Exchange effects in the plasmon dispersion of one-dimensional systems

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The dynamic exchange decoupling method for including exchange in the dielectric function of the homogeneous electron gas has been extended to one-dimensional systems, in both the free-electron and the tight-binding limit. In the free-electron model, the slope of the plasmon branch is almost unaffected by exchange effects. In the tight-binding model, the exchange interaction appreciably lowers this slope, except if the band is almost filled.

I. INTRODUCTION

In recent years, the properties of organic conductors with highly anisotropic electrical conductivity have been extensively studied. The fact that materials like TTF-TCNQ appear metallic along the one-dimensional strands encourages an interpretation of the electronic properties in terms of the one-dimensional electron gas. For this model one expects in the random phase approximation (RPA) that the plasmon frequency increases quadratically with momentum for small wave vectors, and that the long-wavelength plasmon shows an anisotropy of the form $\omega_{p1}(\theta) = \omega_{p1}(0)\cos\theta$, where θ is the angle of propagation relative to the one-dimensional chain.[1]

Although in TTF-TCNQ this predicted anisotropy is in relatively good agreement with experimental data, it is remarkable that the plasmon spectrum is almost dispersionless for $\theta = 45°$ and shows a negative dispersion for $\theta = 0°$.[2]

For other materials, like the $(SN)_x$ polymer, one observes the positive dispersion, expected for the one-dimensional electron gas, but the anisotropic behavior is unusual.[3] For this polymer, the plasmon spectrum can be explained on the basis of a parabolic-band model in any direction if an anisotropic band mass is introduced (the anisotropic mass ratio being $m_\perp/m_\parallel \simeq 1.9$).[4]

The observed anisotropy in TTF-TCNQ is of the form $\omega_{p1}(\theta) = \omega_{p1}(0)\cos\theta$, which characterizes a one-dimensional system. However, the negative dispersion at $\theta = 0°$ suggests that the parabolic-band model is inappropriate. Attempts have been made to understand the plasmon spectrum on the basis of a tight binding model in the RPA.[5] Although for small strand radii this model shows a positive dispersion, a relatively good agreement with experiment could be obtained for $\theta = 0°$ with a strand radius as large as $r \sim 3$ Å. However, no improvement was obtained for the angular dependence of the plasmon dispersion. By extending this model to include interchain coupling,[6] and with nine adjustable parameters, close agreement was obtained for $\theta = 0°$, but for $\theta = 45°$ oscillations occur in the calculated plasmon dispersion which are not present in the experimental data.

In the foregoing approximations, exchange effects were not taken into account. Although in systems of reduced dimensionality with a free-electron-like band these exchange effects might be of minor influence, at least in the long-wavelength limit,[4] the localization in the tight-binding model is expected to enhance the exchange contributions.

In the present paper, the effects of exchange for one-dimensional systems are examined in both the free-electron and the tight-binding model.

In Sec. II, the formalism is presented in which the exchange interaction can be studied. In Sec. III, it is shown that exchange effects are negligible at low wave vector in a one-dimensional electron gas with free-electron-like energy bands. In Sec. IV, the exchange interaction is studied for a one-dimensional tight-binding model. It is shown that substantial contributions of exchange to the plasmon dispersion can occur, depending on the ratio between the conduction-band width and the Fermi energy.

II. DIELECTRIC FUNCTION WITH EXCHANGE

The dielectric function of an electron gas, embedded in a neutralizing homogeneous positive background, is usually written in the form

$$\epsilon(\vec{q}, \omega) = 1 + Q_0(\vec{q}, \omega)/[1 - G(\vec{q}, \omega)Q_0(\vec{q}, \omega)] , \quad (1)$$

where $G(\vec{q}, \omega)$ describes the exchange and correla-

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tion effects, and is supposed to be zero in RPA. $Q_0(\vec{q}, \omega)$ is the Lindhard polarizability[7,8]:

$$Q_0(\vec{q}, \omega) = \frac{4\pi e^2 \hbar}{q^2} \int d^3p \times \frac{N_{\vec{q}}(\vec{p})}{\hbar\omega + i\delta - E(\vec{p}+\hbar\vec{q}/2) + E(\vec{p}-\hbar\vec{q}/2)} . \tag{2}$$

In this expression, $E(\vec{p})$ denotes the one-electron energy associated with the momentum $\vec{p}$, and $N_{\vec{q}}(\vec{p})$ is given by

$$N_{\vec{q}}(\vec{p}) = (2/\hbar)[f^0(\vec{p}+\hbar\vec{q}/2) - f^0(\vec{p}-\hbar\vec{q}/2)] , \tag{3}$$

where $f^0(\vec{p})$ is the equilibrium distribution function, which is $(2\pi\hbar)^{-3}$ if $E(\vec{p})$ lies below the Fermi energy, and zero otherwise.

Neglecting correlation effects, but including the exchange interaction dynamically, the function $G(\vec{q}, \omega)$ in the three-dimensional electron gas is given by[9,10]

$$G(\vec{q}, \omega) = -\frac{1}{2} \frac{4\pi e^2}{q^2} \frac{2\pi e^2 \hbar^4}{Q_0^2(\vec{q}, \omega)} \int d^3p \int d^3p' \frac{N_{\vec{q}}(\vec{p}) N_{\vec{q}}(\vec{p}')}{|\vec{p}-\vec{p}'|^2} \times \frac{[(E(\vec{p}+\hbar\vec{q}/2) - E(\vec{p}-\hbar\vec{q}/2)) - (E(\vec{p}'+\hbar\vec{q}/2) - E(\vec{p}'-\hbar\vec{q}/2))]^2}{[\hbar\omega + i\delta - E(\vec{p}+\hbar\vec{q}/2) + E(\vec{p}-\hbar\vec{q}/2)]^2 [\hbar\omega + i\delta - E(\vec{p}'+\hbar\vec{q}/2) + E(\vec{p}'-\hbar\vec{q}/2)]^2} . \tag{4}$$

Denoting the magnitude of the Fermi wave vector and the Fermi energy by k_F and E_F, it is interesting to note that in the units

$$\vec{q} = \vec{k} k_F, \quad \omega = 2\nu E_F/\hbar , \tag{5}$$

$G(\vec{k} k_F, 2\nu E_F/\hbar)$ reduces to a universal function of $\vec{k}$ and ν.[11] The expressions (2) and (4) can then be written as

$$Q_0(\vec{k} k_F, 2\nu E_F/\hbar) = \frac{e^2 k_F}{2\pi^2 E_F} \frac{1}{k^2} \int d^3\xi \frac{\mathfrak{N}(\vec{\xi}+\vec{k}/2) - \mathfrak{N}(\vec{\xi}-\vec{k}/2)}{\nu + i\delta - \Delta_{\vec{k}}(\vec{\xi})} \tag{6}$$

$$G(\vec{k} k_F, 2\nu E_F/\hbar) = -\tfrac{1}{2} f(\vec{k}, \nu) \int d^3\xi \int d^3\xi' \frac{[\mathfrak{N}(\vec{\xi}+\vec{k}/2) - \mathfrak{N}(\vec{\xi}-\vec{k}/2)][\mathfrak{N}(\vec{\xi}'+\vec{k}/2) - \mathfrak{N}(\vec{\xi}'-\vec{k}/2)]}{|\vec{\xi}-\vec{\xi}'|^2} \times \frac{[\Delta_{\vec{k}}(\vec{\xi}) - \Delta_{\vec{k}}(\vec{\xi}')]^2}{[\nu + i\delta - \Delta_{\vec{k}}(\vec{\xi})]^2 [\nu + i\delta - \Delta_{\vec{k}}(\vec{\xi}')]^2} , \tag{7}$$

where

$$\Delta_{\vec{k}}(\vec{\xi}) = (1/2E_F)[E(\hbar k_F \vec{\xi} + \hbar k_F \vec{k}/2) - E(\hbar k_F \vec{\xi} - \hbar k_F \vec{k}/2)] , \tag{8}$$

$$f(\vec{k}, \nu) = \frac{1}{8} \frac{e^4 k_F^2}{\pi^4 E_F^2 k^2 Q_0^2(\vec{k} k_F, 2\nu E_F/\hbar)} , \tag{9}$$

and where $\mathfrak{N}(\vec{\xi})$ equals unity if $E(\hbar k_F \vec{\xi}) \leq E_F$ and is zero otherwise.

In the three-dimensional electron gas, the effects of the exchange interaction have been discussed from a numerical evalution of the integral (7) for $G(\vec{q}, \omega)$,[11] and the internal consistency of this exchange treatment has been examined.[12]

For the study of strictly one-dimensional systems, we assume that the electrons are bound to a linear chain of positive ions, without interchain coupling:

$$\mathfrak{N}(\vec{\xi}) = \delta(\vec{\xi}_\perp), \quad E(\hbar k_F \xi_z) \leq E_F$$
$$= 0, \quad E(\hbar k_F \xi_z) > E_F . \tag{10}$$

Under this assumption, the plasmon dispersion can be found from Eqs. (6)–(9) if the band structure $E(\vec{p})$ is given. In the following sections, both the free-electron and the tight-binding limit are studied.

III. ONE-DIMENSIONAL FREE-ELECTRON MODEL, INCLUDING EXCHANGE

In the free-electron model the one-electron energies are assumed to be $E(\vec{p}) = p_z^2/2m$. The evaluation of the Lindhard polarizability (6) can then easily be done:

$$Q_0^{\mathrm{FE}}(\vec{k} k_F, 2\nu E_F/\hbar) = \frac{me^2}{\pi^2 \hbar^2 k_F} \frac{1}{k^2 k_z} \left(\ln \left| \frac{\nu^2 - (k_z + k_z^2/2)^2}{\nu^2 - (k_z - k_z^2/2)^2} \right| + i\pi J \right) , \tag{11}$$

where

$$J=+1 \text{ if } |k_z - k_z^2/2| \le \nu \le |k_z + k_z^2/2|$$
$$= -1 \text{ if } -|k_z + k_z^2/2| \le \nu \le -|k_z - k_z^2/2| \quad (12)$$
$$= 0 \text{ otherwise .}$$

The plasmon dispersion relation in RPA, obtained by solving $Q_0(\vec{k}k_F, 2\nu E_F/\hbar) = -1$ for ν, is then given by

$$\nu_{\rm pl}^2(\vec{k})_{\rm RPA} = k_z^2 + \frac{k_z^4}{4} + k_z^3 \coth \frac{k^2 k_z k_F \pi^2 \hbar^2}{2e^2 m} , \quad (13)$$

$$\nu_{\rm pl}^2(\vec{k})_{\rm RPA} \underset{k\to 0}{\longrightarrow} \frac{2e^2 m}{\pi^2\hbar^2 k_F}\left(\frac{k_z}{k}\right)^2 + k_z^2 + \frac{k_z^4}{4} + \frac{1}{3}\frac{\pi^2\hbar^2 k_F}{2e^2 m} k_z^4 k^2 + \cdots . \quad (14)$$

This dispersion has been discussed previously.[5] It should be noted that a second zero of the real part of the RPA dielectric function is given by (13) with the hyperbolic tangent instead of the hyperbolic cotangent. However, one can show that this branch is strongly damped, because it lies in a region where the imaginary part differs from zero.

The integral (7), describing the exchange effects, can be evaluated in this free-electron model. For propagation along the chain axis one obtains

$$G^{\rm FE}_{k_\perp=0}(\vec{k}k_F, 2\nu E_F/\hbar) = -8k^2 f(\vec{k}, \nu)\{\nu k^2/[(\nu + k^2/2)^2 - k^2] \times [(\nu - k^2/2)^2 - k^2]\}^2 . \quad (15)$$

In the long-wavelength limit, these exchange effects yield a contribution of order k^4 to the plasmon dispersion. This is essentially the same conclusion as obtained from the anisotropic mass treatment in the free-electron model for $(\mathrm{SN})_x$.[4] The free-electron model therefore seems not appropriate for reproducing the negative plasmon dispersion in TTF-TCNQ, and no substantial corrections are to be expected from including the exchange interaction, at least in the long-wavelength limit.

IV. ONE-DIMENSIONAL TIGHT-BINDING MODEL, INCLUDING EXCHANGE

For the case of conduction electrons occupying a single one-dimensional tight-binding band, we consider the one-electron energies for wave vector q parallel to the chain axis:

$$E(\hbar q) = 2E_F w(1 - \cos qb) , \quad (16)$$

where w is half the bandwidth in units of twice the Fermi energy, and b is the length of the one-dimensional unit cell. From the definition (8) for the quantity $\Delta_{\vec{k}}(\vec{\xi})$, occuring in the integrals (6) and (7), one obtains

$$\Delta_{\vec{k}}(\vec{\xi}) = 2w \sin\xi\alpha \sin\tfrac{1}{2}k\alpha \quad (17)$$

for $\vec{k}$ and $\vec{\xi}$ parallel to the chain, and where

$$\alpha = bk_F \quad (18)$$

measures the position of the Fermi energy in the band, $\alpha = \frac{1}{2}\pi$ meaning a half-filled band and $\alpha = \pi$ a completely filled band.

By using (10) and (17), and with some elementary substitutions, the expression (6) for the Lindhard polarizability becomes

$$Q_0^{\rm TB}(\vec{k}k_{\hat{F}}, 2\nu E_F/\hbar) = \frac{e^2 k_F}{2\pi^2 E_F}\frac{1}{k^2}\int_{-k_z/2}^{k_z/2} dz \frac{-4w \sin\frac{1}{2}k_z\alpha \sin\alpha \cos z\alpha}{\nu^2 - 4w\nu \sin\frac{1}{2}k_z\alpha \cos\alpha \sin z\alpha + 4w^2 \sin^2\frac{1}{2}k_z\alpha \sin(z+1)\alpha \sin(z-1)\alpha} . \quad (19)$$

Putting

$$\beta = 4w(|\nu^2 - 4w^2 \sin^2\tfrac{1}{2}\alpha k_z|)^{1/2} \sin^2\tfrac{1}{2}\alpha k_z \sin\alpha , \quad (20a)$$

$$\gamma = \nu^2 - 4w^2(\sin^2\alpha + \sin^2\tfrac{1}{2}\alpha k_z)\sin^2\tfrac{1}{2}\alpha k_z , \quad (20b)$$

one obtains by evaluating (19)

$$Q_0^{\rm TB}(\mathrm{k}k_F, 2\nu E_F/\hbar) = -\frac{e^2 k_F}{2\pi^2 E_F}\frac{1}{k^2}\frac{1}{\alpha}\frac{1}{(|\nu^2 - 4w^2\sin^2\frac{1}{2}\alpha k_z|)^{1/2}} \tan^{-1}(\beta/\gamma) \text{ if } |\nu| \ge |2w \sin k_z\alpha| , \quad (20c)$$

$$Q_0^{\rm TB}(\vec{k}k_F, 2\nu E_{\hat{F}}/\hbar = -\frac{e^2 k_F}{2\pi^2 E_F}\frac{1}{k^2}\frac{1}{\alpha}\frac{1}{(|\nu^2 - 4w^2\sin^2\frac{1}{2}\alpha k_z|)^{1/2}}\left(\ln\left|\frac{\gamma+\beta}{\gamma-\beta}\right| + i\pi J\right) \text{ if } |\nu| \le |2w\sin k_z\alpha| , \quad (20d)$$

$$J = 1 \text{ if } \beta > |\gamma|$$
$$= 0 \text{ otherwise .} \quad (20e)$$

For a half-filled band ($\alpha = \frac{1}{2}\pi$) this expression reduces to the result discussed in[5] [Eq. (18) of Ref. 5]. In the long-wavelength limit, the Lindhard polarizability becomes

$$Q_0^{\mathrm{TB}}(\vec{k}k_F, 2\nu E_F/\hbar) \simeq -\frac{(\nu_{\mathrm{pl}}^{\mathrm{TB}})^2}{\nu^2}\cos^2\theta\left[1-\frac{1}{3}\left(\frac{k_z\alpha}{2}\right)^2+\frac{4w^2\sin^2\alpha}{\nu^2}\left(\frac{k_z\alpha}{2}\right)^2+\cdots\right], \tag{21}$$

where

$$(\nu_{\mathrm{pl}}^{\mathrm{TB}})^2=(e^2k_F/2\pi^2E_F)2w\alpha\sin\alpha . \tag{22}$$

Thus the plasmon dispersion in RPA becomes

$$[\nu_{\mathrm{pl}}^{\mathrm{TB}}(\vec{k})]^2_{\mathrm{RPA}} \simeq (\nu_{\mathrm{pl}}^{\mathrm{TB}})^2\cos^2\theta+\frac{1}{3}\left(\frac{k_z\alpha}{2}\right)^2\left[-(\nu_{\mathrm{pl}}^{\mathrm{TB}})^2\cos^2\theta+12w^2\sin^2\alpha\right]+\cdots \tag{23}$$

which for a half-filled band ($\alpha=\frac{1}{2}\pi$) is exactly the expression obtained in[5] [See Eq. (23) of Ref. 5].

From (23) the slope of the plasmon dispersion is not only determined by the ratio between the bandwidth and the plasma frequency, but it also directly depends on the position of the Fermi energy in the band. However, because one expects the band in TTF-TCNQ to be almost half-filled, no substantial corrections arise from this effect.

In order to estimate the influence of the exchange interaction in this model, one has to evaluate (7) under the assumptions (10) and (17). It seems not possible to obtain this integral analytically for arbitrary wave vector and frequency. But in the long-wavelength limit, with $\vec{k}$ parallel to the chain, one obtains

$$\begin{aligned} G^{\mathrm{TB}}_{\vec{k}_\perp=0}(\vec{k}k_F, 2\nu E_F/\hbar) &\underset{k\to 0}{\longrightarrow} -\frac{1}{2}\frac{f(\vec{k},\nu)}{\nu^2}\left(\int_{-1-k/2}^{1-k/2}dz-\int_{-1+k/2}^{1+k/2}dz\right)\left(\int_{-1-k/2}^{1-k/2}dz'-\int_{-1+k/2}^{1+k/2}dz'\right)A_{k,\nu}(z,z')\\ &=-\frac{1}{2}\frac{f(\vec{k},\nu)}{\nu^4}\int_{-k/2}^{k/2}dz\int_{-k/2}^{k/2}dz'[A_{k,\nu}(z-1,z'-1)-A_{k,\nu}(z+1,z'-1)-A_{k,\nu}(z-1,z'+1)+A_{k,\nu}(z+1,z'+1)], \end{aligned} \tag{24}$$

where

$$A_{k,\nu}(z,z')=4w^2\sin^2\frac{k\alpha}{2}\left(\frac{\sin z\alpha-\sin z'\alpha}{z-z'}\right)^2 . \tag{25}$$

To lowest order in k, (25) can be replaced by

$$A_{k,\nu}(z-1,z'-1)=A_{k,\nu}(z+1,z'+1)\simeq 4w^2\alpha^2(\tfrac{1}{2}k\alpha)^2\cos^2\alpha , \tag{26}$$

$$A_{k,\nu}(z-1,z'+1)=A_{k,\nu}(z+1,z'-1)\simeq 4w^2(\tfrac{1}{2}k\alpha)^2\sin^2\alpha , \tag{27}$$

and thus, in the long-wavelength limit (24) becomes

$$G^{\mathrm{TB}}_{\vec{k}_\perp=0}(\vec{k}k_F, 2\nu E_F/\hbar) \underset{k\to 0}{\simeq} -16f(\vec{k},\nu)(w^2/\nu^4)[\cos^2\alpha-(\sin^2\alpha)/\alpha^2](\tfrac{1}{2}k\alpha)^4 . \tag{28}$$

Using this result with the long-wavelength expansion (21) for the Lindhard polarizability in the expression (1) for the dielectric function, one obtains

$$\epsilon^{\mathrm{TB}}_{\vec{k}_\perp=0}(\vec{k}k_F, 2\nu E_F/\hbar) \underset{k\to 0}{\simeq} 1-\frac{(\nu_{\mathrm{pl}}^{\mathrm{TB}})^2}{\nu^2}\left[1-\frac{1}{3}\left(\frac{k\alpha}{2}\right)^2+\frac{1}{\nu^2}\left(\frac{k\alpha}{2}\right)^2\left(4w^2\sin^2\alpha-\tfrac{1}{2}(\nu_{\mathrm{pl}}^{\mathrm{TB}})^2\frac{(\sin^2\alpha)/\alpha^2-\cos^2\alpha}{\sin^2\alpha}\right)\right] \tag{29}$$

and thus the plasmon dispersion for small wave vectors parallel to the chain axis, and including exchange, becomes

$$[\nu_{\mathrm{pl}}^{\mathrm{TB}}(\vec{k})]^2_{\vec{k}_\perp=0} \underset{k\to 0}{\simeq} (\nu_{\mathrm{pl}}^{\mathrm{TB}})^2+\frac{1}{3}\left(\frac{k_z\alpha}{2}\right)^2\left[-(\nu_{\mathrm{pl}}^{\mathrm{TB}})^2+12w^2\sin^2\alpha-\frac{3}{2}\frac{(\nu_{\mathrm{pl}}^{\mathrm{TB}})^2}{\sin^2\alpha}\left(\frac{\sin^2\alpha}{\alpha^2}-\cos^2\alpha\right)\right]. \tag{30}$$

Because

$$(\sin^2\alpha)/\alpha^2-\cos^2\alpha \geq 0 \quad \text{if } \alpha \leq 0.64577\pi \tag{31}$$

the exchange interaction in the tight-binding model thus reduces the slope of the plasmon dispersion if the band is not nearly filled, as can be seen be comparing (30) to the RPA result (23).

Assuming in TTF-TCNQ the numerical values 0.75 eV for the band width,[13] and 0.295π for α from the experimental observation of the $2k_F$

anomaly,[14,15] it then follows that $\omega_p^2(q) \cong \omega_p^2(0) - \gamma(qb/\pi)^2$ with $\gamma = 0.07$ eV^2 in RPA, whereas γ becomes 0.48 eV^2 by including exchange from (30). Thus in the tight-binding model for one-dimensional systems, the slope of the plasmon dispersion for propagation along the chain is drastically influenced by exchange. In TTF-TCNQ, the RPA dispersion is almost dispersionless at small q, but a pronounced negative slope is obtained by including exchange, in at least qualitative agreement with experimental data.

For a quantitative comparison with experiment at finite q and for nonparallel incidence, the exchange effects are to be obtained from numerically integrating (7). This study is in progress and is rather important because at large momentum transfer, substantial further corrections could occur, as possibly indicated by the diffuse $4k_F$ scattering in TTF-TCNQ.[16] Among other interpretations,[17-19] this anomaly has been explained in terms of umklapp scattering of two electrons across the Fermi sea,[20] involving a correlated state of electron charge-density waves. The strong electron correlation needed for this mechanism is not included in the present paper, and the large q plasmon dispersion might reveal the effectiveness of this interaction.

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