Exotic behavior of the dielectric function and the plasmons of an electron gas on a tubule

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The dielectric response of an electron gas confined to the surface of a hollow infinitely long cylinder is calculated in the random-phase approximation. The frequency dependence of the imaginary part of the dielectric function shows a steplike behavior. The dielectric function shows the dimensional crossover from two-dimensional to one-dimensional behavior with decreasing cylinder radius. In the quasi-one-dimensional case, our model does not need any artificial cutoff parameters for the Coulomb potential.

Recent experimental technology, especially nanotechnology, makes it possible to observe many quantum phenomena in narrow or small systems in solid-state physics. In these systems, quantum effects appear clearly. Some "ideal narrow geometrical models" are becoming realizable. A very thin long hollow cylinder is an example of such a model. It may be considered as a simple model of graphene tubules.[1] There are many types of graphene tubules, for example, atomic arrangements of carbon atoms of the so-called armchair fiber type which has a metallic electronic structure, and of the zigzag fiber type whose electronic structure is that of a semiconductor.[2,3]

In this paper, an electronic structure of the former type is treated as an electron gas. We discuss the dielectric function and collective excitations of the electron gas confined to the surface of the cylinder which is empty inside and extends infinitely.

It is efficient to take cylindrical coordinates z and φ, and their canonical momenta, p_Z and p_φ, as shown in Fig. 1. Having the rotational invariance around the cylinder axis, the electronic state of the system is characterized by the momentum along the cylinder axis, $p_Z=\hbar k_Z$, and the z component of the angular momentum $p_\varphi=\hbar l$ (l is an integer). When the cylinder radius R is large enough, the dielectric behavior of the electron gas on a cylinder is expected to reduce to that of a two-dimensional (2D) electron gas.[4,5] On the other hand, when R is sufficiently small, the energy difference between two states which have an adjacent value of the angular momentum gets larger to an order of R^{-2}. The energy dispersion as a function of p_Z does not depend on R if the angular momentum is fixed. Since the Fermi statistics force the number of angular momenta which are occupied by electrons to be small, the discreteness of the angular momentum is reflected clearly in the dielectric function. In a very narrow limit, the occupied angular momentum l is only $l=0$. In the classical mechanics picture, the motion of electrons in the state is restricted only to the direction of the cylinder axis. This state is quasi-one-dimensional. There are some other examples of quasi-1D systems, the quantum wire[6,7] is one. Since the hollow cylinder as a quasi-1D system has a different topology from others, it is expected that its electronic structure is different from that in a quantum wire or the usual 2D electron gas.[4,5] When the cylinder radius R is in the intermediate region, the system becomes neither quasi-1D nor 2D.

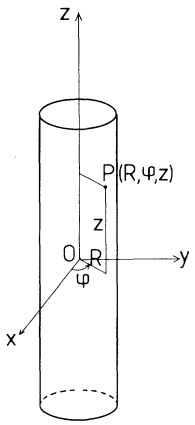

FIG. 1. A schematic illustration of the cylindrical system.

In the 2D electron gas system, the chemical potential μ_0 satisfies the following relations:

$$\mu_0=\frac{\hbar^2k_F^2}{2m}\ , \tag{1}$$

with

$$k_F^2=2\pi n$$

and

$$a_0r_S=1/\sqrt{\pi n}\ .$$

Here k_F is the Fermi wave vector, n the areal electron density, and m the electron mass. The parameter r_S represents the radius of the circle per electron measured in units of the Bohr radius a_0. In the actual solids, the Bohr radius and the electron mass should be replaced by the effective Bohr radius and the effective electron mass, respectively.

In the cylindrical electron-gas case, the relationship

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Eq. (1) between the chemical potential and the electron density is not valid when R is so small that the angular momentum of the system cannot be regarded as continuous. Therefore, the chemical potential of the system depends on R. The energy of the free-electron gas on the cylinder is given by

$$E=\frac{\hbar^2 k_Z^2}{2m}+\frac{\hbar^2 l^2}{2mR^2} . \tag{2}$$

If R is not infinite, each free-electron energy level is split into 1D free-electron energy bands shifted by the energies corresponding to each angular momentum l. The electronic state is quantized around the z axis. This situation is similar to the formation of the Landau level under the magnetic field. But there is a difference in the energy-level splitting between the cylindrical electron gas and the electron gas under the magnetic field. In the former case, the energy difference between the state with angular momentum l and the lowest band state with angular momentum 0 is proportional to l^2. In the latter case, the energy difference between successive Landau levels is usually $\hbar\omega_c$, ω_c being the cyclotron frequency. The real electron density is

$$n=1/\pi a_0^2 r_s^2 . \tag{3}$$

The density of states at energy E for the motion along the z axis is given by

$$\sqrt{2m/\pi^2\hbar^2 E} . \tag{4}$$

Thus the chemical potential μ of the system is determined by

$$2\pi R\times\frac{1}{\pi a_0^2 r_S^2}=\left[\frac{8m}{\pi^2\hbar^2}\right]^{1/2}\left[(\mu)^{1/2}+2\left[\mu-\frac{\hbar^2 1^2}{2mR^2}\right]^{1/2}+\cdots+2\left[\mu-\frac{\hbar^2 l_{\max}^2}{2mR^2}\right]^{1/2}\right] , \tag{5}$$

where $l_{\max}$ is defined by

$$l_{\max}=\max\left\{l:\mu-\frac{\hbar^2 l^2}{2mR^2}>0\right\} . \tag{6}$$

The R dependence of the chemical potential is shown in Fig. 2. This system can be regarded as a quasi-1D system when $R<a_0 r_S/\sqrt{\pi}$. The chemical potential oscillates around the value of the 2D electron gas with increasing R. This behavior can be explained as follows. For very small R, only the $l=0$ band is occupied. With increasing R, the number of particles per unit length along the z axis and the chemical potential become larger. Then the bottoms of the $l=\pm1$ bands go down, and the $l=\pm1$ bands begin to be occupied. The density of states of the 1D band is in inverse proportion to the square root of an energy measured from the band bottom. Since the density of states near the band bottom is very large, electrons prefer to occupy the $l=\pm1$ states rather than the $l=0$ state. Thus the chemical potential decreases when it passes through the band bottom. Now we introduce a quantity q for convenience as

$$\mu=\frac{\hbar^2 q^2}{2m} . \tag{7}$$

q corresponds to the Fermi wave vector which characterizes the motion along the z axis. From Eqs. (6) and (7), $l_{\max}$ is equal to the integral part of Rq. Rq characterizes the dimension of our system. The motion of electrons is in quasi-1D for $Rq<1$, and 2D for $Rq\gg1$. Our system changes from quasi-1D to 2D smoothly as Rq increases.

The Coulomb interaction $V(z,\varphi)$ between two electrons on a cylinder surface is given by

$$V(z,\varphi)=\frac{e^2}{r} , \tag{8}$$

with

$$r=[2R^2(1-\cos\varphi)+z^2]^{1/2} .$$

It should be noted that, in our system, effects of the Coulomb force between two electrons on the motion of the electrons is different from those on a flat surface, since each electron is confined to a curved surface. The component of the Coulomb force normal to the cylindrical surface is canceled out with constraints which keep the electrons on the surface.

The Fourier transform of the Coulomb potential is given by

$$V(k_Z,l)=4e^2R\int_0^{\pi}d\varphi\cos(2l\varphi)K_0(|2Rk_Z\sin\varphi|) . \tag{9}$$

Here $K_0(x)$ is the modified Bessel function of the second kind. This is derived without using any artificial cutoff parameters. Equation (9) can be integrated analytically

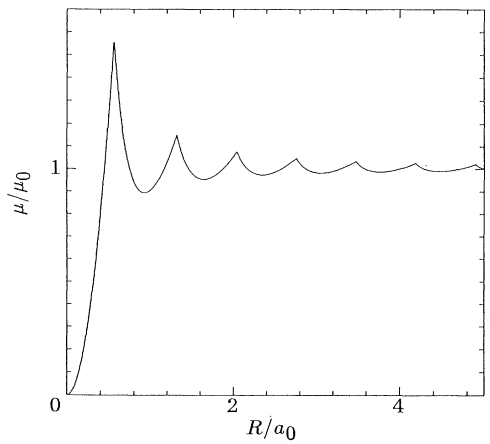

FIG. 2. The R dependence of the chemical potential at $r_S=1$.

for $l=0$ as

$$V(k_Z,0)=4\pi e^2 R I_0(|Rk_Z|)K_0(|Rk_Z|) .$$

In the long-wavelength limit $Rk_Z \ll 1$, we obtain the following asymptotic expression:

$$V(k_Z,0)\simeq -4\pi e^2 R \ln|Rk_Z| .$$

Using the perturbation theory, the lowest-order polarization function $\Pi^{(0)}$ is[8]

$$\Pi^{(0)}(l,k_Z,i\omega)=\frac{2}{\sigma}\sum_{l'}\sum_{k'_Z}\frac{n_F(\xi-\mu)-n_F(\xi'-\mu)}{\xi-\xi'+i\hbar\omega} , \quad (10)$$

where

$$\xi=\frac{\hbar^2 k_Z^2}{2m}\ \frac{\hbar^2 l^2}{2mR^2}$$

and

$$\xi'=\frac{\hbar^2(k_Z+k'_Z)^2}{2m}+\frac{\hbar^2(l+l')^2}{2mR^2} .$$

Here σ is the total area of the cylinder surface, and $n_F(\xi)$ the Fermi distribution function. Performing an analytical continuation, the polarization function can be divided into its real and imaginary parts:

$$\mathrm{Re}\Pi^{(0)}(l,k_Z,\omega)=-\frac{m}{2\pi^2\hbar^2 k_Z R}\sum_{l'}\ln\left|\frac{\alpha^2-(\xi+\beta)^2}{\alpha^2-(\xi-\beta)^2}\right| \quad (11)$$

and

$$\mathrm{Im}\Pi^{(0)}(l,k_Z,\omega)=-\frac{m}{2\pi\hbar^2 k_Z R}\sum_{l'}[\theta(\xi+\alpha+\beta)-\theta(\xi+\alpha-\beta)+\theta(-\xi+\alpha-\beta)-\theta(-\xi+\alpha+\beta)] , \quad (12)$$

with

$$\alpha=\frac{\hbar^2 l l'}{mR^2}-\hbar\omega ,$$

$$\beta=\frac{\hbar^2}{m}k_Z\left[q^2-\frac{l'^2}{R^2}\right]^{1/2} ,$$

and

$$-l_{\max}\le l'\le l_{\max} .$$

The dielectric function $\epsilon(l,k_Z,\omega)$ is given by the random-phase approximation (RPA):[8,9]

$$\epsilon(l,k_Z,\omega)=1-V(l,k_Z)\Pi^{(0)}(l,k_Z,\omega) . \quad (13)$$

The frequency dependence of the dielectric function is shown in Fig. 3 for several R values. We note that Rq is a monotonically increasing function of R. For $Rq\gg 1$, the dielectric function is almost the same as that calculated in the RPA for a usual 2D electron gas.

As R grows smaller, the imaginary part of the dielectric function has definite discrete values, such as a step when k_Z and l are fixed. This can be explained from the expression of the imaginary part of $\Pi^{(0)}(l,k_Z,\omega)$. This function contains only ω in the θ function. As R grows smaller ($1\le Rq\le 10$), the region of the l' summation becomes smaller, then the summation over l' cannot be replaced by an integration. Therefore, the imaginary part of $\epsilon(l,k_Z,\omega)$ cannot have a continuous value as a function of ω. On the other hand, the real part of $\epsilon(l,k_Z,\omega)$ shows some peaks, reflected with logarithmic singularities in each polarization component.

If R is large enough, the l' summation can be replaced by an integral, and the logarithmic singularities are removed. Thus we cannot find any divergent peaks in $\epsilon(l,k_Z,\omega)$. This result is in agreement with that in a 2D electron gas.[4,5] When $0<Rq<1$ is only the $l'=0$ case allowed. Only then can a free-electron state of the system be characterized by a quantum number k_Z, which means

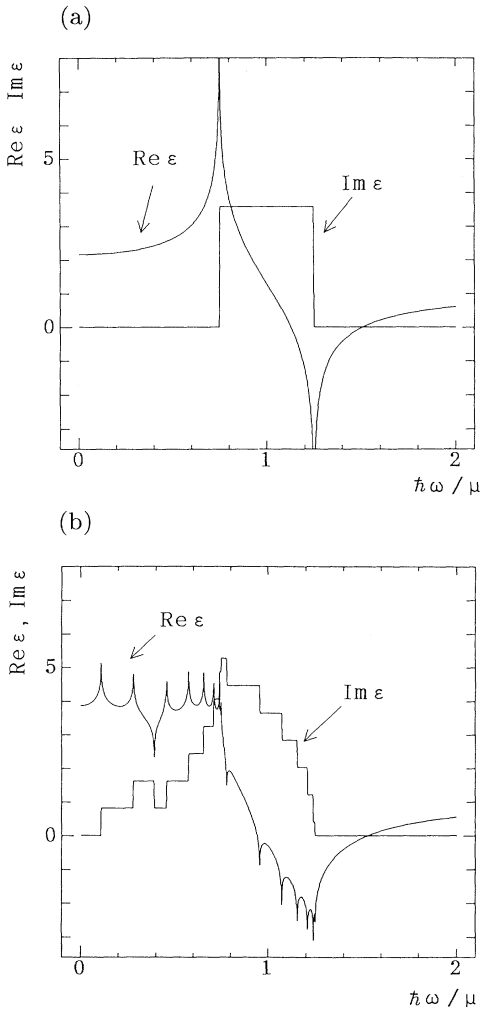

FIG. 3. The frequency dependence of the dielectric function ϵ for several R values at $r_S=1$, $l=0$, and $k_Z=0.5q$. $Rq=$ 0.71 (a), and 7.1 (b).

that the system is quasi-one-dimensional. This extreme case also will correspond to that of the quasi-1D electron systems in quantum wires.[6,7]

For a very slender limit ($0<Rq<1$), we consider only the intraband contribution to $\Pi^0(l,k_Z,\omega)$, i.e., $l=l'=0$. Then the dispersion relation for plasmons can be obtained analytically. By solving equations $\mathrm{Re}\epsilon=0$ and $\mathrm{Im}\epsilon=0$, the plasma frequency ω_p is obtained as

$$\hbar\omega_p=\left[\frac{(\xi_0+\beta_0)^2-\lambda(\xi_0-\beta_0)^2}{1-\lambda}\right]^{1/2}, \tag{14}$$

with

$$\xi_0=\frac{\hbar^2k_Z^2}{2m},$$

$$\beta_0=\frac{\hbar^2k_Zq}{m},$$

and

$$\lambda=\exp\left[-\frac{\pi\hbar^2k_Z}{2me^2\ln(2/R|k_Z|)}\right].$$

The dispersion relation and the single-particle excitation region are shown in Fig. 4. For the long-wavelength limit, we get

$$\omega_p=2ek_Z\left[\frac{q}{\pi m}\left|\ln\frac{Rk_Z}{2}\right|\right]^{1/2}. \tag{15}$$

In this equation, ω_p cannot be expanded in the power series of k_Z. $d\omega_p/dk_Z$ shows a divergence at $k_Z\sim0$, whose degree is weaker than that of a 2D electron gas.[10-12] The plasmon in a 2D electron gas is known to have a frequency ω_p proportional to the square root of a wave number k in the long-wavelength limit. Equation (15) has a structure similar to that of quasi-1D electron systems in quantum wires. If we replace the circumference of $2\pi R$ with the width of the quantum wire in Eq. (15), it is the same as Eq. (2.13) of Ref. 7 in the long-wavelength limit. It should be remarked that we can reproduce the result of the quasi-1D system.

In conclusion, we have reported the dielectric formulation of a cylindrical electron gas. We have calculated the dielectric function of an electron gas confined to the surface of a hollow cylinder which extends infinitely. We also have found the oscillation of the chemical potential with increasing R. The dielectric function obtained shows the dimensional crossover from 2D to 1D with decreasing cylinder radius R. In a slender limit, the plasmon dispersion relation is $\omega_p\sim k_Z|\ln k_Z|^{1/2}$. Our hollow cylindrical model has remarkable superiority as a theoretical model of the quasi-1D system. The Coulomb potential in the quasi-1D system can be introduced naturally, since its Fourier transformation can be performed completely due to the fact that the wave function of the direction around the z axis has a natural periodicity. It is expected that the wave number dependence of the dielectric functions may be observed in graphene tubules.

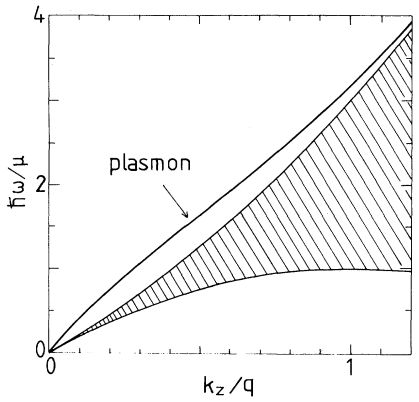

FIG. 4. The plasma dispersion relations for $r_S=1$, $Rq=0.71$. The shaded area shows the single-particle excitation region.

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