Plasmons localized at point charges in semiconductor quantum wells

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The plasmon excitations of inhomogeneous carrier gases in semiconductor quantum wells in the presence of charged impurities are investigated. The random phase approximation for the carrier gas yields an integral equation which expresses the condition that plasmons may be self-consistently localized in the vicinity of the impurity. The localized plasmon is a density wave trapped at the impurity site and exists in the electron (hole) gas only for negative (positive) impurity charge. Bound states of the intersubband plasmon are found for all densities of the carrier gas in a quantum well, a result which differs qualitatively from the bulk case. Numerical results for the binding energies are given for a range of parameters.

I. INTRODUCTION

Both collective effects such as plasmons and also impurity bound states have been of considerable interest in recent studies of semiconductor quantum wells. The confinement provided by the heterostructure permits the investigation of the role of dimensionality on these properties. For example, recent experimental work suggests that plasmons may be bound by neutral donors in quantum wells.[1] The case of a plasmon bound at a point charge in a bulk electron gas was investigated earlier theoretically.[2,3] There it was found[3] that in a doped semiconductor bound plasmon states can exist only for densities below a low threshold, which is not in the regime of physical interest (see Appendix A). The physical picture of a bound plasmon in the bulk case is that the electron density is reduced in the vicinity of the negative point charge which lowers the plasmon energy there. The density nonuniformity causes plasmon scattering and may give rise to a bound plasmon state.[2] The latter is a density wave trapped at the impurity. Such states may have interesting effects on optical and transport properties.

In the case of a semiconductor quantum well (QW) with finite electron or hole density, there are both intrasubband plasmons which are associated with a single carrier subband, and also intersubband plasmons which are associated with carrier transitions between two subbands.[4,5] The dispersion of the intrasubband plasmon begins from zero energy and does not have an upper bound. On the other hand, for intersubband plasmons, as for the bulk plasmons, there is a lower bound to the energy dispersion curve. As will be seen from the discussion below this feature permits the existence of the bound state of the intersubband plasmon. The system which we study here is an electron or hole gas in the presence of a point charge. This model represents physical systems containing various charge configurations. These include single ionized donors or acceptors, which exist in states having one or a few units of charge, or clusters of defects which have a greater charge. The extended intrasubband and intersubband plasma excitations in a quantum well are illustrated schematically in Fig. 1.

The random phase approximation (RPA) is commonly used to derive the collective elementary excitations of the electron gas in a quantum well.[4,5] We have used an approach suggested by Sham[3] to obtain an extension of the RPA for the inhomogeneous electron gas and to derive an integral equation for the bound state of a plasmon. A brief description of our treatment of the quantum well case was presented earlier,[6] where an equation for the bound state was derived and investigated qualitatively by using a separable approximation and sharp cutoff in

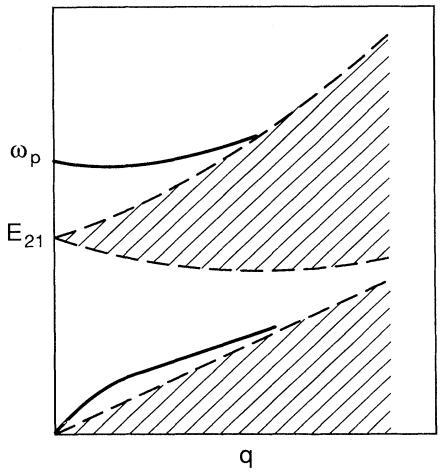

FIG. 1. Sketch of the energies of plasma excitations in a semiconductor quantum well vs wave vector. The lower solid curve represents an intrasubband plasmon, and the upper solid curve represents an intersubband plasmon. E_{21} is the energy separation between two subbands. The lightly hashed areas represent single-particle excitations.

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momentum space for the kernel of the integral equation. Here, a more complete treatment is presented, and the integral equation for the bound state is solved numerically with screening QW form factors properly taken into account. We find that a bound state of the (intersubband) plasmon exists for an arbitrary high density of the electron or hole gas. This behavior is different from that for the bulk case.[2,3] Explicit results for the binding energies are obtained as functions of doping density, QW width, and carrier effective mass.

This paper is organized as follows. In Sec. II the model of the electron or hole gas in a QW is defined, and the necessary formalism is described. In Sec. III an equation for the collective excitations is derived, and the approximations used are described. The numerical solution for the bound state is given in Sec. IV for ranges of parameters. The results are discussed in Sec. V. A brief description of the problem in the bulk case is presented in Appendix A. The discussion there makes clear the qualitative differences between plasmon localization by a charge in a bulk semiconductor and in a quantum well. The interaction matrix elements and form factors for the Coulomb interaction in the quantum well are given in Appendix B, and the parameters describing the long-wavelength dispersion of free QW plasmons are given in Appendix C.

II. RPA FOR AN INHOMOGENEOUS ELECTRON GAS IN A QUANTUM WELL

In real space the position of the carrier is given by a three-dimensional (3D) vector $\mathbf{R}=(\mathbf{r},z)$, where $\mathbf{r}$ is a 2D vector and z is taken along the growth direction. Let $c^{\dagger}(\mathbf{r},z)$ be a carrier creation operator in second quantization. The density operator is given by $\hat{\rho}(\mathbf{r}z)=c^{\dagger}(\mathbf{r},z)c(\mathbf{r},z)$. Calculations will be performed in the basis $|n,\mathbf{k}\rangle$ where n is a QW subband index, and $\mathbf{k}$ is a 2D wave vector. Correspondingly,

$$c(\mathbf{r},z)=A^{-1/2}\sum_{\mathbf{k}} c_n(\mathbf{k})\exp(i\mathbf{k}\cdot\mathbf{r})\xi_n(z) , \tag{2.1}$$

where $\xi_n(z)$ is a subband wave function of a one-dimensional confining potential and can always be chosen as real; A is the normalization area.

To derive a linear-response equation for the inhomogeneous QW system, we introduce an off-diagonal density operator,

$$\hat{\rho}(\mathbf{r},z_1,z_2)=c^{\dagger}(\mathbf{r},z_1)c(\mathbf{r},z_2) . \tag{2.2}$$

In the $|n,\mathbf{r}\rangle$ basis,

$$\hat{\rho}(\mathbf{r},z_1,z_2)=\sum_{nm} f_{nm}(z_1,z_2)\hat{\rho}_{nm}(\mathbf{r}) , \tag{2.3}$$

where

$$f_{nm}=\xi_n(z_1)\xi_m(z_2) ,$$

$$\hat{\rho}(\mathbf{r})=c_n^{\dagger}(\mathbf{r})c_m(\mathbf{r}) ,$$

and in the $|n,\mathbf{k}\rangle$ basis

$$\hat{\rho}(\mathbf{r},z_1,z_2)=A^{-1}\sum_{\mathbf{q},nm}\exp(-i\mathbf{q}\cdot\mathbf{r})f_{nm}(z_1,z_2)\hat{\rho}_{nm}(\mathbf{q}) ,$$

$$\hat{\rho}_{nm}(\mathbf{q})=\sum_{\mathbf{k}} c_n^{\dagger}(\mathbf{k}+\mathbf{q})c_m(\mathbf{k}) .$$

A weak external charge distribution described by the operator $\rho^{\rm ext}$ with matrix elements $\rho_{ij}^{\rm ext}(\mathbf{r})$ couples to the carrier gas and changes the Hamiltonian H to $H+H_{\rm ext}$ with

$$H_{\rm ext}=\int d\mathbf{r}\,dz\,dz'\rho(\mathbf{r},z)V(\mathbf{r},z,z')\rho^{\rm ext}(\mathbf{r},z') ,$$

where V is the Coulomb interaction. This external perturbation induces a change $\delta\rho_{nm}(\mathbf{r})$ in the subband matrix elements of the operator $\hat{\rho}(\mathbf{r};z,z')$, and the usual derivation of the linear response[7] gives

$$\delta\rho_{nm}(\mathbf{r},t)=\hbar^{-1}\int dt\,d\mathbf{r}'d\mathbf{r}''\sum_{plij} D_{nm,pl}(\mathbf{r},\mathbf{r}';t-t')\times V_{pl,ij}(\mathbf{r}'-\mathbf{r}'')\delta\rho_{ij}^{\rm ext}(\mathbf{r}'') , \tag{2.4}$$

where the retarded density response function D is defined as

$$D_{nm,pl}(\mathbf{r},\mathbf{r}';t-t')=-i\theta(t-t')\langle[\hat{\rho}_{nm}(\mathbf{r},t),\hat{\rho}_{pl}^{\dagger}(\mathbf{r}',t')]\rangle . \tag{2.5}$$

Here, $\hat{\rho}(\mathbf{r},t)$ is a Heisenberg operator $e^{-iHt}\hat{\rho}(\mathbf{r})e^{iHt}$, and in case of zero temperature the expectation value is taken in a ground state of H. The interaction matrix element is defined by

$$V_{mn,ij}(\mathbf{r})=\int dz\,dz'V(\mathbf{r};zz')\xi_m(z)\xi_n(z)\xi_i(z')\xi_j(z') .$$

In the $|n,\mathbf{k}\rangle$ basis and after Fourier transformation in time,

$$\delta\rho_{nm}(\mathbf{k},\omega)=(A\hbar)^{-1}\sum_{ijpl}\sum_{\mathbf{k}'} D_{nm,pl}(\mathbf{k},\mathbf{k}';\omega)V_{pl,ij}(\mathbf{k}')\delta\rho_{ij}^{\rm ext}(\mathbf{k}',\omega) . \tag{2.6}$$

The change of the total carrier density in the presence of $H_{\rm ext}$ is

$$\delta\rho_{nm}^{T}(\mathbf{k},\omega)=\delta\rho_{nm}(\mathbf{k},\omega)+\delta\rho_{nm}^{\rm ext}(\mathbf{k},\omega) .$$

We define the off-diagonal dielectric operator $\hat{\varepsilon}$ in the momentum space in analogy to that in the homogeneous system[7] in the operator form as

$$\hat{\varepsilon}^{-1}=\hbar^{-1}\hat{D}\hat{V}+\hat{I} ,$$

so that

$$\delta\rho_{nm}^{T}(k,\omega)=\sum_{mn,\mathbf{k}'}\varepsilon_{nm,ij}^{-1}(\mathbf{k},\mathbf{k}';\omega)\delta\rho_{ij}^{\rm ext}(\mathbf{k}',\omega) . \tag{2.7}$$

Inverting Eq. (2.7) and defining the collective excitations by the condition $\delta\rho^{\rm ext}=0$ while $\delta\rho^{T}\neq 0$, we obtain an equation for the collective excitations of the system H,

$$\int d\mathbf{k}'\sum_{ij}\varepsilon_{mn,ij}(\mathbf{k},\mathbf{k}';\omega)\delta\rho_{ij}^{T}(\mathbf{k}',\omega)=0 . \tag{2.8}$$

Here, and elsewhere, the $\mathbf{k}$ sums are converted to the 2D integrals by

$$\sum_k \rightarrow (2\pi)^{-2} A \int d\mathbf{k} \ .$$

Our next task is the evaluation of $\varepsilon(\mathbf{k},\mathbf{k}';\omega)$ for an electron or hole gas in a QW in the presence of a fixed point charge. Here we will be interested in bound states of the intrasubband and intersubband plasmons, and thus we will include only the first two levels in a symmetric quantum well with only the lowest level occupied by carriers. Tunneling into the barrier will be neglected in this calculation.

The Hamiltonian for the system in second quantization is

$$\begin{aligned}
&H = H_c + H_{c\text{-}i} \ , \\
&H_c = K + H_{\text{int}} = \sum_{\mathbf{k};n=1,2} \varepsilon_n(\mathbf{k}) c_n^\dagger(\mathbf{k}) c_n(\mathbf{k}) + (2A)^{-1} \sum_{\mathbf{q}\neq 0} [V_{11,11}(\mathbf{q})\hat{\rho}_1(\mathbf{q})\hat{\rho}_1(-\mathbf{q}) + 2V_{11,22}\hat{\rho}_2(\mathbf{q})\hat{\rho}_2(-\mathbf{q})] \\
&\quad + (2A)^{-1} \sum_{\mathbf{k}\mathbf{k}'q} \{ [V_{12,12}(\mathbf{q}) c_1^\dagger(\mathbf{k}) c_2(\mathbf{k}+\mathbf{q}) c_1^\dagger(\mathbf{k}') c_2(\mathbf{k}'-\mathbf{q}) + (1 \leftrightarrow 2)] \\
&\qquad + [V_{12,21}(\mathbf{q}) c_1^\dagger(\mathbf{k}) c_2(\mathbf{k}+\mathbf{q}) c_2^\dagger(\mathbf{k}') c_1(\mathbf{k}'-\mathbf{q}) + (1 \leftrightarrow 2)] \} \ , \\
&H_{c\text{-}i} = -A^{-1} \sum_{\mathbf{q}\neq 0;n} Z V_{nn}(\mathbf{q}) \hat{\rho}_n(\mathbf{q}) \ .
\end{aligned} \tag{2.9}$$

H_c represents a system of charged carriers including the carrier-carrier Coulomb interactions; $H_{c\text{-}i}$ represents the interaction of carriers with impurity of charge Ze. The Coulomb matrix elements are given by

$$V_{ij,mn}(\mathbf{q}) = \int dz\, dz' \xi_i(z)\xi_j(z) V_q(z-z') \xi_m(z')\xi_n(z') \tag{2.10}$$

and

$$V_{mn}(\mathbf{q}) = \int dz\, \xi_m(z) V_q(z) \xi_n(z) \ , \tag{2.11}$$

where $V_q(z)$ is a 2D Fourier transformation of the Coulomb potential energy $V(\mathbf{r},z-z')$ and is given by[4]

$$V_q(z) = (2\pi e^2/\varepsilon_\infty q) \exp(-q|z|) \ . \tag{2.12}$$

In this equation the background dielectric constant is taken to be the high-frequency value for the frequencies larger than LO-phonon frequency ω_{LO}. In the isotropic effective-mass approximation,

$$\varepsilon_n(\mathbf{k}) = \hbar^2 k^2/2m + E_n \ ,$$

where E_n is a QW subband energy. The density operator $\hat{\rho}_n$ is a diagonal part of $\hat{\rho}_{nm}$ in momentum space,

$$\hat{\rho}_n(\mathbf{q}) = \sum_{\mathbf{k}} c_n^\dagger(\mathbf{k}+\mathbf{q}) c_n(\mathbf{k}) \ . \tag{2.13}$$

In actual calculations we will take

$$\begin{aligned}
\xi_1(z) &= \sqrt{2/L} \cos(\pi z/L)\theta(L/2-|z|) \ , \\
\xi_2(z) &= \sqrt{2/L} \sin(2\pi z/L)\theta(L/2-|z|) \ .
\end{aligned} \tag{2.14}$$

Explicit expressions for the interaction matrix elements in this model are given in Appendix B.

A detailed treatment of the homogeneous electron gas in a QW can be found in Ref. 4. In order to extend it to the present case which lacks the translational invariance in the QW plane, we define a time-ordered Green's function which is off diagonal in $\mathbf{k}$ space,

$$\hbar G_{nm}(\mathbf{k},\mathbf{k}';t) = -i\langle \Psi_0 | T c_n(\mathbf{k},t) c_m^\dagger(\mathbf{k}',0) | \Psi_0 \rangle \ , \tag{2.15}$$

where $c_n(\mathbf{k},t)$ is a Heisenberg operator $e^{-iHt} c_n(\mathbf{k}) e^{iHt}$. In order to derive a perturbation theory formalism for H, we rewrite Eq. (2.9) as

$$\begin{aligned}
&H = H_0 + H_{\text{int}} \ , \\
&H_0 = K + H_{c\text{-}i} \ .
\end{aligned}$$

Dyson's equation and the RPA then can be derived in close analogy to the homogeneous QW case.[4,5] We define a density propagator as a time-ordered correlation function,

$$D^T_{nm,ij}(\mathbf{k},\mathbf{k}';t) = -i\langle \Psi_0 | T \hat{\rho}_{nm}(\mathbf{k},t) \hat{\rho}_{ij}^\dagger(\mathbf{k}',0) | \Psi_0 \rangle \ . \tag{2.16}$$

It satisfies the usual Dyson's equation in operator form,[7]

$$D^T = \Pi + \Pi V D^T \ ,$$

where Π is an irreducible part of D^T, and V is the bare Coulomb interaction. The lowest-order term in the perturbation expansion of the irreducible part is given by

$$\begin{aligned}
&\Pi^0_{nm}(\mathbf{k},\mathbf{k}';\omega) \\
&\quad = (2\pi)^{-4} \int d\mathbf{q}\, d\mathbf{q}' \int_{-\infty}^{\infty} d\omega' G_n(\mathbf{q},\mathbf{q}';\omega+\omega') \\
&\qquad \times G_m(\mathbf{k}+\mathbf{q},\mathbf{k}'+\mathbf{q}';\omega') \ ,
\end{aligned} \tag{2.17}$$

where $G_n(\mathbf{k},\mathbf{k}';\omega)$ is the (n,n) component of the electron propagator for $H_0 = K + H_{c\text{-}i}$, i.e., for the system of independent electrons interacting with the impurity. This term is shown diagrammatically in Fig. 2. The RPA is derived by same general arguments as in a homogeneous bulk case. We define the operator Π^R by

$$\begin{aligned}
&\text{Re}\Pi^R(\omega) = \text{Re}\Pi^0(\omega) \ , \\
&\text{Im}\Pi^R(\omega) = (\text{sgn}\omega)\text{Im}\Pi^0(\omega) \ .
\end{aligned} \tag{2.18}$$

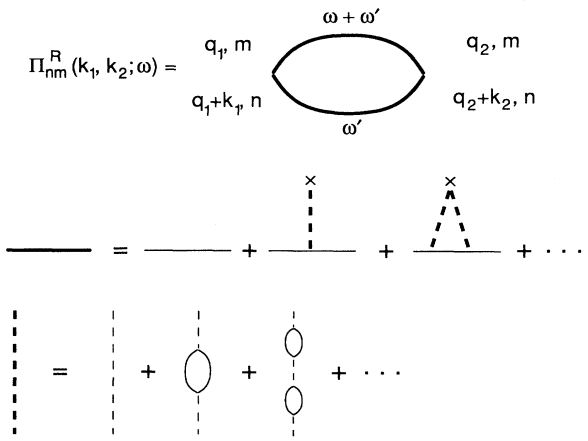

FIG. 2. The random-phase approximation for the density propagator Π_{nm}. The thick solid line represents the one-particle propagator of the system of independent carriers in the presence of impurity. In the approximation employed here the impurity-carrier interaction is separately screened in the RPA.

Then, from Dyson's equation for D^T and the definition of the inverse dielectric operator $\hat{\varepsilon}^{-1}$, we obtain the RPA for ε in operator form,

$$\hat{\varepsilon}=I-\Pi^R V \ . \tag{2.19}$$

We substitute this expression into Eq. (2.8) and obtain a system of coupled integral equations. Omitting the explicit ω dependence,

$$\begin{aligned}&\sum_{\mathbf{k}'}[\delta_{\mathbf{k}\mathbf{k}'}-\Pi^R_{12}(\mathbf{k},\mathbf{k}')V_{12,12}(k')]\delta\rho^T_{12}(\mathbf{k}')\\ &\qquad+\sum_{\mathbf{k}'}[-\Pi^R_{12}(\mathbf{k}\mathbf{k}')V_{12,21}(k')\delta\rho^T_{21}(\mathbf{k}')]=0\ ,\\ &\sum_{\mathbf{k}'}[-\Pi^R_{21}(\mathbf{k},\mathbf{k}')V_{21,12}(k')\delta\rho^T_{12}(\mathbf{k}')]\\ &\qquad+\sum_{\mathbf{k}'}[\delta_{\mathbf{k}\mathbf{k}'}-\Pi^R_{21}(\mathbf{k},\mathbf{k}')V_{21,21}(k')\delta\rho^T_{21}(\mathbf{k}')]=0\ .\end{aligned} \tag{2.20}$$

According to Eq. (2.10),

$$V_{12,12}(k)=V_{12,21}(k)=V_{21,21}(k)\ .$$

The two coupled integral equations (2.20) are decoupled simply by adding and subtracting them. By defining

$$\chi=\Pi^R_{12}+\Pi^R_{21} \tag{2.21}$$

and

$$g(\mathbf{k})=\delta\rho^T_{12}(\mathbf{k})+\delta\rho^T_{21}(\mathbf{k})\ , \tag{2.22}$$

we obtain an integral equation for the intersubband collective excitations

$$\sum_{\mathbf{k}'}[\delta_{\mathbf{k}\mathbf{k}'}-\chi(\mathbf{k},\mathbf{k}')V_{12,12}(\mathbf{k}')]g(\mathbf{k}')=0\ . \tag{2.23}$$

The carrier density in the $|\mathbf{k},z\rangle$ basis is related to the function $g(\mathbf{k})$ as

$$\delta\rho^T(\mathbf{k},z)=\xi_1(z)\xi_2(z)g(\mathbf{k})+\xi_1^2(z)\delta\rho^T_{11}(\mathbf{k})\ , \tag{2.24}$$

where ξ_i is a subband envelope wave function.

III. EVALUATION OF Π_{12} AND AN INTEGRAL EQUATION FOR THE LOCALIZED INTERSUBBAND PLASMON

In order to obtain an explicit integral equation from Eq. (2.23), we have to evaluate the polarization propagator $\Pi_{nm}(\mathbf{k},\mathbf{k}';\omega)$. In principle, we could use Eq. (2.17) if we knew $G(\mathbf{k},\mathbf{k}';\omega)$. However, for the gas of independent electrons interacting with an impurity via the Coulomb potential an exact expression for the one-particle Green's function is not known. Here we will develop an approximation for Π_{nm} using a spectral representation and evaluate it with what amounts to an infinite sequence of sum rules, as was suggested by Sham in the case of the bulk system.[3] In this way we shall derive in the next section a reasonable approximation for the kernel of the integral equation (2.23) together with a criterion for its validity.

As a digression we note that if one were to choose to model the carrier's interaction with an impurity by the point potential $\delta(\mathbf{r})$, an exact expression for $G(\mathbf{k},\mathbf{k}';\omega)$ in Eq. (2.17) would be available.[7] But even then the direct evaluation of Eq. (2.17) would still be very cumbersome.

The polarization propagator $\hbar\Pi_{nm}(\mathbf{k},\mathbf{k}';\omega)$ in the RPA is a time Fourier transformation of the retarded density-density correlation function,

$$D^R_{nm,nm}(\mathbf{k},\mathbf{k}';t)=-i\theta(t)\langle[\hat{\rho}_{nm}(\mathbf{k},t),\hat{\rho}^\dagger_{nm}(\mathbf{k}',0)]\rangle\ ,$$

which is a momentum Fourier transformation of the density-density response function $D(\mathbf{r},\mathbf{r}';t)$ defined in Eq. (2.5). Therefore it has a spectral representation easily derived by using the identity

$$\theta(t)=-\int_{-\infty}^{\infty}\frac{d\omega}{2\pi i}\frac{e^{-i\omega t}}{\omega+i\eta}$$

with $\eta\to+0$. We then have

$$\hbar\Pi^R_{nm}(\mathbf{k},\mathbf{k}';\omega)=\int_{-\infty}^{\infty}\frac{d\nu}{2\pi}\frac{\sigma_{nm}(\mathbf{k},\mathbf{k}';\nu)}{\omega-\nu+i\eta}\ , \tag{3.1}$$

where we have defined the spectral function per unit area as

$$\begin{aligned}&\sigma(\mathbf{k},\mathbf{k}';\omega)=\int_{-\infty}^{\infty}dt\,e^{i\omega t}\tilde{\sigma}(\mathbf{k},\mathbf{k}';t)\ ,\\ &\tilde{\sigma}(\mathbf{k},\mathbf{k}';t)=A^{-1}\langle[\hat{\rho}_{nm}(\mathbf{k},t),\hat{\rho}^\dagger_{nm}(\mathbf{k}',0)]\rangle\ .\end{aligned} \tag{3.2}$$

In terms of a complete set of eigenstates $|\alpha\rangle$ of the Hamiltonian H_0 defined as

$$H_0=K+H_{c\text{-}i}\ , \tag{3.3}$$

the spectral function at zero temperature is given by the following expression:

$$\sigma_{nm}(\mathbf{k},\mathbf{k}';\omega)=2\pi\sum_{\alpha}\{[\hat{\rho}_{nm}(\mathbf{k})]_{0\alpha}[\hat{\rho}_{nm}(\mathbf{k}')]^{*}_{0\alpha}\times\delta(E_{\alpha}-E_0-\omega)-[\hat{\rho}_{nm}(\mathbf{k})]_{\alpha 0}[\hat{\rho}_{nm}(\mathbf{k}')]^{*}_{\alpha 0}\times\delta(E_{\alpha}-E_0+\omega)\}\ , \tag{3.4}$$

where $[\hat{\rho}_{nm}]_{\alpha 0}\equiv\langle\alpha|\hat{\rho}_{nm}|0\rangle$ and $|0\rangle$ is being a ground state of H_0. The part diagonal in k is obviously real,

$$\sigma_{nm}(\mathbf{k},\mathbf{k};\omega)=2\pi\sum_{\alpha}|[\hat{\rho}_{nm}(\mathbf{k})]_{\alpha 0}|^2[\delta(E_{\alpha}-E_0-\omega)-\delta(E_{\alpha}-E_0+\omega)]\ .$$

Equations (3.4) and (3.1) constitute the Lehmann representation of Π^R. To keep the notation simpler, we omit the superscript R in Π^R. The off-diagonal part of $\sigma(\mathbf{k},\mathbf{k}';\omega)$, in general, is a complex number, and so is the polarization propagator. We shall use only the real part of the polarization Π in Eq. (2.23). Then, the solution will have a finite lifetime because for the general solution $\mathrm{Im}\omega\neq 0$. The lifetime will be estimated as in Ref. 2. Now we want an expression for $\mathrm{Re}\Pi_{nm}(\omega)$ in terms of $\sigma(\omega)$. From its definition, $\Pi(\omega)$ is an analytical function of ω in the upper half-plane and vanishes at infinity. Therefore, we can use the Kramers-Kronig relation which we substitute into (3.1) and obtain

$$\Pi(\omega)=P\int\frac{d\omega'}{2\pi}\frac{\sigma(\omega')}{\omega-\omega'}-iP\int\frac{d\omega'}{2\pi}P\int\frac{d\omega''\sigma(\omega'')}{2\pi(\omega'-\omega)(\omega'-\omega'')}\ .$$

If we expand $\sigma(\mathbf{k},\mathbf{k}';\omega)$ in a Taylor series in $\mathbf{k}$ and $\mathbf{k}'$ and find that to some order the expression $P\int d\omega'\sigma(\omega')/(\omega-\omega')$ is real, then it follows that to the same order in $\mathbf{k}$ and $\mathbf{k}'$,

$$\mathrm{Re}\Pi(\mathbf{k},\mathbf{k}';\omega)=P\int_{-\infty}^{\infty}\frac{d\nu}{2\pi}\frac{\sigma(\mathbf{k},\mathbf{k}';\nu)}{(\nu-\omega)}\ .$$

Now, we formally expand $(\omega-\nu)^{-1}$ in powers of ν and obtain

$$\int_{-\infty}^{\infty}\frac{d\nu}{2\pi}\frac{\sigma_{nm}(\nu)}{(\omega-\nu)}=(2\pi)^{-1}\sum_{p=1}^{\infty}\omega^{-p}\int_{-\infty}^{\infty}d\nu\,\nu^{p-1}\sigma_{nm}(\nu)\ . \tag{3.5}$$

We evaluate the right-hand side of this equation by using the Fourier transformation

$$(2\pi)^{-1}\int_{-\infty}^{\infty}d\nu\,\nu^{p}\sigma_{nm}(\nu)=(-i)^{p}\frac{\partial^{p}}{\partial t^{p}}\sigma_{nm}(t)|_{t=+0} \tag{3.6}$$

and evaluate this from the equations of motion for the Heisenberg operators $\rho(t)$, $\rho^{\dagger}(t)$,

$$i\hbar\frac{\partial\hat{\rho}}{\partial t}=[\hat{\rho},H_0]\ ,$$

with H_0 given by Eq. (3.3). In this way we obtain an infinite sequence of sum rules.[3]

It is clear on physical grounds that upon resummation we should end up with the expansion of $\Pi_{21}(\omega)$ in inverse powers of $(\omega^2-E_{21}^2)$, and indeed that will turn out to be the case. Evaluating the commutator $[\rho_{nm}(\mathbf{k}),\rho_{nm}(\mathbf{k}')]$ we obtain the first sum rule in terms of the Schrödinger operators,

$$(2\pi)^{-1}\int_{-\infty}^{\infty}d\nu\,\sigma_{nm}(\mathbf{k},\mathbf{k}';\nu)=\tilde{\sigma}_{nm}(\mathbf{k},\mathbf{k}';t=0)=A^{-1}\langle\hat{\rho}_{nn}(\mathbf{k}-\mathbf{k}')-\hat{\rho}_{mm}(\mathbf{k}-\mathbf{k}')\rangle\ . \tag{3.7}$$

Recall that in terms of c and $c^{\dagger}$,

$$\hat{\rho}_{nm}(\mathbf{k})=\sum_{\mathbf{q}}c_n^{\dagger}(\mathbf{k}+\mathbf{q})c_m(\mathbf{q})\ ,$$

$$\hat{\rho}(\mathbf{r})=A^{-1}\sum_{\mathbf{k}}e^{i\mathbf{k}\cdot\mathbf{r}}\hat{\rho}(\mathbf{k})\ .$$

We define the macroscopic density $n_j(\mathbf{r})$ as

$$n_j(\mathbf{r})=\langle\hat{\rho}_{jj}(\mathbf{r})\rangle \tag{3.8}$$

and

$$n_j(\mathbf{k})=A^{-1}\langle\hat{\rho}_{jj}(\mathbf{k})\rangle=A^{-1}\int d^2r\,e^{i\mathbf{k}\cdot\mathbf{r}}n(\mathbf{r})\ , \tag{3.9}$$

so the first sum rule in Eq. (3.7) can be written as

$$(2\pi)^{-1}\int_{-\infty}^{\infty}d\nu\,\sigma_{nm}(\mathbf{k},\mathbf{k}';\nu)=n_n(\mathbf{k}-\mathbf{k}')-n_m(\mathbf{k}-\mathbf{k}')\ . \tag{3.10}$$

The second sum rule is evaluated from Eq. (3.6) with $p=1$ and the repeated application of the equation of motion which yields

$$(2\pi)^{-1}\int_{-\infty}^{\infty}d\nu\,\nu\sigma_{nm}(\mathbf{k},\mathbf{k}';\nu)=E_{mn}[n_n(\mathbf{k}-\mathbf{k}')-n_m(\mathbf{k}-\mathbf{k}')]+(\hbar^2/2m)\mathbf{k}\cdot\mathbf{k}'[n_n(\mathbf{k}-\mathbf{k}')+n_m(\mathbf{k}-\mathbf{k}')]-ZA^{-1}\sum_{q\neq 0}[V_{mm}(\mathbf{q})-V_{nn}(\mathbf{q})][n_n(\mathbf{k}-\mathbf{k}'-\mathbf{q})-n_m(\mathbf{k}-\mathbf{k}'-\mathbf{q})]\ , \tag{3.11}$$

where $E_{mn}=E_m-E_n$ is the difference between the energies of the subbands m and n. From these and higher sum rules we learn that our expansion turns out to be also an expansion in powers of $\mathbf{k}$ and $\mathbf{k}'$. The corresponding expansion in the bulk case[3] starts with $O(\mathbf{k}\cdot\mathbf{k}')$ as seen in Appendix A. In contrast, the QW intersubband expansion starts with $O(1)$ in every sum rule for Eq. (3.6). The orders $O(k^2)$, $O(k'^2)$, and $O(\mathbf{k}\cdot\mathbf{k}')$ will be collectively referred to as $O(k^2)$. We only write down $O(1)$ orders in k explicitly in the higher sum rules.

We introduce the following notation:

$$\Delta V_{mn}(k)=V_{mm}(k)-V_{nn}(k)\ ,$$
$$\Delta n_{mn}(\mathbf{k})=n_m(\mathbf{k})-n_n(\mathbf{k})\ . \tag{3.12}$$

The next two sum rules to leading order in k are

$$(2\pi)^{-1}\int_{-\infty}^{\infty}d\nu\,\nu^2\sigma_{nm}(\mathbf{k},\mathbf{k}';\nu)=E_{mn}^2\Delta n_{nm}(\mathbf{k}-\mathbf{k}')-2ZE_{mn}A^{-1}\sum_{\mathbf{q}}\Delta n_{nm}(\mathbf{k}-\mathbf{k}'-\mathbf{q})\Delta V_{mn}(q)$$
$$+Z^2A^{-2}\sum_{\mathbf{q}\mathbf{q}'}\Delta n_{nm}(\mathbf{k}-\mathbf{k}'-\mathbf{q}-\mathbf{q}')\Delta V_{mn}(q)\Delta V_{mn}(q')+O(k^2) \tag{3.13}$$

and

$$(2\pi)^{-1}\int_{-\infty}^{\infty}d\nu\,\nu^3\sigma_{nm}(\mathbf{k},\mathbf{k}';\nu)=E_{mn}^3\Delta n_{nm}(\mathbf{k}-\mathbf{k}')-3ZE_{mn}^2A^{-1}\sum_{\mathbf{q}}\Delta n_{nm}(\mathbf{k}-\mathbf{k}'-\mathbf{q})\Delta V_{mn}(q)$$
$$+3Z^2E_{mn}A^{-2}\sum_{\mathbf{q}\mathbf{q}'}\Delta n_{nm}(\mathbf{k}-\mathbf{k}'-\mathbf{q}-\mathbf{q}')\Delta V_{mn}(q)\Delta V_{mn}(q')$$
$$-Z^3A^{-3}\sum_{\mathbf{q}\mathbf{q}'\mathbf{q}''}\Delta n_{nm}(\mathbf{k}-\mathbf{k}'-\mathbf{q}-\mathbf{q}'-\mathbf{q}'')\Delta V_{mn}(q)\Delta V_{mn}(q')\Delta V_{mn}(q'')+O(k^2)\ . \tag{3.14}$$

Substitution of these sum rules into the right-hand side (rhs) of Eq. (3.5) generates an expansion in powers of Z. Note that the part of the density $n(\mathbf{k})$ induced by the impurity charge Ze is itself $O(Z)$, but for now we classify the terms in the sum rules by the order of Z that explicitly appears as a factor in the expansion. Now we resum the rhs of Eq. (3.5) to all orders of frequency ω in each given order of Z. First, we resum all $O(Z^0)$ terms,

$$\Delta n_{nm}\omega^{-1}+\Delta n_{nm}E_{mn}\omega^{-2}+\Delta n_{nm}E_{mn}^2\omega^{-3}+\cdots=\Delta n_{nm}(\omega-E_{mn})^{-1}\ . \tag{3.15}$$

The corresponding term in the expansion of $\chi_{mn}=\Pi_{mn}+\Pi_{nm}$ will be

$$\Delta n_{nm}(\omega-E_{mn})^{-1}+\Delta n_{mn}(\omega-E_{nm})^{-1}=2\Delta n_{nm}E_{mn}(\omega^2-E_{mn}^2)^{-1}\ . \tag{3.16}$$

The series on the left-hand side (lhs) of Eq. (3.15) is convergent only if

$$|\omega/E_{mn}|>1\ . \tag{3.17}$$

In the case of intersubband plasmons of particular interest here, $n=1$, $m=2$, and Eq. (3.17) restricts the validity of the expansion to the physically reasonable region $\omega>E_{21}$. The terms to $O(Z)$ can be resumed as follows:

$$[-Z\omega^{-2}-2ZE_{mn}\omega^{-3}-3ZE_{mn}^2\omega^{-4}-\cdots]\sum_{\mathbf{q}}\Delta n_{nm}(\mathbf{k}-\mathbf{k}'-\mathbf{q})\Delta V_{mn}(q)=-Z(\omega-E_n)^{-2}\sum_{\mathbf{q}}\Delta n_{nm}(\mathbf{k}-\mathbf{k}'-\mathbf{q})\Delta V_{mn}(q)\ . \tag{3.18}$$

This contributes to χ_{nm} the following term:

$$-\frac{Z}{\omega^2-E_{mn}^2}\left[1+\frac{2E_{mn}^2}{\omega^2-E_{mn}^2}\right]A^{-1}\sum_{\mathbf{q}}\Delta n_{nm}(\mathbf{k}-\mathbf{k}'-\mathbf{q})\Delta V_{mn}(q)\ . \tag{3.19}$$

Similarly, the summation can be performed for every set of $O(Z^n)$ terms. This yields an expression for χ_{nm} as an expansion in orders of Z. Each term of the expansion involves successive convolutions in momentum space. The polarization χ can be written as

$$\chi_{nm}=\sum_{j=0}^{\infty}\{[t_{nm}]_j+[t_{mn}]_j\}\ , \tag{3.20}$$

where

$$[t_{nm}]_j=\frac{(-Z)^j}{(\omega-E_{mn})^{j+1}}A^{-j}$$
$$\times\sum_{\mathbf{q}_1\cdots\mathbf{q}_j}\Delta n_{nm}(\mathbf{k}-\mathbf{k}'-\mathbf{q}_1-\cdots-\mathbf{q}_j)$$
$$\times\Delta V_{mn}(q_1)\cdots\Delta V_{mn}(q_j)\ . \tag{3.21}$$

By transforming to the real space it is possible to perform the summation in Eq. (3.20). The Fourier transform

of ΔV can be written as a 1D integral. For example, for $n=1$, $m=2$, using Eqs. (3.12), (2.11), and (2.12) we obtain

$$\Delta V_{21}(\mathbf{r})=(2e^2/\varepsilon_\infty L)\int dz[\xi_1^2(z)-\xi_2^2(z)](z^2+r^2)^{-1/2} , \tag{3.22}$$

where $\xi_{1,2}$ is the QW envelope functions. The density Fourier transformation is defined in Eq. (3.9). So the leading term in the long-wavelength approximation takes the following form:

$$\chi_{nm}(\mathbf{k},\mathbf{k}';\omega)=(2\pi)^{-2}\int d^2r\, e^{(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}}\tilde{\chi}(\mathbf{r},\omega) ,$$
$$\tilde{\chi}(\mathbf{r},\omega)=2\Delta n_{nm}(\mathbf{r})\frac{E_{mn}-Z\Delta V_{mn}(\mathbf{r})}{\omega^2-[E_{mn}-Z\Delta V_{mn}(\mathbf{r})]^2} . \tag{3.23}$$

This leading term turns out to be a function of $\mathbf{k}-\mathbf{k}'$. Terms that would appear to $O(k^2)$ and higher order depend on k and k' differently, as seen in Eq. (3.11). Representation of χ by Eq. (3.23) produces an expression for the kernel of the integral equation which makes a numerical investigation quite complicated. A considerable simplification is achieved if $|Z\Delta V/E_{21}|$ is small enough to neglect $j\geq 1$ terms in Eq. (3.20). The criterion for this to be valid will be formulated below in terms of the momentum space functions.

In our model only the first QW level is occupied, so that $n_2=0$, and $\Delta n_{12}=n(\mathbf{k})$. Let us write the electron density as

$$n(\mathbf{k})=n_0\delta_{k,0}+\delta n(\mathbf{k}) ,$$
$$n(\mathbf{r})=n_0(\mathbf{r})+\delta n(\mathbf{r}) , \tag{3.24}$$

where $\delta n(\mathbf{r})$ is a change in the electron density due to the presence of impurity of charge Z^*e, where $Z^*=Z/\varepsilon_\infty$, an external charge screened by the dielectric background. It is the same charge density that appears in the Poisson equation for the response potential ϕ_{res} when an external perturbation ϕ_{ext} is applied. Using Eq. (2.3) we can write

$$\nabla^2\phi_{\text{res}}(\mathbf{r},z)=4\pi e\,\delta n(\mathbf{r})\xi_1^2(z) ,$$
$$\phi_T(\mathbf{r},z)=\phi_{\text{ext}}(\mathbf{r},z)+\phi_{\text{res}}(\mathbf{r},z) . \tag{3.25}$$

For the case of the hole gas one should replace e by $-e$ in this equation and in the definition of the impurity charge. Equation (3.25) implies that the impurity-carrier interaction is screened statically as indicated in Fig. 2. We define the QW average by

$$\bar{\phi}(\mathbf{k})=\int dz\,\phi(\mathbf{k},z)\xi_1^2(z)$$

and then the static screening of the impurity-carrier interaction is given by

$$\bar{\phi}_T(\mathbf{k})=\bar{\phi}_{\text{ext}}(\mathbf{k})/\varepsilon(k) . \tag{3.26}$$

We assume that the point charge is placed at the center of QW. From Eqs. (3.25) and (3.26) we obtain the linear screening approximation[3] for δn as

$$\delta n(k)=\frac{Z^*S(k)}{F(k)}\left[1-\frac{1}{\varepsilon(k)}\right] , \tag{3.27}$$

where

$$S(k)=\int dz\, e^{-k|z|}\xi_1^2(z) . \tag{3.28}$$

The form of $\varepsilon(k)$ for a QW static screening is given by[8]

$$\varepsilon(k)=1+(k_{\text{TF}}/k)F(k)G(k) , \tag{3.29}$$

where the screening form factor $F(k)$ is defined by

$$F(k)=\int dz\,dz'\xi_1^2(z)\xi_1^2(z')e^{-k|z-z'|} \tag{3.30}$$

and the function $G(k)$ takes into account the finite size of the Fermi surface,

$$G(k)=1 \text{ if } k<2k_F ,$$
$$G(k)=1-[1-(2k_F/k)^2]^{1/2} \text{ if } k>2k_F . \tag{3.31}$$

In these equations, k_F is a 2D Fermi momentum and k_{TF} is a 2D Thomas-Fermi momentum equal to the inverse of the 2D Bohr radius. Explicit expressions for the factors $S(k)$ and $F(k)$ are given in Appendix B.

Now we can formulate in momentum space a criterion for neglecting the $j\geq 1$ terms in Eq. (3.20) and thus retaining only the term given by Eq. (3.16) in the expansion of the polarizability. From Eqs. (3.23), (3.16), and (3.19) we deduce the following criterion:

$$|Z^*\langle\Delta V\rangle/E_{21}|\ll 1 ; \quad \langle\Delta V\rangle\equiv\sum_{\mathbf{k}}\Delta V_{12}(k)\delta n(\mathbf{k}) \tag{3.32}$$

and from Eqs. (3.27) and (3.29),

$$\langle\Delta V\rangle=(2\pi)^{-2}\int d^2k[V_{11}(k)-V_{22}(k)]\times\frac{S(k)G(k)}{k/k_{\text{TF}}+G(k)F(k)} . \tag{3.33}$$

The quantity $\langle\Delta V\rangle/E_{21}$ is shown in Fig. 3 as a function of QW width L for two typical carrier mass values. For given m and ε_∞ there exist a range of QW widths where

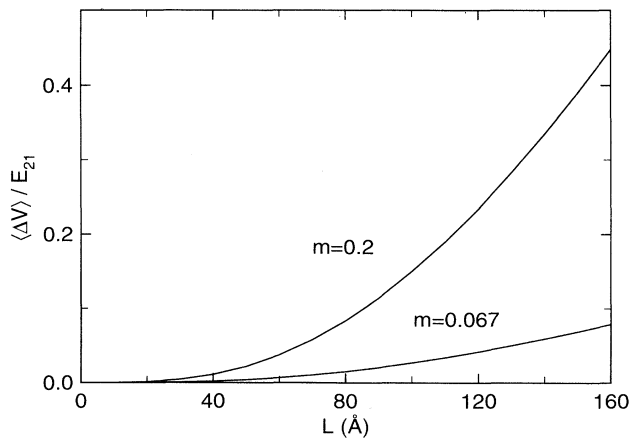

FIG. 3. The interaction parameter $\langle\Delta V\rangle/E_{21}$ defined in Eq. (3.32) is shown here as a function of QW width for volume density $n_v=1\times10^{18}$ cm^{-3}, $\varepsilon_\infty=10.9$, and two different values of carrier mass m/m_0.

$$|Z\langle\Delta V\rangle/E_{21}|<\tfrac{1}{2}\ .$$

Therefore, we suggest that for such range of parameter values the $j=0$ term in Eq. (3.20) is the dominant one. It is the term given by Eq. (3.16).

Now, Eqs. (3.24) and (3.23) are substituted into (2.23) to obtain an integral equation for the function $g(\mathbf{k})$ defined in (2.22). In the long-wavelength approximation for terms containing the unperturbed density $n_0\delta_{k,0}$ we need only the diagonal part $\chi(k)$ but to $O(k^2)$ in order to take proper account of the free plasmon dispersion.[2,3] With these approximations we obtain the following equation:

$$[k^2-(\mu E_{21}/\sigma)k-\mathcal{E}]g(\mathbf{k})+\frac{\alpha}{2n_0\sigma}\int\frac{d^2k'}{(2\pi)^2}2E_{21}\delta n(\mathbf{k}-\mathbf{k}')g(\mathbf{k}')=0\ , \tag{3.34}$$

where the energy parameter is defined as

$$\mathcal{E}=\frac{(\omega^2-\omega_0^2)\hbar^2\varepsilon_\infty}{4\pi e^2 n_0\sigma(\omega)}\ , \tag{3.35}$$

where ω_0 is the frequency of the intersubband plasmon at $k=0$ in the absence of impurity and is obtained from Eq. (C7) as $\omega_{\rm pl}(k=0)$; α, μ, and $\sigma(\omega)$ are coefficients in the long-wavelength approximation (LWA) expansion for plasmon dispersion and are defined in Appendix C in Eqs. (C2) and (C5). The LWA is compared to the full RPA for the free plasmon in Fig. 4. It is seen that the LWA, which will be used here for plasmon dispersion, gives a good approximation for the RPA at long wavelengths. The intersubband plasmon dispersion has a lower bound given by $\min\{\omega_{\rm pl}(k)\}$, and thus bound states may exist below it. Accordingly, for bound states,[2,3] $\mathcal{E}<0$. Expanding $g(\mathbf{k})$ in 2D spherical harmonics gives

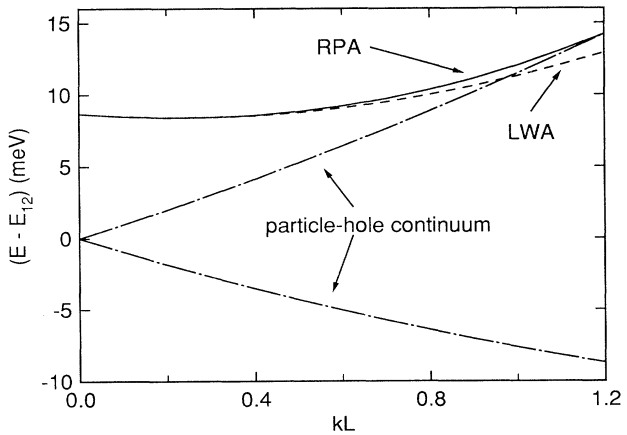

FIG. 4. Dispersion relations of the free intersubband plasmons in a QW. The system parameters here are $L=100$ Å, $\varepsilon_\infty=10.9$, $m=0.2m_0$, and the volume density is $n_v=1\times10^{18}$ cm^{-3}. Exact RPA is given by the solid curve, LWA is given by the dashed curve. The region for which there are single-particle intersubband excitations is indicated.

$$g(\mathbf{k})=\sum_{l=0}^{\infty}f_l(k)k^{-1/2}e^{il\theta} \tag{3.36}$$

and we obtain for the $l=0$ component the following integral equation:

$$[k^2-(\mu E_{21}/\sigma)k+|\mathcal{E}|]f_0(k)=-\frac{Z\alpha E_{21}}{2\pi n_0\sigma}\int_0^\infty dk'K_0(k,k')f_0(k')\ , \tag{3.37}$$

where

$$K_0(k,k')=\pi^{-1}\int_0^\pi d\theta(kk')^{1/2}\frac{G(\Delta k)S(\Delta k)}{\Delta k/k_{\rm TF}+F(\Delta k)G(\Delta k)}\ , \tag{3.38}$$

$$\Delta k\equiv|\mathbf{k}-\mathbf{k}'|=(k^2+k'^2-2kk'\cos\theta)^{1/2}\ .$$

By substituting

$$\phi_0(k)=f_0(k)[k^2-(\mu E_{21}/\sigma)k+|\mathcal{E}|]^{1/2} \tag{3.39}$$

we transform Eq. (3.37) into the integral equation with the symmetric kernel

$$\phi_0(k)=\int_0^\infty dk'K(k,k')\phi_0(k')\ , \tag{3.40}$$

$$K(k,k')=-\frac{Z^*\alpha E_{21}}{2\pi n_0\sigma}K_0(k,k')\times[k^2-(\mu E_{21}/\sigma)k+|\mathcal{E}|]^{-1/2}\times[k'^2-(\mu E_{21}/\sigma)k'+|\mathcal{E}|]^{-1/2}\ .$$

This equation has solutions only for $Z<0$. Recall that, by definition, here the impurity charge is Ze for the electron gas and $-Ze$ for the hole gas. If $|\mathcal{E}|=|\mathcal{E}_c|\equiv\mu^2E_{21}^2/4\sigma^2$ the kernel $K(k,k')$ will be singular. It follows then that by taking $\mathcal{E}$ sufficiently close to $\mathcal{E}_c$ a bound-state solution will be found at an arbitrary density.[6] This situation differs qualitatively from the bulk case for which a solution exists only for densities below a cutoff at some low value.[3]

IV. SOLUTION OF THE INTEGRAL EQUATION FOR THE BOUND STATE

In our previous work[6] we used a separable approximation for the kernel $K_0(\mathbf{k},\mathbf{k}')$ so as to reduce an integral equation to a simple transcendental equation. That required use of a cutoff in momentum space. That treatment of Eq. (3.40) would be adequate only at high density where binding is weak. Here, we will not use this separable approximation and instead we will solve Eq. (3.40) numerically "exactly" retaining the full QW screening in Eq. (3.38).

We define the eigenvalues λ of the integral equation (3.40) in a conventional way,[2]

$$\phi(k)=\lambda\int_0^\infty dk\,K(k,k')\phi(k') \tag{4.1}$$

so that λ^{-1} is an eigenvalue of the integral operator. Discretizing the momentum space turns this equation into a matrix equation. We define the binding energy as the difference between the minimum of the free plasmon energy $\omega_{\rm pl}(k)$ and the energy of the bound state,

$$\hbar\omega_b = \min\{\hbar\omega_{\rm pl}(k)\} - \hbar\omega \ , \tag{4.2}$$

where ω is related to the energy parameter $\mathcal{E}$ through Eq. (3.35). Equation (4.1) has a discrete (infinite) set of eigenvalues,

$$\lambda_0 < \lambda_1 < \lambda_2 < \cdots \ .$$

If we treat the binding energy ω_b as a parameter and plot each eigenvalue as a function of ω_b, solutions of the integral equation will be found from the equation $\lambda_i(\omega_b)=1$. We find that every inverse eigenvalue λ_i^{-1} is a monotonically decreasing function of the binding energy, which is similar to the bulk case.[2] It follows then that the lowest-lying state corresponds to the lowest eigenvalue λ_0 and that its binding energy $\hbar\omega_b$ is found from the following equation:

$$\lambda_0(\hbar\omega_b)=1 \ . \tag{4.3}$$

We find that λ_0 corresponds to a nodeless eigenfunction $\phi_0(k)$ which is shown in Fig. 5 for two different values of the QW width L. This function is related to the $l=0$ component of the function $g(\mathbf{k})$ defined in Eq. (2.24) through

$$g_0(k) = f_0(k)k^{-1/2} = k^{-1/2}[k_2 - (\mu E_{21}/\sigma k + |\mathcal{E}|]^{-1/2}\phi_0(k) \ . \tag{4.4}$$

The binding energy found from numerical solution of Eqs. (4.1) and (4.3) is shown in Fig. 6 for several values of the well width, dielectric constant, and carrier mass. In Fig. 6(a) the binding energy is displayed as a function of inverse volume density $1/n_V$ and in Fig. 6(b) as a function of the effective two-dimensional density $n_S = n_0$ obtained from the simple relation $n_S = Ln_V$. The important qualitative result obtained here is that for quantum well systems there is a finite plasmon binding for all densities with the binding energy approaching zero for very high densities [Fig. 6(a)]. This in contrast to the bulk case for which nonzero binding occurs only for densities below a low density cutoff.

The bound state has a finite lifetime due to decay into single-particle excitations. Let us write the dielectric function at complex frequency $\omega_1 + i\omega_2$ in Eq. (2.8) as a sum of the real and imaginary parts. Then, omitting the subband indices we obtain

$$\varepsilon(\mathbf{k},\mathbf{k}';\omega_1+i\omega_2) = \varepsilon_1(\mathbf{k},\mathbf{k}';\omega_1+i\omega_2) + i\varepsilon_2(\mathbf{k},\mathbf{k}';\omega_1+i\omega_2) \ . \tag{4.5}$$

We expand ε_1 and ε_2 in powers of ω_2, substitute in Eq. (2.8), and separate real and imaginary parts. The real part will give us an integral equation which was derived in Sec. III; the imaginary part retained to linear order in ω_2 will give an expression for ω_2 in terms of $\varepsilon_1(k,k';\omega_1)$ and $\varepsilon_2(k,k';\omega_1)$. Following Ref. 2 we use only the diago-

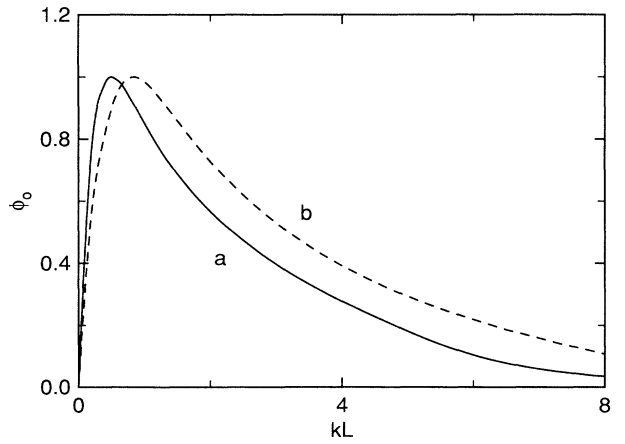

FIG. 5. Eigenfunctions of integral Eq. (3.40) corresponding to the lowest S state of the bound plasmon for two values of QW width: (a) $L=100$ Å, (b) $L=130$ Å. Both are normalized to max $\phi_0(k)=1$. The system parameters are volume density $n_v = 1\times10^{18}$ cm^{-3}, $\varepsilon_\infty = 10.9$, $m = 0.2m_0$, $|Z^*|=2$.

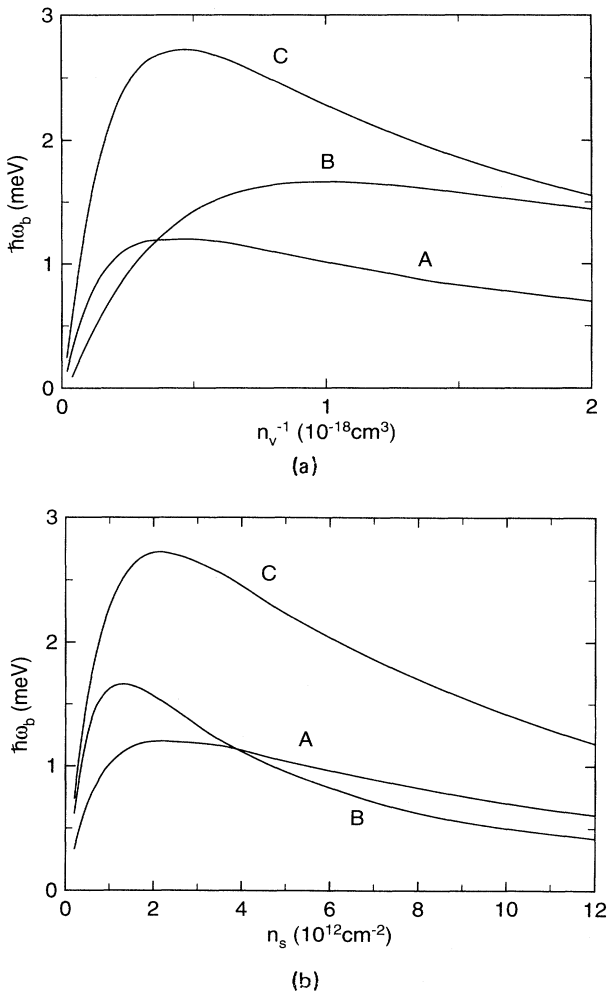

FIG. 6. The plasmon binding energy defined in Eq. (4.2) is shown here as a function of the inverse volume density (a) and as a function of the effective two-dimensional density $n_s = n_V L$ (b). The quantum-well systems illustrated here are the following: (A) well width $L=100$ Å, $m=0.2m_0$, $\varepsilon_\infty=10.9$, $|Z^*|=2$; (B) $L=130$ Å, $m=0.2m_0$, $\varepsilon_\infty=10.9$, $|Z^*|=2$; (C) $L=100$ Å, $m=0.16m_0$, $\varepsilon_\infty=7.3$, $|Z^*|=2$.

nal part of the dielectric function for an estimate of ω_2 and obtain an inverse lifetime from $\hbar/\tau=\omega_2$. In terms of the function $f_0(k)$ in Eq. (4.4), we obtain

$$\hbar/\tau \approx -\frac{\int dk\, f_0^2(k)\varepsilon_2(k,\omega)}{\int dk\, f_0^2(k)\frac{\partial\varepsilon_1}{\partial\omega}(k,\omega)} \tag{4.6}$$

evaluated at the eigenfrequency of the bound S state. In this equation we use the diagonal dielectric function for the QW evaluated in Ref. 4. For the parameter range indicated in Fig. 6 we find that the inverse lifetime is comparable to the binding energy ω_b. Therefore $\omega_2 \ll \omega$, and the bound plasmon is relatively stable against decay into single-particle excitations. Because $\omega_2 \sim \omega_b$, however, the linewidth of the bound state is comparable to the binding energy.

V. DISCUSSION

Let us summarize the results presented in previous sections. We have generalized the equations for plasma excitations[4,5] to the case of an inhomogeneous electron gas in a quantum well. By extending the RPA to this inhomogeneous case we obtained an integral equation given by (2.23) for the intersubband plasmons. By evaluating to leading order an infinite sequence of sum rules we have derived an explicit expression for the long-wavelength approximation for the kernel of the integral equation for the quantum well gas of charged carriers interacting with a charged center, and the result is given in Eq. (3.34). This equation has both scattering solutions[2] and bound-state solutions. The latter exist only when impurity has a charge the same sign as the carriers. For such a case we have derived an equation for the S state of the localized intersubband plasmon, which is given by Eq. (3.37).

In the corresponding bulk case[2,3] it was found that bound states exist only for densities below a certain threshold. As shown in Appendix A this threshold density is so low for bulk semiconductors that the plasmon itself will not be observable. The situation in a quantum well is qualitatively different in that the solution of the bound-state equation (3.37) exists in principle at arbitrary densities as indicated in Fig. 6(a). To understand this behavior qualitatively, let us neglect the linear term in k in the long-wavelength approximation of the interaction matrix element. Let M be a plasmon "mass" defined by the inverse curvature of the plasmon dispersion at $k=0$ in Eq. (C7). Then, the integral equation to leading order is similar to Schrödinger's equation for a particle of mass M in an attractive 2D screened Coulomb potential with an effective charge,

$$e^*=\frac{\alpha Z^* E_{21} me}{2\pi M n\sigma} ,$$

and this potential has a bound state at arbitrary e^*.

The results obtained here, which are illustrated in Fig. 6, suggest that bound plasmons below the intersubband transition energy in semiconductor quantum-well systems are of physical interest and may be directly observable depending on the parameters of the system. We find that the binding enregy is larger for larger carrier masses and for wider wells. Thus, for example, the binding will be small for the electron gas in a GaAs quantum well with its relatively small carrier mass but will be larger for holes in GaAs wells with their greater mass. The binding in some II-VI materials with their larger electron masses and smaller dielectric constants also will be greater. The binding energy is greater for larger impurity charge Z and smaller background dielectric constant ε_∞. We find that for Z/ε_∞ on the order of unity the binding enregy can be a few meV. Thus we expect that for semiconductors, which typically have dielectric constants in the range of five to ten, the binding energy of the plasmons at impurity charges of one or two units will be too small to be observed. On the other hand, clusters of defects having charges on the order of 10 can give rise to bound plasmons states with observable binding energies. In all cases there will also be scattering states of the plasmons. We might note that the carriers in compound semiconductors also interact with the longitudinal-optical-phonon modes, and thus the elementary excitations in these systems are couled plasmon-phonon modes.[9] The problem of bound states of coupled plasmon-phonon modes interacting with an impurity will be addressed in a future publication.

ACKNOWLEDGMENT

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APPENDIX A: BULK PLASMONS IN THE PRESENCE OF CHARGED IMPURITY

The possibility of plasmon localization by a Coulomb center in 3D bulk systems was investigated by Sziklas[2] and Sham.[3] Sziklas used the first Born approximation for impurity scattering in order to obtain the lowest-order term in the expansion of the dielectric matrix $\varepsilon(\mathbf{k},\mathbf{k}';\omega)$ in powers of $\mathbf{k}$ and $\mathbf{k}'$. We prefer to use Sham's approach which consists of an expansion of the spectral representation in powers of frequency and an evaluation of the resulting integrals by using Heisenberg's equation of motion for the density operator. This approach allows us to obtain terms to higher orders in the impurity charge. The equations for the inhomogeneous electron gas in 3D can be obtained, in fact, from the equations of Secs. II and III by considering the intrasubband case $n=m$ and changing 2D momenta to 3D momenta. The first three sum rules are much simpler than in the QW case:

$$\int_{-\infty}^{\infty} d\omega\, \sigma(\omega)=0 , \tag{A1}$$

$$(2\pi)^{-1}\int_{-\infty}^{\infty} d\omega\, \omega\sigma(\mathbf{k},\mathbf{k}';\omega)=(\hbar^2/m)\mathbf{k}\cdot\mathbf{k}' n(\mathbf{k}-\mathbf{k}') , \tag{A2}$$

$$\int_{-\infty}^{\infty} d\omega\, \omega^2\sigma(\omega)=0 , \tag{A3}$$

where $n(k)$ is a Fourier transform of the 3D density, and, as in Eq. (3.24), we write

$$n(\mathbf{k})=n_0\delta_{k,0}+\delta n(\mathbf{k}) , \tag{A4}$$

where δn is a change of the electron gas density due to

the presence of an impurity. These first three sum rules are exact and are the only ones derived in Ref. 3. In the limit of infinite volume $\Omega\to\infty$ and in units where $\hbar=1$ we obtain the next sum rule

$$(2\pi)^{-1}\int d\omega\,\omega^3\sigma(\mathbf{k},\mathbf{k}';\omega)$$
$$=(Z/m^2)\Omega^{-1}\sum_{\mathbf{q}}V(k)(\mathbf{k}\cdot\mathbf{q})(\mathbf{k}'\cdot\mathbf{q})\delta n(\mathbf{k}-\mathbf{k}'-\mathbf{q})$$
$$-(3/m^3)(\mathbf{k}\cdot\mathbf{k}')\Omega^{-1}\sum_{\mathbf{q}}(\mathbf{k}\cdot\mathbf{q})^2 f_q+O(k^6)\ , \tag{A5}$$

where $V(k)=4\pi e^2/\varepsilon_\infty k^2$ and f_k is the momentum probability distribution

$$f_k\equiv\langle c_{\mathbf{k}}^\dagger c_{\mathbf{k}}\rangle=f_k^0+\delta f_k\ . \tag{A6}$$

At zero temperature, $f_k^0=\theta(k-k_F)$, and δf_k includes effects of the impurity on the one-electron levels. Applying Heisenberg's equation of motion and defining

$$S_n(\mathbf{k},\mathbf{k}')=(2\pi)^{-1}\int d\nu\,\nu^n\sigma(\mathbf{k},\mathbf{k}';\nu)\ ,$$

we find that for even n, this S_n does not contribute to $O(k^2)$ while for odd n it contributes to the polarization $\Pi(\mathbf{k},\mathbf{k}';\omega)$ in second order of k and k', a term that is $O[(ZV)^{(n-1)/2}\delta n/\omega^{n+1}]$. By retaining terms of fourth order in k that are proportional to the homogeneous density n_0 and terms of second order in k for the rest, we obtain the following expansion for the real part of the polarization (in units of $\hbar=1$):

$$\mathrm{Re}\Pi(\mathbf{k},\mathbf{k}';\omega)=\left[\frac{n_0}{m\omega^2k^2}+\frac{3n_0k^4u_F^2}{5m\omega^4}\right]\delta_{\mathbf{k},\mathbf{k}'}+\frac{\mathbf{k}\cdot\mathbf{k}'}{m\omega^2}\delta n(\mathbf{k}-\mathbf{k}')+\frac{Z}{m^2\omega^4}\Omega^{-1}\sum_{\mathbf{q}}V(q)(\mathbf{k}\cdot\mathbf{q})(\mathbf{k}'\cdot\mathbf{q})\delta n(\mathbf{k}-\mathbf{k}'-\mathbf{q})$$
$$+\frac{Z^2}{m^3\omega^6}\Omega^{-2}\sum_{\mathbf{q}\mathbf{q}'}V(\mathbf{q})V(\mathbf{q}')(\mathbf{k}'\cdot\mathbf{q})(\mathbf{k}\cdot\mathbf{q}')(\mathbf{q}\cdot\mathbf{q}')\delta n(\mathbf{k}-\mathbf{k}'-\mathbf{q}-\mathbf{q}')+\cdots\ , \tag{A7}$$

where for $\delta n(k)$ we will use the Thomas-Fermi formula

$$\delta n(k)=\frac{Z^*}{1+k^2/k_{\mathrm{TF}}^2}\ , \tag{A8}$$

where $Z^*=Z/\varepsilon_\infty$.

Let us define $\delta\rho^T(\mathbf{k},\omega)$ as the change of the total electron density in the presence of a weak external perturbation. Application of the linear-response theory then gives an integral equation for this function. The derivations in Refs. 2 and 3 neglect the terms of order $O(Z/\omega^4)$ and higher in Eq. (A7). We will do likewise here and comment on the effect of the neglected terms at the end of this section. We define the function ϕ and the energy parameters $\mathcal{E}$ and Λ as follows:

$$\phi(\mathbf{k})=k\delta\rho^T(\mathbf{k})\ ,$$
$$\mathcal{E}=\frac{5}{9}\frac{\omega^2}{\omega_0^2}\left[\frac{\omega^2}{\omega_0^2}-1\right]k_{\mathrm{TF}}^2\ , \tag{A9}$$
$$\Lambda=\frac{5}{9}\frac{\omega^2}{\omega_0^2}\frac{k_{\mathrm{TF}}^2Z^*}{(2\pi)^3n_0}\ ,$$

where ω_0 is the plasma frequency at $k=0$. The function ϕ then satisfies the following integral equation:

$$(k^2-\mathcal{E})\phi(\mathbf{k})=-\Lambda\int d^3k'K(\mathbf{k},\mathbf{k}')\phi(\mathbf{k}') \tag{A10}$$

with the kernel given by the expression

$$K(\mathbf{k},\mathbf{k}')=\frac{\mathbf{k}\cdot\mathbf{k}'}{kk'}\delta n(\mathbf{k}-\mathbf{k}')\ . \tag{A11}$$

This is the equation studied by Sziklas.[2] The solutions with the continuous spectrum are the scattering states. The investigation of the solutions was facilitated greatly by the fact that the dispersion of the bulk plasmons is quadratic, so that Eq. (A10) can be cast in the form of the Lippman-Schwinger equation for a particle of definite mass.[2] If the impurity's charge Ze is negative for an electron gas (positive for a hole gas), Eq. (A10) may also have discrete spectrum solutions with $\mathcal{E}<0$. If the impurity is at the origin of real space, the system is rotationally invariant, and decomposition into spherical harmonics yields an integral equation with orbital momentum $\hbar l$. For each value of l, Eq. (A10) reduces to a one-dimensional integral equation with a kernel that is finite even for $|\mathcal{E}|=0$. Therefore, there is a threshold in Z/n for the existence of a bound state. We confine the following remarks to the $l=0$ solutions. If Λ is viewed as an eigenvalue and $\mathcal{E}$ as a parameter, $\Lambda(\mathcal{E})$ is a monotonically increasing function, and the largest binding energy will be found from the lowest eigenvalue Λ. The interparticle spacing parameter is defined as

$$r_s=\left[\frac{3}{4\pi a^3n_0}\right]^{1/3}\ .$$

Here, the effective Bohr radius for an electron with an effective mass m is related to the vacuum Bohr radius a_0 by

$$a=a_0\varepsilon_\infty m_0/m\ .$$

For a given value of $|Z^*|$ the binding energy is nonzero only when r_s exceeds a certain value r_s^c. Using the numerical results in Ref. 2 we obtain for $|Z^*|=1$ a value $r_s^c\approx5.5$. Taking, for example, bulk GaAs we set the material parameters to be $m_e=0.067m_0$, $m_h=0.5m_0$, and $\varepsilon_\infty=10.9$. Then, at the threshold density, the plasma energy $\hbar\omega_0$ is 0.5×10^{-2} meV for electron gas and 3.7×10^{-2} meV for hole gas. These values are too small for the plasmon itself to be observable.

In the derivation of Eq. (A10) an infinite sequence of terms of the order of $O(Z/\omega^4)$ and higher in Eq. (A7) was neglected. It is easy to see that the cumulative effect of these terms will be to reduce the binding of the putative bound state, thus reducing the threshold value of the density even further.

APPENDIX B: INTERACTION MATRIX ELEMENTS AND FORM FACTORS

The Coulomb matrix elements defined in Eqs. (2.10) and (2.11) are easily evaluated for a QW with infinite potential barriers and are given by

$$V_{12,12}(k)=\frac{2e^2L}{\varepsilon_\infty\pi}\left[\frac{1}{1+k^2L^2/\pi^2}+\frac{1}{9+k^2L^2/\pi^2}-\frac{128kL}{\pi^2}\frac{1+e^{-kL}}{(1+k^2L^2/\pi^2)^2(9+k^2L^2/\pi^2)^2}\right],$$

$$V_{11}=\frac{8e^2}{\varepsilon_\infty k(4+k^2L^2/\pi^2)}\left[\frac{kL}{\pi}+\frac{2\pi(1-e^{-kL/2})}{kL}\right],$$

$$V_{22}(k)=\frac{16\pi e^2(1-e^{-kL/2})}{\varepsilon_\infty k^2L(4+k^2L^2/4\pi^2)}.$$

The form factors defined in Eqs. (3.28) and (3.30) are given for an infinite QW by

$$S(k)=\frac{2(1-e^{-kL/2})}{kL}+\frac{2kL(1+e^{-kL/2})}{k^2L^2+4\pi^2},$$

$$F(k)=kL\left[\frac{2}{k^2L^2}+\frac{1}{k^2L^2+4\pi^2}\right]-\frac{32\pi^4(1-e^{-kL})}{k^2L^2(k^2L^2+4\pi^2)^2}.$$

APPENDIX C: LONG-WAVELENGTH APPROXIMATION FOR THE FREE INTERSUBBAND PLASMONS

In the absence of scattering centers the free intersubband plasmons are given by

$$1-V_{12,12}(k)\chi(\mathbf{k},\omega)=0 \tag{C1}$$

which is, in fact, the diagonal part of Eq. (2.23). The expansion of V in powers of k can be obtained from the expression in Appendix B and is given by

$$V_{12,12}(k)=(2\pi e^2/\varepsilon_\infty)(\alpha-\mu k+\gamma k^2)+O(k^3), \tag{C2}$$

where the coefficients are

$$\alpha=\frac{10}{9\pi^2}L,$$

$$\mu=\frac{256}{81\pi^4}L^2,$$

$$\gamma=\frac{46}{81\pi^4}L^3.$$

The expansion for $\chi(k)$ is[4]

$$\chi(k,\omega)=\frac{2n}{\hbar^2(\omega^2-\Omega_{21}^2)}[\hbar\Omega_{21}+c(\omega)k^2]+O(k^4), \tag{C3}$$

where Ω_{21} is the intersubband frequency $E_{21}/\hbar$, n is a 2D carrier density, and $c(\omega)$ is given by

$$c(\omega)=\frac{\hbar^2}{2m}+\frac{1}{\omega^2-\Omega_{21}^2}\left[\tfrac{3}{4}u_F^2\hbar\Omega_{21}+\frac{\hbar^2\Omega_{21}^2}{m}\right]+\frac{u_F^2\hbar\Omega_{21}^3}{(\omega^2-\Omega_{21}^2)^2}. \tag{C4}$$

The parameter σ that appears in the integral equation (3.34) is related to $c(\omega)$

$$\sigma(\omega)=\alpha c(\omega)+\gamma\hbar\Omega_{21}. \tag{C5}$$

To obtain the plasmon dispersion $\omega_{\rm pl}(k)$ from Eq. (C1) to the order $O(k^2)$, one needs $c[\omega(k)]$ only to order $O(1)$. Denoting this as c_0 we obtain

$$c_0=\frac{\hbar^2}{2m}+\frac{\hbar^2\varepsilon_\infty}{4\pi ne^2\alpha\hbar\Omega_{21}}\left[\tfrac{3}{4}u_F^2\hbar\Omega_{21}+\frac{\hbar^2\Omega^2}{m}\right]+\frac{u_F^2\hbar^3\Omega_{21}\varepsilon_\infty^2}{(4\pi ne^2\alpha)^2}. \tag{C6}$$

Then we obtain the LWA for the free plasmon dispersion $\omega_{\rm pl}(k)$ to $O(k^2)$,

$$\omega_{\rm pl}^2=\Omega_{21}^2+\frac{4\pi ne^2\alpha\Omega_{21}}{\hbar\varepsilon_\infty}-\left[\frac{4\pi ne^2\Omega_{21}\mu}{\hbar\varepsilon_\infty}\right]k+\left[\frac{4\pi ne^2\sigma_0}{\hbar^2\varepsilon_\infty}\right]k^2, \tag{C7}$$

where

$$\sigma_0=\alpha c_0+\gamma\hbar\Omega_{21}. \tag{C8}$$

Equations (C6)–(C8) were used to determine the bottom of the plasmon dispersion in Eq. (4.2) and also to compare the LWA with the exact RPA (Ref. 4) for the free plasmon dispersion in Fig. 4. Equations (C4) and (C5) were used to determine the coefficients in Eq. (3.34).

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