Optical properties of a two-dimensional electron gas: Evolution of spectra from excitons to Fermi-edge singularities

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The evolution of the absorption and emission spectrum from an exciton to a Fermi-edge singularity as a function of a quasi-two-dimensional electron-gas density is examined. Band-gap renormalization, screening, shake up of the Fermi sea, and the effect of the finite hole mass are included. The real-time response of the Fermi sea to the creation and annihilation of the hole in the valence band is treated nonperturbatively. The time evolution of the self-energy and vertex corrections is shown to be governed by a set of nonlinear differential equations, which allows for a very efficient numerical solution. The effect of the finite hole mass is to wash out the Fermi-edge singularity in absorption.

I. INTRODUCTION

An absorption of a photon in a semiconductor creates an electron in the conduction band and a hole in the valence band. The interacting electron hole pair forms an "atomic" exciton. The absorption spectrum is proportional to the density of states of an exciton, with a distinct peak, corresponding to the bound state of the exciton, shifted below the continuum be the exciton binding energy E_b. If N free carriers are present in the conduction band, the absorption process involves correlation of the hole with $N+1$ electrons. When the number of carriers N is small, the electron and a hole form atomic complexes. For example, with only one electron in the conduction band and a localized hole, the lowest excitonic transition would be lowered by the energy $2E_b-U$, where U is the Coulomb interaction energy between two electrons in a bound exciton state. When the number of particles N is large enough to think of the ground state of electrons in the absence of the hole as the Fermi sea of electrons, Mahan[1] has shown that the absorption spectrum develops a singularity at the Fermi energy. We study here how the spectrum evolves from that of an atomic exciton to the Fermi-edge singularity as a function of free carrier density in quasi-two-dimensional systems. The quasi-two-dimensional systems are of special interest because the Fermi energy E_F for a typical carrier density is comparable to the atomic exciton binding energy E_b. In GaAs for carrier density $n=5\times10^{11}$ cm^{-2}, the Fermi energy E_F is approximately 20 meV, i.e., it is equal to the two-dimensional (2D) exciton binding energy E_b (for infinite hole mass). Such densities are obtained in gated heterojunctions,[2] modulation-doped quantum wells,[3] and double-barrier resonant-tunneling structures,[4] for which absorption and emission spectra as a function of carrier density have been extensively studied.[2-4] Theoretical interpretations[5-9] are either qualitative[5] or incomplete. They either include model interactions and dynamical response of the Fermi sea,[8,9] or static screening and band-gap renormalization but no response of the Fermi sea.[6,7] Neither approach gives both the line shape and position of the spectrum. We incorporate band-gap renormalization, screening, and dynamical response of the Fermi sea to study the absorption and emission spectrum as a function of carrier density. Our approach follows the Combescot and Nozieres (CN) (Ref. 10) exact formulation of the x-ray absorption in metals.

II. THEORY OF ABSORPTION

An exact expression for the absorption spectrum for the localized hole (with infinite mass) in a noninteracting gas of fermions was derived by CN,[10] subsequently rederived by Ohtaka and Tanabe,[9] and generalized to include approximately finite hole mass by Unoyama and Sham.[8]

The starting point for calculation of the absorption spectrum are the initial-state H_i and final-state H_f Hamiltonians. The initial-state Hamiltonian describes N noninteracting quasiparticles in the conduction subband with single-particle Hamiltonians t_i, a quasiparticle energy spectrum e_k, and single-particle states $|k\rangle$. The energy spectrum e_k includes approximately electron-electron interactions via static self-energy: the "Coulomb-hole" term and screened exchange. The final-state Hamiltonian describes the kinetic energy T of $N+1$ quasiparticles, interaction energy with the valence hole via a screened Coulomb interaction V, and the valence hole Hamiltonian h [$H=T+V(r_h)+h(r_h)$]. Screening of the valence hole potential is assumed to take place instantaneously.[11] The dynamics of the switching-on of the valence hole potential during absorption process is then incorporated in the Mahan-Nozieres-DeDominicis (MND) Hamiltonian:

$$H=\sum_k e_k a_k^\dagger a_k+\sum_{k,k',q,q'} V_{k,k'}^{q,q'} a_k^\dagger a_{k'} c_q^\dagger c_{q'}+\sum_q h_q c_q^\dagger c_q \ . \tag{1}$$

Here $a_k^\dagger$ creates a conduction-band quasiparticle in a state $|k\rangle$ with energy e_k, $c_q^\dagger$ creates a valence hole in a state $|q\rangle$ with energy h_q, and $V_{k,k'}^{q,q'}$ scatters the electron from state $|k\rangle$ to state $|k'\rangle$, while the valence hole

scatters from state $|q\rangle$ to state $|q'\rangle$. The absorption spectrum at zero temperature is related to the real-time current-current correlation function $A(t)$:

$$A(t)=\sum_{k,k',q,q'} M_{k',q'}\langle i|e^{iHt}a_{k'}c_{q'}e^{-iHt}a_k^\dagger c_q^\dagger|i\rangle M_{k,q} \ . \quad (2)$$

Here $M_{k,q}=P_{vc}\langle k|q\rangle$ are optical-transition matrix elements, P_{vc} is an interband momentum matrix element, and $\langle k|q\rangle$ is the envelope wave-function overlap between the electron and hole states. The envelope wave-function overlap between the electron and hole states assures that only s angular-momentum channel contributes to absorption. The initial state $|i\rangle$ is the ground state of the system prior to the absorption of a photon. It is a product of the ground state of N electrons $|0_i\rangle$ and a vacuum for the hole. We can rewrite Eq. (2) as

$$A(t)=\sum_{k,k',q,q'} M_{k',q'}e^{iE_it}\langle q'|\otimes(\langle 0_i|a_{k'})e^{-iHt}(a_k^\dagger|0_i\rangle)\otimes|q\rangle M_{k,q} \ , \quad (3)$$

where the initial-state energy E_i is the ground-state energy of N quasiparticles in the absence of the hole. Following Combescot and Nozieres,[10] we go back to first quantization and define the state $|\Psi_k\rangle=a_k^\dagger|0_i\rangle$ as a Slater determinant of $N+1$ electrons occupying N lowest states in the Fermi sea (states p with $p<k_F$, where k_F is the Fermi wave vector) and one state $|k\rangle$ above the Fermi surface. The second step is to separate the Hamiltonian H into the $N+1$ electrons part $T+V(r_h)$, which is the sum of single-particle Hamiltonians, describing electrons scattering of the hole potential, with the hole localized at r_h, and the hole Hamiltonian $h(r_h)$:

$$A(t)=\sum_{k,k',q,q'} M_{k',q'}e^{iE_it}\langle q'|\otimes\langle\psi_{k'}|e^{-i[T+V(r_h)]t}S(t)|\psi_k\rangle\otimes|q\rangle M_{k,q} \ , \quad (4)$$

where the S matrix $S(t)=e^{+i[T+V(r_h)]t}e^{-i[T+V(r_h)+h(r_h)]t}$ describes the propagation of the hole in the electron system and satisfies the equation of motion:

$$\frac{\partial S(t)}{\partial t}=-ie^{+i[T+V(r_h)]t}h(r_h)e^{-i[T+V(r_h)]t}S(t) \quad (5)$$

with an initial condition $S(0)=1$. Inserting a complete set of states $|\Psi_\beta\rangle|q\rangle$ of the operator $T+h$ for the hole and $N+1$ electrons into Eqs. (4) and (5) gives the final expression for the absorption:

$$A(t)=\sum_{k,k',q,q'} M_{k',q'}M_{k,q}e^{iE_it}\sum_{\beta,q''} F_{k',\beta}^{q',q''}(t)S_{\beta,k}^{q'',q}(t) \quad (6)$$

with the S matrix satisfying equation of motion

$$\frac{\partial}{\partial t}S_{\beta,k}^{q'',q}(t)=-i\sum_{\alpha,\alpha',q',q'''} F_{\beta,\alpha}^{q'',q'}(-t)h_{q'}F_{\alpha,\alpha'}^{q',q'''}(t)S_{\alpha',k}^{q''',q}(t) \ . \quad (7)$$

We have defined the F and S matrices as follows:

$$F_{k',\beta}^{q',q''}(t)=\langle q'|\langle\psi_{k'}|e^{-i[T+V(r_h)]t}|\psi_\beta\rangle|q''\rangle \ ,$$
$$S_{\beta,k}^{q'',q}(t)=\langle q''|\langle\psi_\beta|S(t)|\psi_k\rangle|q\rangle \ . \quad (8)$$

Hence the calculation of the absorption spectrum is reduced to the calculation of matrix F.

III. ABSORPTION FROM THE LOCALIZED STATE

We first consider a special case when transitions involve only a single strongly localized valence hole state $|q_0\rangle$. Such a state can be associated with an acceptor impurity in a quantum well, or potential fluctuations in the width of a quantum well. With this assumption, the summation over all intermediate states $|\Psi_\alpha\rangle$ in Eq. (7) can be carried through exactly, and the S matrix has a very simple form

$$S_{\beta,k}^{q_0,q_0}(t)=\delta_{\beta,k}e^{-ih_{q0}t} \ . \quad (9)$$

By bringing the valence hole to the origin, one can show that matrix F separates into a time-dependent part corresponding to the scattering of electrons by the valence hole localized at the origin and a static form factor:

$$F_{k',k''}^{q',q''}(t)=\langle\psi_{k'}|e^{-i[T+V(0)]t}|\psi_{k''}\rangle\langle q'|e^{i(k'-k'')r_h}|q''\rangle$$
$$=F_{k',k''}(t)\langle q'|e^{i(k'-k'')r_h}|q''\rangle \ .$$

The real-time current-current correlation function $A(t)$ is finally given by a CN formula:

$$A(t)=\sum_{k,k'>k_F} M_{k'}M_k e^{iE_it}e^{-ih_{q_0}t}F_{k,k'}(t)$$
$$\times\langle q_0|e^{i(k-k')r_h}|q_0\rangle \ , \quad (10)$$

where $F_{k,k'}(t)$ is the probability that the $(N+1)$-electron system, initially with one electron above the Fermi surface in state $|k'\rangle$, can be found at a time t measured from the switching on of the valence hole potential at $r_h=0$, in the state with N electrons in the Fermi sphere and one

electron in a different state $|k\rangle$. $F_{k,k'}(t)$ can be expressed in terms of a single particle matrix elements $\varphi_{p,p'}$:

$$F_{k,k'}(t)=e^{-iC(t)}\left[\varphi_{k,k'}(t)-\sum_{p,p'<}\varphi_{k,p}(t)(\varphi^{-1})_{p,p'}\varphi_{p',k'}(t)\right],$$
$$\varphi_{k,k'}(t)=\langle k|e^{-ith(0)}|k'\rangle\ , \tag{11}$$

where $h(0)$ is the single-electron Hamiltonian in the presence of a valence hole potential at the origin, and φ^{-1} is the inverse of the matrix $\varphi_{p,p'}$ with $p,p'<k_F$. The first term ($\exp[-iC(t)]=\mathrm{Det}(\phi)$) describes the response of N electrons to the switching of the valence hole potential and represents the dynamical self-energy of the valence hole. The second term corresponds to the vertex corrections and describes the scattering of the optically injected electron above the Fermi sphere. The first term in the vertex corrections $\varphi_{k,k'}$ corresponds to a direct scattering of the electron above the Fermi surface by the valence hole potential, while in the second term the scattering is mediated by electrons *inside* the Fermi sea via exchange processes. Note that the CN formula for absorption involves only single-particle states k,k' unoccupied in the initial single-particle basis.

The numerical calculation of the time evolution of the current-current correlation function $A(t)$ is nontrivial due to Anderson orthogonality and infrared divergencies, i.e., singularities in the long-time behavior of the system.[1] The long-time behavior in the CN formulation involves invertions of large matrices $\varphi_{p,p'}$, or a solution of a set of singular integral equations.[1] An alternative approach to a similar class of problems in terms of differential equations has been proposed by Schonhammer and Gunnarson.[12] The formulation in terms of differential equations is implemented in this work in the final single-particle basis $|\lambda\rangle$, where states $|\lambda\rangle$ and energies E_λ are the eigenstates and eigenvalues of the single-particle Schrödinger equation $h(0)|\lambda\rangle=E_\lambda|\lambda\rangle$. To obtain the CN formula we neglect the wave-vector dependence of the hole density [the last term in Eq. (10)]. Using the identity[13] $\varphi_{k,k'}(t)=\sum_\lambda\langle k|\lambda\rangle e^{-itE_\lambda}\langle\lambda|k\rangle$, the definition of the matrix $F_{k,k'}$ in the final basis as $F_{k,k'}=\sum_{\lambda,\lambda'}\langle k|\lambda\rangle F_{\lambda,\lambda'}\langle\lambda'|k'\rangle$, and the definition of the effective matrix element $m_\lambda=\sum_{k>k_F}M_k\langle k|\lambda\rangle$, the formula for absorption [Eq. (11)] in the s channel of the final basis can be written as

$$A(t)=\sum_{\lambda,\lambda'}m_\lambda e^{iE_it}e^{-ih_{q_0}t}F_{\lambda,\lambda'}(t)m^*_{\lambda'}\ ,$$
$$F_{\lambda,\lambda'}(t)=e^{iC(t)}[\delta_{\lambda,\lambda'}-G_{\lambda,\lambda'}(t)]e^{-itE_{\lambda'}}\ . \tag{12}$$

In Eq. (12) all final single-particle states contribute to the absorption spectrum at a given time. This is to be contrasted with the original CN formula [Eq. (10)] which appears to suggest that only empty initial electron states appear to play a role. The actual strength of each final-state contribution is determined by the time evolution of the self-energy and vertex corrections. The vertex correction contribution from the states below the chemical potential cancels the direct term so there is no response for frequencies lower than the chemical potential. The self-energy corrections $C(t)$ and vertex corrections $G(t)$ satisfy a set of *nonlinear differential equations*:

$$\frac{\partial}{\partial t}G_{\lambda,\lambda'}(t)=-iE_\lambda G_{\lambda,\lambda'}(t)+i\sum_{\lambda''}G_{\lambda,\lambda''}(t)E_{\lambda''}G_{\lambda'',\lambda'}(t)\ ,$$
$$\frac{\partial}{\partial t}C(t)=2\sum_\lambda E_\lambda G_{\lambda,\lambda}(t)\ , \tag{13}$$

with initial conditions $G_{\lambda,\lambda'}(0)=\sum_{k<k_F}\langle\lambda|k\rangle\langle k|\lambda\rangle$. The initial condition contains the information about the filling of phase space prior to absorption (phase-space filling).

In Eqs. (12) and (13) absorption involves an electron with a spin opposite to the given spin of the hole. Hence vertex corrections involve exchange processes with only one spin component of the Fermi sea. All electrons respond to the appearance of the charge of the hole and both spin components contribute to the hole self-energy and screening. Hence the factor of 2 in the equation for $C(t)$.

The overlap matrix elements $\langle k|\lambda\rangle$ between the initial and the final states are solutions of the Wannier equation with attractive, screened electron-hole interaction:

$$e_k\langle k|\lambda\rangle-\sum_{k'}\langle k|V|k'\rangle\langle k'|\lambda\rangle=E_\lambda\langle k|\lambda\rangle\ . \tag{14}$$

The spectrum E_λ contains bound and scattering states. These states are built out of *all* plane wave states, empty and occupied. Only s states are retained as they give a finite overlap with the hole localized at the origin. The bound state for an attractive potential in two dimensions *always* exists, irrespective of the form of the potential.[14] Since the effect of free carriers is to screen the interaction the bound state exists for all carrier densities. This conclusion remains true even when exchange and correlation are accounted for.[14] By contrast, in three dimensions a finite strength of the potential is required to bind a particle, and bound are not expected to play an important role for sufficiently high densities of free carriers.

The quasiparticle spectrum e_k is modified by the Coulomb hole term and screened exchange terms due to the repulsive electron-electron interaction:

$$e_k=\frac{\hbar^2k^2}{2m}+\tfrac{1}{2}\sum_{k'}(V^s_{k,k'}-V^b_{k,k'})-\sum_{k'<k_F}V^s_{k,k'}\ , \tag{15}$$

where the bare interactions $V^b_{k,k'}=2\pi e^2/\epsilon_0|\mathbf{k}-\mathbf{k}'|$ and the screened interaction $V^s_{k,k'}=V^b_{k,k'}/\epsilon(|\mathbf{k}-\mathbf{k}'|)$ are given in terms of the dielectric function ϵ:

$$\epsilon(|\mathbf{k}-\mathbf{k}'|)=1+\frac{2g(|\mathbf{k}-\mathbf{k}'|)}{a_0|\mathbf{k}-\mathbf{k}'|}\ ,$$
$$g(|\mathbf{k}-\mathbf{k}'|)=\begin{cases}1 & \text{if } |\mathbf{k}-\mathbf{k}'|<2k_F\ ,\\ 1-\sqrt{1-2k_F/|\mathbf{k}-\mathbf{k}'|} & \text{if } |\mathbf{k}-\mathbf{k}'|>2k_F\ .\end{cases} \tag{16}$$

Here a_0 is the bulk effective Bohr radius, ϵ_0 is the static dielectric constant, and m is the electron mass.

IV. ABSORPTION FROM THE VALENCE BAND

We now consider a hole in a valence band with energy spectrum $h_q=\hbar^2q^2/2m_h$ and a plane-wave basis of states $|q\rangle$. For a hole originating from the valence band, the static Coulomb hole self-energy of the valence state has to be included in the band-gap renormalization. This is done by removing the factor of $\frac{1}{2}$ in Eq. (15). With only direct transitions allowed the transition matrix element gives wave-vector conservation $M_{k,q}=M_k\delta_{q,-k}$. The main task is to calculate the F and S matrices approximately. Recall that the F matrix contains all scattering processes for the localized hole while the S matrix describes the propagation of the valence hole as it drags with it excitations of the Fermi sea. This can be done in a systematic way by expanding all intermediate excited states of the $(N+1)$-electron systems in terms of states with the specific number of electron-hole pair excitations of the Fermi sea. We first demonstrate the results for the no pair excitation spectrum. In the first step the complete space of excited intermediate states of the $(N+1)$-electron system is restricted to the set of states with N electrons in the Fermi sea and one electron occupying a state $|k_\beta\rangle$ above the Fermi surface: $|\psi_\beta\rangle\rightarrow|\psi_{k_\beta}\rangle$. Next we define the final basis of electronic states as the basis for a hole localized at the origin. Note that this is *not* an excitonic basis, but rather an impurity basis. After proving the identity $F^{-k,-k'}_{k,k'}(t)=\langle\psi_k|e^{-i[T+V(0)]t}|\psi_{k''}\rangle=F_{k,k'}(t)$, the equation of motion for the S matrix in the final basis can be obtained from Eq. (7). Substituting this result into Eq. (6) and transforming all quantities into the final basis as in the localized hole case, we arrive at the absorption spectrum in the final single-electron basis:

$$A(t)=e^{iE_it}e^{-itE_g}\sum_{\lambda,\lambda'}m_\lambda(0)F_{\lambda,\lambda'}(t)m^*_{\lambda'}(t)\ . \tag{17}$$

Equation (17) differs from the localized hole result, Eq. (12), by the presence of a time-dependent transition matrix element $m_\lambda(t)$. This factor mutes the infrared singularities in the absorption spectrum. It satisfies the equation of motion:

$$\frac{\partial}{\partial t}m^*_\lambda(t)=-i\sum_{\beta,\alpha}[\delta_{\lambda,\beta}-G_{\lambda,\beta}(0)]h_{\beta\alpha}(t)m^*_\alpha(t)\ . \tag{18}$$

The effective time-dependent hole Hamiltonian $h_{\alpha\gamma}$ in the final basis is given by

$$h_{\beta,\alpha}(t)=\sum_{\beta',\alpha'}F^\dagger_{\beta,\beta'}(t)h_{\beta',\alpha'}F_{\alpha',\alpha}(t)\ . \tag{19}$$

The matrix F is given by Eqs. (12) and (13). Hence the time evolution of the hole is determined by the time evolution of the electron system via the time dependence of the electron response function F. The strength of the approximate formula for the absorption is that it reproduces *exactly* the infinite mass result, Eq. (12), when we neglect the hole kinetic energy and identify the hole energy with the band gap E_g. When there are no free carriers in the conduction band, vertex corrections vanish ($G_{\lambda,\lambda'}=0$), the matrix F has a form $F_{\lambda,\lambda'}(t)=\delta_{\lambda,\lambda'}\exp(-itE_{\lambda'})$, and an effective hole Hamiltonian takes on a simple form $h_{\alpha,\beta}(t)=\exp(itE_\alpha)h_{\alpha,\beta}\exp(-itE_\beta)$. By going into the excitonic basis one can now demonstrate that the correlation function $A(t)$ in the absence of free carriers reduces to the single electron-hole pair (exciton) solution. Clearly, while the approximate formula for absorption appears to interpolate between the two exactly known results, the only way to test it is to include higher-order excited electron-hole pair intermediate states.

V. EMISSION SPECTRUM

After absorption of a photon the $(N+1)$-electron system and a hole relax to the lowest energy state $|f\rangle$. The stimulated emission spectrum involves the emission of a photon with simultaneous annihilation of a valence hole and one of the electrons from the conduction band. It is given by a correlation function $E(t)$ [*different* from absorption $A(t)$]:

$$E(t)=\sum_{k,k',q,q'}M_{k',q'}\langle f|e^{iHt}a^\dagger_kc^\dagger_qe^{-iHt}a_{k'}c_{q'}|f\rangle M_{k,q}\ . \tag{20}$$

The main difficulty is the calculation of the ground state $|f\rangle$. Of course, when a single localized state is involved, the ground state is the Slater determinant of bound and scattered single-particle states $|\lambda\rangle$. The calculation for the localized hole has been carried out by CN in the basis of scattered states. We note that again it is best to do the calculation in the final basis for emission, i.e., plane-wave states $|k\rangle$. The result is now very similar to absorption:

$$E(t)=\sum_{k,k'}M_ke^{iE_ft}e^{ih_{q_0}t}e^{-iC(t)}e^{+ie_kt}G_{k,k'}(t)M_{k'}\ , \tag{21}$$

where E_f is the ground-state energy of the $(N+1)$-electron system in the presence of the hole potential, and $G_{k,k'}$ and $C(t)$ are vertex and self-energy corrections. Note that the summation is over all plane-wave states, irrespective whether they are occupied in the final ground state or not. Which single-particle states contribute is solely determined by the dynamical vertex correction. Again, a set of nonlinear differential equations describes the time evolution of the vertex $G_{k,k'}(t)$ and self-energy $C(t)$ corrections:

$$\frac{\partial}{\partial t}G_{k,k'}(t)=-iE_kG_{k,k'}(t)+i\sum_{k''}G_{k,k''}(t)E_{k''}G_{k'',k'}(t)\ , \tag{22}$$

$$\frac{\partial}{\partial t}C(t)=2\sum_kE_kG_{k,k}(t)\ ,$$

with initial conditions $G_{k,k'}(0)=\sum_{\lambda<\lambda_F}\langle k|\lambda\rangle\langle\lambda|k'\rangle$. Hence the filling of phase space in the initial basis enters via the initial condition. The Fourier transform of $E(t)$ gives emission as a function of frequency $E(\omega)=2\,\mathrm{Re}\int_0^\infty dt\,e^{-i\omega t}E(t)$.

VI. RIGID-FERMI-SURFACE APPROXIMATION

The dynamical response of the Fermi surface, i.e., dynamical vertex and self-energy corrections, makes calculations of the optical properties difficult. Hence the rigid-Fermi-surface approximation is commonly used. We shall discuss its validity for the localized hole case. Let us start with absorption Eqs. (10) and (11). The absorption of photon corresponds to injection of a carrier into empty states $|k\rangle$ above the Fermi surface. In the rigid-Fermi-surface approximation one neglects the response of all other electrons, except for instantaneous screening of the hole potential. This means we neglect the vertex corrections $G(t)$ and the self-energy correction $C(t)=E_i$ cancels the ground-state energy of the initial state E_i. The absorption $A_R(t)$ in the rigid-Fermi-surface approximation is given by the scattering of an injected electron by the hole potential in the subspace of empty states of the initial basis:

$$A_R(t)=\sum_{k,k'>k_F} M_k\langle k|e^{-ih(0)t}|k'\rangle M_{k'} . \tag{23}$$

The single-particle Hamiltonian $h(0)$ (including the localized hole) operates only in the subspace of empty states of the initial Hamiltonian. By diagonalizing $h(0)$ in this subspace, a simple formula for absorption is obtained:

$$A_R(t)=\sum_m |\psi_m|^2 e^{-itE_m} e^{-ith_{q_0}} , \tag{24}$$

where ψ_m is related to the Fourier transform of exciton wave function in real space $\psi_m=\sum_{k>k_F} M_k\langle k|m\rangle$. The exciton states $\langle k|m\rangle$ (Mahan excitons) are built out of empty plane-wave states in the initial basis and are solutions of the generalized Wannier equation:

$$e_k\langle k|m\rangle-\sum_{k'>k_F}\langle k|V|k'\rangle\langle k'|m\rangle=E_m\langle k|m\rangle \quad \text{with } k,k'>k_F . \tag{25}$$

The lowest Mahan exciton state evolves in a continuous way from a bare exciton state in the absence of free carriers to a bound state below the Fermi surface. When the density of free carriers is high and the hole self-energy has been added by hand in Eq. (24) from Fumi's theorem, Eq. (24) provides a reasonable approximation. However, the continuous evolution of the Mahan exciton toward the atomic exciton as the density of carriers is lowered is clearly an artifact of the rigid-Fermi-surface approximation, and should be rejected. The notion of unbinding of excitons in a Fermi sea is clearly unfounded in view of exact results presented earlier. We also point out that excitons in the rigid Fermi sea do not satisfy exact sum rules[13] and should not be used for extracting carrier density from, e.g., absorption spectra. Mahan excitons described here are often used in calculations of absorption.[3,7]

Let us now discuss Mahan excitons for emission. In emission, we start with electrons occupying bound and scattered states $|\lambda\rangle$ for $E_\lambda<\mu$. The emission process destroys an electron in an occupied state and a localized hole. The missing state below the Fermi surface is a "hole" in the final-state basis. All states $|\lambda\rangle$ for $E_\lambda>\mu$ are holes in the conduction band. Hence interband emission corresponds to the injection of an additional hole above the Fermi surface of holes.[13] We now freeze the Fermi sea of holes, and consider only a response of an extra hole to the switching-off of the valence hole potential. The final result gives a simplified formula for emission:

$$E_R(t)=\sum_m |\psi_m|^2 e^{+itE_m} e^{+ith_{q_0}} ,$$
$$\psi_m=\sum_{\lambda<\lambda_F} M_\lambda\langle\lambda|m\rangle , \tag{26}$$

where the matrix elements $\langle\lambda|m\rangle$ satisfy a generalized Wannier equation in a final basis:

$$E_\lambda\langle\lambda|m\rangle+\sum_{\lambda'<\lambda_F}\langle\lambda|V|\lambda'\rangle\langle\lambda'|m\rangle=E_m\langle\lambda|m\rangle \quad \text{with } E_\lambda,E_{\lambda'}<E_F . \tag{27}$$

This approximation gives resonant states *above* the Fermi energy. If only one $1s$ state is occupied prior to emission, the photon energy is increased by the exciton binding energy in this approximation, while for the exact solution the photon energy is reduced by the binding energy. Clearly, an exact solution is again necessary for low carrier densities.

VII. RESULTS

Numerical results for emission and absorption are obtained in three steps. First the Wannier equation [Eq. (14)] for s states is solved on a finite set of energy levels with Gaussian weights. Energy is measured in bulk Rydbergs. We have found that typically a cutoff in energy of 48 Ry and a set of 100 points yielded a reasonable convergence for a few of the lowest eigenvalues and eigenvectors. Next the initial conditions for $G_{\lambda,\lambda'}$ and effective matrix elements m_λ are constructed. We find that $G_{\lambda,\lambda'}$ is almost diagonal for eigenvalues lower than the Fermi level except for the significant overlap of the bound state and states in the vicinity of the Fermi surface. $G_{\lambda,\lambda'}$ becomes very small for states above the Fermi surface. The matrix elements m_λ are significant for the bound state, are very small for occupied states, and show a drastic increase as we cross the Fermi level μ. The relative weight of the bound state versus the states at the Fermi level changes with density of free carriers. This is shown in Fig. 1, which illustrates m_λ^2 as a function of energy E_λ for $E_F=1,2,4,8$. We shall use the Fermi energy of free carriers $E_F=k_F^2/2m$ as a convenient measure both of carrier density and implicitly of the Fermi wave vector k_F. The Fermi energy $E_F=2\pi n a_0^2$ Ry is directly proportional to the density of electrons n. It is to be distinguished from the Fermi level μ which is the energy of the highest occupied quasiparticle state.

The time evolution of the emission and absorption spectrum is then calculated using a standard Runge-Kutta routine. The spectra are calculated over a finite

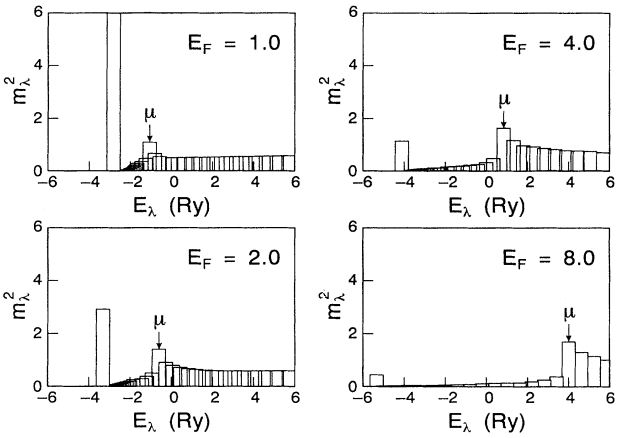

FIG. 1. The distribution of effective transition-matrix elements m_λ^2 as a function of transition energies E_λ for Fermi energies $E_F=1,2,4,8$. Note the decrease of the weight of the bound state and the increase of the structure in the vicinity of Fermi level. Energy is measured in bulk Rydbergs. 1 Ry gives binding energy of exciton in the bulk for localized hole. Matrix elements are measured in M_0^2, where M_0 is a constant interband matrix element.

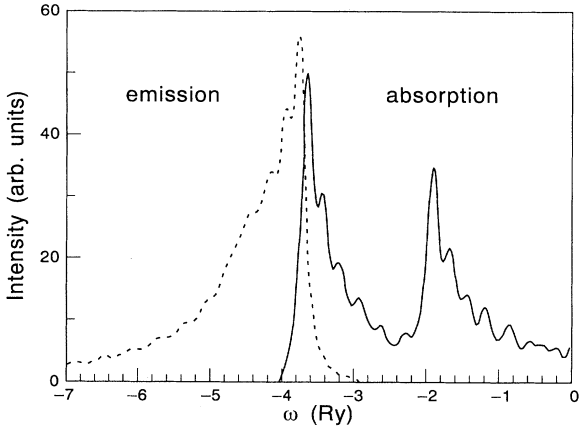

FIG. 2. Emission (dashed line) and absorption (solid line) for $E_F=1.0$ for the localized hole. Note the two peaks in absorption and a broad peak in emission with the width exceeding Fermi energy.

time interval $[0,T_{\max}]$. The typical time cutoff giving a reasonable convergence was approximately 40 Ry^{-1}. Shorter times were sufficient for higher carrier densities. The real part of the hole self-energy correction $C(t)$ has a long-time behavior $C(t)=C_0 t$ superimposed with oscillations associated with the presence of the bound state. The energy shift C_0 is calculated from the long-time behavior of the time derivative of $C(t)$. The frequency spectrum of, e.g., absorption is then calculated as follows:

$$A(\omega)=2\,\mathrm{Re}\sum_\lambda\left[\int_0^{T_{\max}} e^{i\omega_\lambda t}[g_\lambda(t)-g_\lambda(T_{\max})]dt + \frac{ig_\lambda(T_{\max})}{\omega_\lambda}\right],$$

$$g_\lambda(t)=\sum_{\lambda'} m_{\lambda'}[\delta_{\lambda,\lambda'}-G_{\lambda,\lambda'}(t)]m_\lambda e^{-i[C(t)-tC_0]}, \quad (28)$$

$$\omega_\lambda=\omega-(C_0-E_i)-E_\lambda-h_{q_0}+i\gamma\ .$$

In Eq. (28) dynamical vertex corrections assure contribution only from unoccupied states while the self-energy correction (C_0-E_i) imparts an overall shift in frequency. A small imaginary part of the frequency has been added for convergence.

In Fig. 2 we show a typical absorption and emission spectrum for low carrier density with Fermi energy $E_F=1.0$ Ry. The exciton binding energy in the absence of free carriers $E_b=4$ Ry, where Ry is the binding energy of the exciton in the bulk for a infinite hole mass. The transition energies are measured relative to the localized level energy. The absorption line consists of two peaks. The small oscillatory structure comes from the use of a discrete set of energy levels, and is smoothed in all remaining figures. The exact positions of both peaks can be inferred directly from Eq. (2). The lowest peak is the main singularity at energy $\omega_1=E_f-E_i+\mu$ and the second peak is at $\omega_2=\omega_1+\mu-E_s$. Here E_s is the lowest eigenvalue (bound state) of the screened Wannier equation [Eq. (14)], E_f-E_i is the difference in ground-state energy of N electrons due to the presence of the hole, and μ is the energy of the highest occupied level. The second peak involves transitions to excited states with a single electron-hole pair in the Fermi sea. The threshold is associated with a hole in the bound state E_s as discussed by CN. Note that the position of the first peak is unrelated to either the position of the bound state E_s or the Mahan exciton. The emission line is at lower frequency. The line shape is asymmetric, with a low-frequency tail extending to all frequencies smaller than the threshold frequency ω_1. There is no signature of the Fermi surface in the emission spectrum. The interesting point is that the position ω_1 of the main peak in absorption and emission is close to the value of the unscreened exciton at -4 Ry. This is illustrated in Fig. 3 which shows the transition frequency ω_1, the renormalized single-particle band gap, the Fermi level μ, and the bound-state energy E_s. The bound-state energy starts at -4 Ry, shifts rapidly toward higher energies to eventually saturate and follow the bottom of the band at higher densities. The transition energy ω_1 appears to be quite insensitive to carrier density (Fermi energy), with a value close to the bare 2D exciton energy, eventually following the shift toward higher energies of the top of the band at higher density. Hence the emission spectrum deceptively evolves from what appears to be a *broadened* atomic exciton peak at frequency E_b.

The evolution of the emission spectrum as a function of free carrier density is shown in Fig. 4. For E_F up to approximately 2 Ry the emission spectrum resembles that of a bare atomic exciton with an asymetric low-frequency tail. For higher densities the spectrum broadens, the

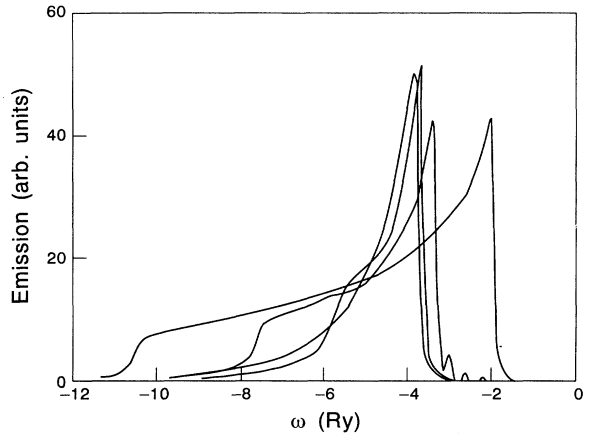

FIG. 3. The dependence of the absorption threshold ω_1, highest occupied level μ, the bottom of the band, and bound-state energy E_s, as a function of Fermi energy E_F.

higher energy part follows ω_1, while the lower frequency part develops a step at frequency $\omega_3=\omega_1-(e_{k_F}-e_0)$, corresponding to the bottom of the single-particle band.

Finally, we turn our attention to the effect of a finite hole mass on the absorption spectrum. For small carrier density the effect is mainly to renormalize the exciton energy and wave function. For higher carrier density, finite hole mass leads to the destruction of the Fermi-edge singularity. The absorption spectrum for $E_F=8$ Ry and hole masses: $m_h=1000m$, $m_h=10m$, and $m_h=4m$ (appropriate for GaAs) are shown in Fig. 5. While the Fermi-edge singularity is visible for a very heavy-hole mass, it becomes shifted toward higher energies and broadened as the mass decreases. This case corresponds to an ultraclean two-dimensional electron gas in GaAs quantum wells. We note that the rigid-Fermi-surface (ladder) approximation with finite hole mass leads to a

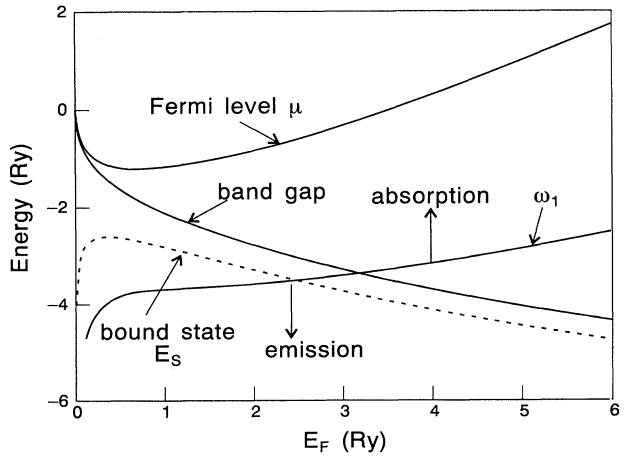

FIG. 4. The emission spectrum for a localized hole for different Fermi energies $E_F=1,2,4,8$. Note that the position of the peak coincides with bare exciton transition at $E_b=-4$ Ry.

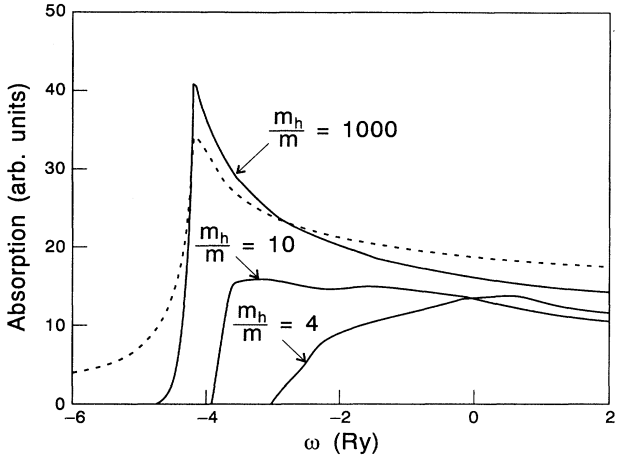

FIG. 5. The absorption spectrum for valence-to-conduction-band transitions for $E_F=8.0$ Ry for two different ratios of the hole to electron masses: $m_h=1000m$, $m_h=10m$, $m_h=4m$. The effect of the finite hole mass is to remove the excitonic enhancement at the Fermi energy. The dashed line shows the absorption when vertex corrections are neglected (but the same shift as the heavy mass case is retained). We see that vertex corrections give rise to the enhancement at the Fermi energy and remove transitions to occupied states.

logarithmic divergence at the Fermi energy and a weak bound state below the Fermi energy.[5,7] Hence the ladder approximation predicts an enhancement at the Fermi level, while our approximation does not. We are inclined to believe that the enhanced absorption in the vicinity of the Fermi level observed experimentally is due to hole localization. This is supported by the fact that no Fermi-edge singularity was observed in extremely clean GaAs quantum wells.[15] The absorption spectrum shown in Fig. 5 contains the static Coulomb hole self-energy contributions to the valence hole energy, and is measured relative to the bare band gap.

VIII. SUMMARY

We have used a Combescot and Nozieres approach to develop a numerically tractable method to calculate low-temperature absorption and emission spectra of modulation-doped quantum wells involving localized holes. The calculation takes into account band-gap renormalization, static screening, and dynamical response of the Fermi sea. We show the evolution of the spectra as the Fermi energy is varied over a wide range when compared to the exciton binding energy. The absorption and emission spectra are pinned to the Fermi level in the conduction band. However, when the hole self-energy is included, the position of the actual emission (absorption) line falls close to the bare excitonic transition. Hence, the net result of correct treatment of dynamical self-energy and vertex corrections are spectra which resemble closely an asymetrically broadened exciton line. Additional information is available due to the second peak structure in the absorption spectrum. The second peak is

due to the bound exciton state. When carrier density increases, absorption spectrum evolves into a blue-shifting Fermi-edge singularity while the emission spectrum begins to resemble the single-particle density of states in the conduction band, with enhancement at the Fermi level.

The effect of the finite hole mass is to wash out the Fermi-edge singularity. For parameters corresponding to the high-mobility GaAs quantum wells, no enhancement at the Fermi level is expected.

The major shortcoming of our approach is the neglect of dynamical screening and mutual interaction of localized electrons. The static treatment of electron-electron interactions in the absence of the hole gives a reasonable description of extended states and band-gap renormalization. It is however insufficient to treat the bound state in the final basis. The more realistic treatment of electron-electron interactions, finite hole mass, and finite temperatures should be investigated in the future.

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