Effect of Finite Hole Mass on Edge Singularities in Optical Spectra

T. Uenoyama and L. J. Sham

Department of Physics, B-019, University of California, San Diego, La Jolla, California 92093

(Received 13 June 1990)

A theory of optical transitions from a valence state to the conduction band taking into account the dynamical response of the Fermi sea is given using the functional-integral method. The method yields an approximation for the effects of the finite hole mass and finite temperature on the Mahan edge singularities. Magneto-optical spectra are calculated for n-doped quantum wells, which explain the range of observed behavior corresponding to finite-to-infinite hole mass at various temperatures.

PACS numbers: 78.70.Dm, 78.65.−s, 78.70.En

In transitions between valence and conduction bands in a metal or doped semiconductor, the dynamical response of the Fermi sea to the presence of the valence hole gives rise to a high density of states of conduction-band electron-hole pairs near the Fermi level, which manifest their presence as a singularity in the optical spectrum at the Fermi edge, if the valence hole is infinitely heavy.[1] Finite temperature, in smearing out the Fermi distribution, dampens the edge singularity.[2] The finite valence hole mass which has a similar effect is, however, difficult to treat theoretically and so the theories have been qualitative,[3,4] or in the boson approximation.[5] A theory of the optical spectra which treats the dynamical response of the Fermi sea taking into account the finite hole mass and finite-temperature effects is both a theoretical challenge and currently of great interest in view of recent experiments on the optical spectra in n-doped semiconductor quantum wells. The behavior of the spectra ranges widely. In both InGaAs and GaAs quantum wells, some samples[6–8] show the edge singularity behavior in both absorption and luminescence while other samples show the singularity in the absorption spectra[7,9] but not in the luminescence spectra.[9,10] Theories[7,11] which use only the exciton channel to explain the edge singularities in the spectra fail to account for the delicate balance between the ladder diagrams (the electron-hole attraction) and the crossing diagrams (the valence hole exciting the conduction electron-hole pairs) and for the competition between the Mahan exciton effect and the orthogonal catastrophe.[1]

We present a theory in which the valence-band dispersion is present *ab initio*. To include the initial- (or final-) state effect in emission (or absorption) of the Fermi sea reacting to the presence to the mobile valence hole, we use the functional-integral method of coherent fermion states.[12] The temperature is taken into account in the ensemble average. In analogy with the polaron theory, the degrees of freedom of the conduction Fermi sea and those of the valence hole can be treated separately without, however, making boson approximations for the former. The valence hole propagation in an arbitrary coherent state of the conduction Fermi sea is solved by a cumulant expansion in the electron-hole interaction to first order. The conduction-band degrees of freedom are then integrated in the presence of the dynamic potential due to the hole. Explicit expressions for the optical spectra are shown to reduce correctly to the exact solution[13] in the infinite-hole-mass limit. Our theory is used to compute the optical spectra of quantum wells in strong normal magnetic fields. The calculated dependence of the emission and absorption spectra on the hole mass and on temperature is compared with experiment, giving a theoretical underpinning to the understanding of the range of observed behavior described above.

The Hamiltonian is taken to include a conduction band of electrons with energy ε_p^e and chemical potential μ^e and a valence hole band with energy dispersion ε_q^h. Only the interband Coulomb interaction $V_{qq'}^{pp'}$ is taken into account.[1] Electron interaction within the conduction band is neglected. In the states considered, there is either zero or one valence hole. We consider first the emission spectrum, given in terms of the conduction-electron-valence hole pair-correlation function $\pi_{p,p'}^{q,q'}(\tau)$. For emission, the ensemble average is over the initial states with one valence hole and a sea of conduction electrons.

As an illustration of the method, we first evaluate the partition function, which may be written in the functional-integral form as[12]

$$Z=\int \mathcal{D}(\xi_p^*\xi_p)e^{-S^e}Z_h(\xi_p^*,\xi_p)\,, \tag{1}$$

where the action of the conduction electrons is given by

$$S^e=\int_0^\beta d\tau\left\{\sum_p \xi_p^*\frac{\partial}{\partial\tau}\xi_p+\sum_p(\varepsilon_p^e-\mu_e)\xi_p^*\xi_p\right\}, \tag{2}$$

β is the reciprocal temperature, and the Grassmann variables ξ_p are the coherent-state eigenvalues of the conduction-electron annihilation operators. The functional integration over ξ_p is separated from the integration over the valence hole Grassmann variables η_q contained in Z_h, the effective hole partition function for a given conduction-electron coherent state, given by

$$Z_h(\xi_p^*,\xi_p)=\sum_{q'}\int\prod_q d\eta_{q,1}^* d\eta_{q,1}\, d\eta_{q,2}^* d\eta_{q,2}\exp\left(-\sum_q(\eta_{q,1}^*\eta_{q,1}+\eta_{q,2}^*\eta_{q,2})\right)\eta_{q',1}\eta_{q',2}^*$$
$$\times\int_{\eta_{q,2}}^{\eta_{q,1}^*}\mathcal{D}[\eta_q^*\eta_q]\exp\left\{\sum_q\eta_q^*(\beta)\eta_q(\beta)-S^h\right\}, \tag{3}$$

where the valence hole action is given by

$$S^h=\int_0^\beta d\tau\left\{\sum_q\left[\eta_q^*\frac{\partial}{\partial\tau}\eta_q+\varepsilon_q^h\eta_q^*\eta_q\right]-\sum_{qq'}U_{qq'}(\tau)\eta_q^*\eta_{q'}\right\}, \tag{4}$$

with the effective potential

$$U_{qq'}(\tau)=\sum_{pp'}V_{qq'}^{pp'}\xi_p^*(\tau)\xi_{p'}(\tau). \tag{5}$$

In the hole partition function, Eq. (3), the first integral contains the projection operators of the form

$$\int\prod_p d\eta_p^*\, d\eta_p\exp\left(-\sum_p\eta_p^*\eta_p\right)\eta_q \tag{6}$$

which reduce the coherent valence hole states at the terminal points of the path integral to states with a single hole.

Since the hole action in Eq. (4) is quadratic in the hole Grassmann variables, the functional integral for the hole partition function Z_h may be evaluated as

$$Z_h(\xi_p^*,\xi_p)=\mathrm{Tr}[\mathbf{K}^h(\beta,0)] \tag{7}$$

in terms of the hole propagator $K_{qq'}^h(\tau,\tau')$, defined by the matrix equation

$$\frac{\partial}{\partial\tau}\mathbf{K}^h(\tau,\tau')=[-\mathbf{E}^h+\mathbf{U}(\tau)]\mathbf{K}^h(\tau,\tau'), \tag{8}$$

with the boundary condition of $\mathbf{K}^h(\tau,\tau)$ equal to the unit matrix. The matrix $\mathbf{E}^h$ is a diagonal matrix of hole energies. The cumulant expansion to first order in $\mathbf{U}$ yields

$$K_{qq'}^h(\beta,\tau)\simeq\begin{cases}e^{-\varepsilon_q^h(\beta-\tau)}\exp\left(\int_\tau^\beta d\tau' U_{qq}(\tau')\right), & q=q',\\ e^{\varepsilon_{q'}^h\tau}\left[\exp\left(\int_\tau^\beta d\tau' e^{-\varepsilon_q^h(\beta-\tau')}U_{qq'}(\tau')e^{-\varepsilon_{q'}^h\tau'}\right)-1\right], & q\neq q'.\end{cases} \tag{9}$$

The justification for this approximation is in reproducing the correct infinite-hole-mass limit (see below). The hole partition function Z_h, and, hence, the total partition function Z, is a Gaussian form in the electron variables ξ_p. Thus, Z may be evaluated to be

$$Z=\sum_q e^{-\beta\varepsilon_q^h}\prod_p[1+e^{-\beta[\tilde{\varepsilon}_p^e(q)-\mu^e]}], \tag{10}$$

where $\tilde{\varepsilon}_p^e(q)$ is the electron eigenenergy in the presence of the potential $V_{qq'}^{pp'}$. In later computation, we assume for simplicity that the potential is independent of q, which does not change the essential features of the spectra.

Using the same procedure of integrating over the hole variables first, we obtain the expression for the electron-hole correlation

$$\pi_{p'',p'}^{q,q'}(\tau)=\int\mathcal{D}(\xi_p^*\xi_p)e^{-S^e}\xi_{p''}^*(\tau)\xi_{p'}(0)K_{q'q}^h(\beta,\tau). \tag{11}$$

Further integration over the electron variable yields an expression in terms of the matrix $\mathbf{K}_{qq'}^e$ which is the electron propagator defined by the matrix equation

$$\frac{\partial}{\partial\tau}\mathbf{K}_{qq'}^e(\tau,\tau')=[-\mathbf{E}^e+\mathbf{V}_{qq'}(\tau)]\mathbf{K}_{qq'}^e(\tau,\tau'), \tag{12}$$

with

$$[\mathbf{E}^e]^{pp'}=(\varepsilon_p^e-\mu^e)\delta_{pp'}, \tag{13}$$

$$[\mathbf{V}_{qq'}(\tau)]^{pp'}=e^{-\varepsilon_q^h\{\beta(1-\delta_{qq'})-\tau\}}V_{qq'}^{pp'}e^{-\varepsilon_{q'}^h\tau}. \tag{14}$$

The initial condition is the same as $\mathbf{K}^h$.

The emission spectrum is given by the Fourier transform with respect to the imaginary time of

$$E(\tau)=\sum_{pq}(M_{pp}^*M_{qq}/Z)\{e^{-\varepsilon_p^h\beta}\delta_{pq}+(1-\delta_{pq})\}e^{\varepsilon_p^h\tau}\det[\mathbf{I}+e^{-\mathbf{E}^e\tau}\mathbf{K}_{pq}^e(\beta,\tau)]$$
$$\times\sum_r[\mathbf{K}_{pq}^e(\beta,\tau)]^{pr}\{[\mathbf{I}+e^{-\mathbf{E}^e\tau}\mathbf{K}_{pq}^e(\beta,\tau)]^{-1}\}^{rq}, \tag{15}$$

where M_{pp} is the band-to-band transition-matrix element. Similarly, the absorption is given by

$$A(\tau)=\sum_{pq}(M_{pp}^{*}M_{qq}/Z)e^{-\varepsilon_p^h\tau}\det[\mathbf{I}+e^{-\mathbf{E}^e(\beta-\tau)}\mathbf{K}_{pq}^e(\tau,0)]\times\sum_r[\mathbf{K}_{pq}^e(\tau,0)]^{pr}\{[\mathbf{I}+e^{-\mathbf{E}^e(\beta-\tau)}\mathbf{K}_{pq}^e(\tau,0)]^{-1}\}^{rq}. \quad (16)$$

The finite-mass case has been reduced to the single-particle problem of calculating the electron propagator $\mathbf{K}_{qq'}^e$ in the time-dependent $\mathbf{V}_{qq'}(\tau)$ as a function of the hole state. Note that the off-diagonal elements of $\mathbf{V}_{qq'}(\tau)$ include the recoil process in which the hole in the q' state is scattered to the q state by the electron-hole interaction. In emission, the hole distribution $\exp(-\varepsilon_p^h\beta)$ effectively decreases the transition matrix in the diagonal terms and the electron-hole interaction in the off-diagonal term in Eq. (15). The absorption spectrum is independent of the hole distribution since the initial state has no hole. When the hole mass is infinite, $\mathbf{V}_{qq'}(\tau)$ becomes independent of time. The hole, when it is present, provides a constant potential for the electrons. In the limit of infinite hole mass and zero temperature, our formulas for emission and absorption reduce to those in Ref. 13.

The theory of spectra is applied to an n-doped quantum well in a magnetic field $\mathbf{B}$ normal to the interface plane. One conduction and one valence subband are taken with parabolic dispersion and a state in a Landau level is characterized by the Landau-level number n and angular momentum m about the magnetic-field axis,[14] in place of p or q. The electron-hole interaction is approximated by a separable potential

$$V_{n_3m_3,n_4m_4}^{n_1m_1,n_2m_2}=V_0u_e(n_1m_1)u_e(n_2m_1)u_h(n_3m_3)u_h(n_4m_3)\delta_{m_1m_2}\delta_{m_3m_4}, \quad (17)$$

with the cutoff function $u_j(nm)=\theta(m_c-m)$. The matrix equations for the propagators are then solved with six Landau levels in each of the two subbands.

Figure 1 shows the calculated emission and absorption spectra as functions of the temperature T, the hole mass m_h^*, and the strength of the electron-hole interaction V_0. The cutoff m_c is determined by fitting the emission spectrum calculated for the infinite hole mass with the model interaction $V_0=0.3$ to the corresponding spectrum calculated using the true Coulomb potential for the electron-hole interaction. Energy and mass are measured in units of the electron cyclotron energy and the free-electron mass, respectively. The parameters in the calculation are $m_c=3$, $B=5$ T, with the Fermi energy lying between the third and fourth electron Landau levels. The electron mass m_e^* is 0.067 times the free mass. The line spectra are broadened by the introduction of a damping coefficient δ in the frequency $\omega-i\delta$, with $\delta=0.2$. The ratio of the peak intensities is unchanged by the introduction of δ.

In Fig. 1(a), the increase of peak strength towards the Fermi energy in both emission and absorption for infinite hole mass at the lowest temperature corresponds to the edge singularity at zero magnetic field. The emission spectrum has the same form as the observed magnetoluminescence spectrum for the InGaAs quantum well,[15] in agreement with the suggestion of optical transition to a localized hole. As temperature increases, the peak strength is moved away from the Fermi level in both directions, blurring the edge singularity. The trend is in agreement with the zero-field case.[2] Figure 1(b) shows that as the hole mass is lowered, while the absorption spectrum moves the intensity gradually from the Fermi level, the strength near the Fermi level in the emission spectrum is drastically reduced. The change of the emis-

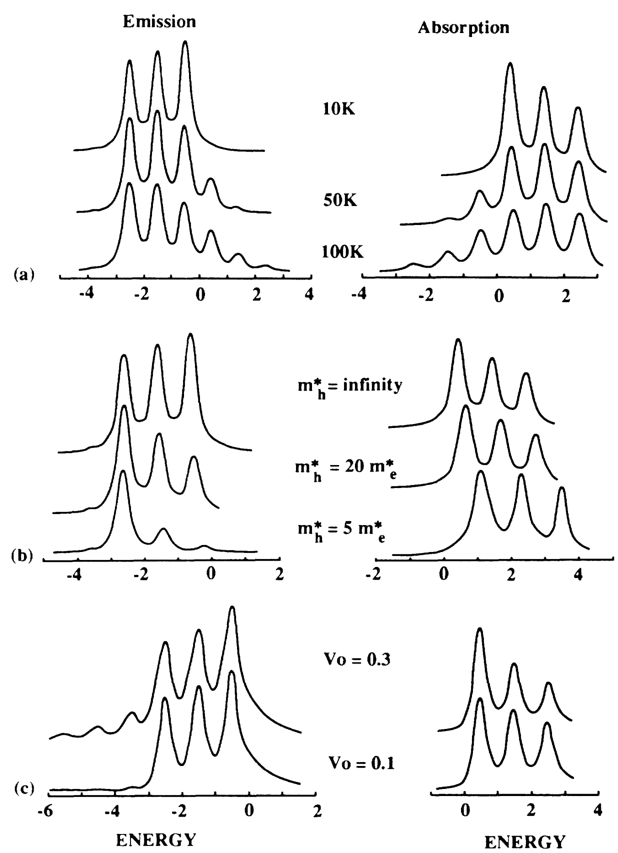

FIG. 1. Emission and absorption spectra (a) for various temperatures with $V_0=0.1$ (in units of the cyclotron energy), $m_h=\infty$; (b) for three values of the hole mass with $V_0=0.1$, $T=10$ K; (c) for two values of V_0 with $m_h=\infty$, $T=10$ K. The zero energy is at the Fermi energy.

sion spectrum is brought about by two effects of the finite valence-subband dispersion: the hole recoil and the temperature distribution of the initial hole state. The latter effect is inoperative in absorption. The low hole-mass emission spectrum has the same form as the observed one in the GaAs quantum well by Smith *et al.*,[16] suggesting the removal of the edge singularity by the finite valence-subband dispersion. The less drastic change in absorption may explain why vestiges of the edge singularity are observed in absorption.[7,9] The GaAs[8] and InGaAs[9] quantum wells in which edge singularities are seen in both emission and absorption are thought to have localized hole levels. The evidence is in the width of their emission spectrum being a little less than the Fermi energy in the conduction subband whereas in the samples where the emission spectra are more indicative of finite-hole-mass effects the emission bandwidth is the sum of the conduction- and valence-subband energies at the Fermi vector.[9,10]

Figure 1(c) shows that when the interaction strength is increased the edge singularity becomes stronger and shakeup peaks appear in the emission spectrum below the band edge. The shakeup processes involve final states with electron-hole pairs in the conduction band.

We have shown how the modern functional-integral method may be straightforwardly used to include the finite hole band dispersion in the theory of dynamical response to the Fermi sea to optical transitions. Our calculated magneto-optic spectra demonstrate the change of the spectra due to the finite hole mass, more drastically in the emission than in the absorption spectrum. From these results, we give an explanation of the diverse behavior observed in the quantum wells. Our calculations may be refined for low magnetic fields.

This work is supported by NSF Grant No. DMR 88-15068. We thank Dr. A. Houghton for helpful comments. One of us (T.U.) is grateful to Dr. H. Mizuno, T. Kajiwara, and T. Onuma for their encouragement.

[1]A comprehensive and up-to-date review of the theory is given by its originator, G. Mahan, *Many-Particle Physics* (Plenum, New York, 1990), 2nd ed., Sec. 8.3.

[2]K. Ohtaka and Y. Tanabe, Phys. Rev. B **39**, 3054 (1989).

[3]J. Gavoret, P. Nozières, B. Roulet, and M. Combescot, J. Phys. (Paris) **30**, 987 (1969).

[4]A. E. Ruckenstein and S. Schmitt-Rink, Phys. Rev. B **35**, 7551 (1987).

[5]E. Müller-Hartmann, T. V. Ramkrishnan, and G. Toulouse, Phys. Rev. B **3**, 1101 (1971).

[6]M. S. Skolnick, J. M. Rorison, K. J. Nash, D. J. Mowbray, P. R. Tapster, S. J. Bass, and A. D. Pitt, Phys. Rev. Lett. **58**, 2130 (1987).

[7]G. Livescu, D. A. B. Miller, D. S. Chemla, M. Ramaswamy, T. Y. Chang, N. Sauer, A. C. Gossard, and J. H. English, IEEE J. Quantum Electron. **24**, 1677 (1988).

[8]J. S. Lee, Y. Iwasa, and N. Miura, Semicond. Sci. Technol. **2**, 675 (1987).

[9]R. Cingolani, W. Stolz, and K. Ploog, Phys. Rev. B **40**, 2950 (1989); Y.-H. Zhang, D.-S. Jiang, R. Cingolani, and K. Ploog, Appl. Phys. Lett. **56**, 2197 (1990).

[10]A. Pinczuk, J. Shah, C. Miller, A. C. Gossard, and W. Wiegman, Solid State Commun. **50**, 735 (1984).

[11]J. M. Rorison, J. Phys. C **20**, L311 (1987).

[12]J. W. Negele and H. Orland, *Quantum Many-Particle Systems* (Addison-Wesley, Reading, MA, 1988).

[13]M. Combescot and P. Nozières, J. Phys. (Paris) **32**, 913 (1971).

[14]T. Uenoyama and L. J. Sham, Phys. Rev. B **39**, 11044 (1989).

[15]M. S. Skolnick, K. J. Nash, S. J. Bass, P. E. Simmonds, and M. J. Kane, Solid State Commun. **67**, 637 (1988).

[16]M. C. Smith, A. Petrou, C. H. Perry, J. M. Worlock, and R. L. Aggarwal, in *Proceedings of the Seventeenth International Conference on the Physics of Semiconductors, San Francisco, 1984,* edited by D. J. Chadi and W. A. Harrison (Springer-Verlag, New York, 1985).