendix A, the Fourier components of the effective scalar potentials satisfy the following equation in the RPA:

$$\varphi_{eff}(\mathbf{k}, \omega) \left(1 - \frac{D4\pi e^2}{k^2 \hbar} \frac{1}{(2\pi)^3} \int d^3\mathbf{q} \, F(\mathbf{q}, \mathbf{q} + \mathbf{k}) \frac{\theta(E_F - E_{\mathbf{q}}) - \theta(E_F - E_{\mathbf{q}+\mathbf{k}})}{\omega + (E_{\mathbf{q}} - E_{\mathbf{q}+\mathbf{k}})/\hbar + i\eta} \right) = \varphi_{ext}(\mathbf{k}, \omega),$$

$$\therefore F(\mathbf{q}, \mathbf{q} + \mathbf{k}) = \left| \langle \psi_{\mathbf{q}} | e^{-i\mathbf{k} \cdot \mathbf{r}} | \psi_{\mathbf{q}+\mathbf{k}} \rangle \right|^2, \tag{23}$$

where the 3D Coulomb potential was used and only the conduction band $s = 1$ was considered. The term in the parenthesis of the left side of Equation (23) corresponds to the dielectric function $\varepsilon(\mathbf{k}, \omega)$. Under high frequency conditions at $k \to 0$, the following approximations can be used in Equation (23):

$$\frac{1}{\omega + (E_{\mathbf{q}} - E_{\mathbf{q}+\mathbf{k}})/\hbar + i\eta} \approx \frac{1}{\omega}\left(1 + \frac{\gamma}{\hbar\omega}\frac{\mathbf{k} \cdot \mathbf{q}}{q}\right), F(\mathbf{q}, \mathbf{q} + \mathbf{k}) \approx 1. \tag{24}$$

Then, the dielectric function is given by

$$\varepsilon(\mathbf{k}, \omega) = 1 - \omega_b^2/\omega^2,$$

$$\because \omega_b = \sqrt{\frac{8e^2 v_F}{3\hbar\pi}}k_F = \sqrt{\frac{8e^2 v_F}{3\hbar\pi}}\left(\frac{6\pi^2}{D}n_{3D}\right)^{1/3} \propto (n_{3D})^{1/3}, \tag{25}$$

where ω_b is the bulk plasmon frequency and the 3D Fermi wave number k_F is given by

$$\frac{D}{(2\pi)^3}\int\limits_{|\mathbf{k}|\leq k_F} \mathrm{d}^3\mathbf{k} = n_{3D} \rightarrow k_F = \left(\frac{6\pi^2}{D}n_{3D}\right)^{1/3}. \tag{26}$$

The dielectric function $\varepsilon(\mathbf{k}, \omega) = 1 - \omega_b^2/\omega^2$ has no k dependence and has the same formula as that for the Schrödinger fermions under high frequency conditions at $k \rightarrow 0$. The bulk plasmon frequency, however, is different from the conventional one $\sqrt{4\pi e^2 n_{3D}/m_e}$ for the Schrödinger fermions.

For the 2D Weyl fermions such as in a single layer graphene, similar calculations gave the same planar plasmon frequency at 2D wave number $k \rightarrow 0$ as that previously reported [23], where $\hat{k}_z = 0$, $D = 4$ and the 2D Coulomb potential were used in Equation (23), and k_F is the 2D Fermi wave number:

$$\omega_{pl} = \sqrt{\frac{2e^2 v_F k_F k}{\hbar}} = \sqrt{\frac{2e^2 v_F}{\hbar}}(\pi n_{2D})^{1/4}\sqrt{k} \propto (n_{2D})^{1/4}\sqrt{k}. \tag{27}$$

The wave number and nanodisk radius dependencies of the plasmon frequencies at $k \rightarrow 0$ are summarized in Table 1. The plasmon frequencies depend on the kind of fermions (Schrödinger or Weyl), the dimensions (2D or 3D) and the structures (uniform or nanodisk).

Table 1. Two-dimensional (2D) and 3D plasmon frequencies at $k \rightarrow 0$. The frequencies for the 2D Weyl fermion, i.e., the graphene case, have already been reported in previous studies [9,23].

	Dimension	Bulk/Planar	Surface/Edge
Schrödinger	3D	$(n_{3D})^{1/2}$	$(n_{3D})^{1/2}$
fermion	2D	$(n_{2D})^{1/2}\sqrt{k}$	$(n_{2D})^{1/2}/\sqrt{a}$
Weyl	3D	$(n_{3D})^{1/3}$	$(n_{3D})^{1/3}$
fermion	2D	$(n_{2D})^{1/4}\sqrt{k}$ [23]	$(n_{2D})^{1/4}/\sqrt{a}$ [9]

It is assumed in Table 1 that the surface plasmon for the 3D Weyl fermion has the same electron density dependence as that of the bulk plasmon for the Schrödinger fermions because the formula of the dielectric function is the same as that for the Schrödinger fermions under high frequency conditions at $k \rightarrow 0$. It has been theoretically and experimentally reported, however, that the new surface states in the form of Fermi-arc appear for the 3D Weyl semimetals [24,25]. The effect of the surface states on the surface plasmon should be investigated in future studies.

3. Conclusions

The theory of the planar and edge plasmons for 2D metal nanostructures with the Schrödinger fermions has been derived from the 3D one in the RPA under high frequency conditions. The wave number and nanodisk radius dependences of the plasmons have been calculated at small wave number limit. It was found that the plasmon frequencies strongly depended on the kind of fermions (Schrödinger or Weyl), the dimensions (2D or 3D) and the structures (uniform or nanodisk). However, this should be improved because several approximations such as Equations (4) and (13) were used.

The plasmon frequencies for uniform 2D and 3D Weyl fermions were also calculated at small wave number limit using the RPA under high frequency conditions, which were compared with those for the Schrödinger fermions. A theory of the plasmons for the Weyl fermion nanostructures,

however, has not yet been derived by our previous method. These are future problems that should be further studied.

Part of this work has been presented at the international conference on Atomically Controlled Surfaces, Interfaces and Nanostructures ACSIN2016 held in Frascati, Rome Italy on 9–15 October 2016 [26].

Conflicts of Interest: The author declares no conflict of interest.

Appendix A

Considering an effective scalar potential $\varphi_{eff}(\mathbf{r_2}, \omega)$ within the electron gas in metal nanostructures, an electron charge density $\rho_{ind}(\mathbf{r_1}, \omega)$ induced by the effective scalar potential [15] is given in the frequency ω expression by

$$\rho_{ind}(\mathbf{r_1}, \omega) = \int d\mathbf{r_2} e^2 \, P_0(\mathbf{r_1}, \mathbf{r_2}, \omega) \varphi_{eff}(\mathbf{r_2}, \omega). \tag{A1}$$

The polarization of the non-interacting electron gas $P_0(\mathbf{r_1}, \mathbf{r_2}, \omega)$ is given by

$$P_0(\mathbf{r_1}, \mathbf{r_2}, \omega) = \frac{D}{\hbar} \sum_{n,n'} \psi_n^*(\mathbf{r_1}) \cdot \psi_n(\mathbf{r_2}) \cdot \psi_{n'}^*(\mathbf{r_2}) \cdot \psi_{n'}(\mathbf{r_1}) \frac{\theta(E_F - E_n) - \theta(E_F - E_{n'})}{\omega + (E_n - E_{n'})/\hbar + i\eta}, \tag{A2}$$

where the infinitesimal imaginary term $i\eta$ is required by the causality of the one-particle Green's function for a single electron. $\psi_n(\mathbf{r})$ is the single-electron wave function in the metal nanostructure, which satisfies the following Schrödinger equation:

$$\left[-\frac{\hbar^2}{2m_e} \nabla^2 + V(\mathbf{r}) \right] \psi_n(\mathbf{r}) = E_n \psi_n(\mathbf{r}). \tag{A3}$$

In Equations (A2) and (A3), $\theta(E_F - E_n)$ is the step function, E_F is the Fermi energy, m_e and $-e$ are the electron mass and charge, and E_n is the electron energy in the nanostructure with the local potential energy $V(\mathbf{r})$. Then, the induced scalar potential $\varphi_{ind}(\mathbf{r}, \omega)$ is given by

$$\varphi_{ind}(\mathbf{r}, \omega) = \int d\mathbf{r_1} \frac{\rho_{ind}(\mathbf{r_1}, \omega)}{|\mathbf{r} - \mathbf{r_1}|} = \iint d\mathbf{r_1} d\mathbf{r_2} \frac{e^2 P_0(\mathbf{r_1}, \mathbf{r_2}, \omega) \varphi_{eff}(\mathbf{r_2}, \omega)}{|\mathbf{r} - \mathbf{r_1}|}, \tag{A4}$$

where $e^2/|\mathbf{r} - \mathbf{r_1}|$ is the 3D Coulomb potential between the electrons. When an external scalar potential $\varphi_{ext}(\mathbf{r}, \omega)$ is considered, the effective scalar potential satisfies

$$\varphi_{eff}(\mathbf{r}, \omega) = \varphi_{ext}(\mathbf{r}, \omega) + \iint d\mathbf{r_1} d\mathbf{r_2} \frac{e^2 P_0(\mathbf{r_1}, \mathbf{r_2}, \omega) \varphi_{eff}(\mathbf{r_2}, \omega)}{|\mathbf{r} - \mathbf{r_1}|}. \tag{A5}$$

The above self-consistent integral equation is equivalent to that calculated in the RPA, which gives the well-known dielectric function for the uniform electron gas with translational invariance [27].

A high-frequency condition of $|E_n - E_{n'}|/\hbar\omega << 1$ is considered valid for collective excitations, such as plasmons that have excitation energies much larger than single-electron excitation energies [14]. The right-side denominator of Equation (A2) can then be approximated as

$$\frac{1}{\omega + (E_n - E_{n'})/\hbar} \approx \frac{1}{\omega} \left[1 - \frac{(E_n - E_{n'})}{\hbar\omega} \right], \tag{A6}$$

where ω is assumed to include the infinitesimal imaginary term $i\eta$. Using a similar method to that given previously [14], where Equation (A3), the completeness of the single-electron wave function

$\sum_n \psi_n^*(\mathbf{r}_1) \cdot \psi_n(\mathbf{r}_2) = \delta(\mathbf{r}_1 - \mathbf{r}_2)$, and integration by parts were used, the calculation of Equation (A5) using Equation (A6) gives Equation (1).

Appendix B

The 3D Coulomb potential is given using the cylindrical coordinate by [28]

$$
\begin{aligned}
\frac{1}{|\mathbf{r}-\mathbf{r}_1|} &= \sum_{m=-\infty}^{\infty} \exp[im(\phi - \phi_1)] \int_0^{\infty} dk J_m(kX) J_m(kX_1) \exp(-k|z-z_1|), \\
&= \frac{1}{\pi\sqrt{XX_1}} \sum_{m=-\infty}^{\infty} \exp[im(\phi - \phi_1)] Q_{m-\frac{1}{2}} \left[\frac{X^2 + X_1^2 + (z-z_1)^2}{2XX_1} \right],
\end{aligned}
\tag{B1}
$$

where m is the integer, $J_m(s)$ is the Bessel function of the first kind and $Q_{m-\frac{1}{2}}(s)$ is the odd-half-integer degree Legendre function of the first kind. The 2D Coulomb potential is given by putting $z = z_1 = 0$ in Equation (B1), which becomes, however, divergent at $X = X_1$ because the Legendre function $Q_{m-\frac{1}{2}}(s)$ has an infinite value at $s = 1$. To remove the divergence, the small positive value α is introduced as shown in Equation (13). This is considered valid because the actual materials are not pure 2D ones but have 3D properties for the Coulomb potential where the term $\exp(-k|z-z_1|)$ removes the divergence at $X = X_1$.

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