PHYSICAL REVIEW B VOLUME 48, NUMBER 16 15 OCTOBER 1993-II

Interlevel optical transitions in quantum wells

A. G. Petrov and A. Shik
Ioffe Physical-Technical Institute, 194021 St. Petersburg, Russia

(Received 28 December 1992)

A general expression for optical matrix elements describing interlevel absorption in size-quantized systems in the presence of electric and magnetic fields is derived. For rectangular and triangular confining potentials, this approach does not require detailed knowledge of the electron wave function and considerably simplifies the problem. As a result, selection rules and analytical expressions for the matrix elements are obtained for many cases where the standard procedure is much more complicated. As examples, optical matrix elements and selection rules are calculated for some particular shapes of quantum wells: triangular, single, and double asymmetric rectangular. The problem is generalized to the case of heterostructures with effective-mass mismatch. A similar approach to quantum wires and dots is also considered. Interlevel absorption spectra for quantum wells in a parallel magnetic field are calculated.

I. INTRODUCTION

Interlevel optical transitions in quantum wells (QW) have attracted significant attention in recent years and have found an important application in infrared photodetectors.[1] To describe these transitions theoretically, one must calculate the momentum matrix elements between corresponding electron states. For the intricately shaped QW actively studied in recent years, this problem is rather complicated, especially in the presence of strong electric and/or magnetic fields. In the present paper a theory is given expressing these matrix elements through the values of wave functions at the heterointerfaces, which simplifies the problem considerably and excludes the necessity of a wave-function calculation in the entire space followed by integration. This allows us to obtain new analytical results as well as to generalize the problem to the cases of quantum wires and dots.

II. GENERAL EXPRESSIONS

We begin with the general Hamiltonian of the system with some potential relief $U(\mathbf{r})$ and the magnetic field characterized with the vector potential $\mathbf{A}$:

$$\mathcal{H}=\frac{\mathcal{P}^2}{2m}+U(\mathbf{r})\ , \quad \mathcal{P}=-i\hbar\nabla+\frac{e\,\mathbf{A}}{c}\ . \tag{1}$$

Let ε_i be the eigenvalues of the Hamiltonian. To describe the optical properties of the system, we must calculate matrix elements of the generalized momentum $(\mathcal{P}_\alpha)_{fi}$ (f and i mean the final and initial states, $\alpha=x,y,z$).

For further calculations, it is worth deriving a useful general formula for $(\mathcal{P}_\alpha)_{fi}$. To do so, let us calculate the time derivative of the operator $\mathcal{P}_x$. If there is no explicit time dependence of $\mathcal{P}_x$ and the magnetic field $\mathbf{H}=\operatorname{rot}\mathbf{A}$ is uniform, then

$$\begin{aligned}\frac{d\mathcal{P}_x}{dt}=\frac{i}{\hbar}[\mathcal{H},\mathcal{P}_x]&=-\frac{i\hbar e}{2mc}[\nabla^2,A_x]-\frac{i\hbar e}{mc}\left[\mathbf{A}\nabla,\frac{\partial}{\partial x}\right]\\&\quad+\frac{e^2}{2mc^2}\left[A^2,\frac{\partial}{\partial x}\right]\\&\quad-\frac{e^2}{mc^2}[\mathbf{A}\nabla,A_x]-\left[U-eE\mathbf{r},\frac{\partial}{\partial x}\right]\\&=-\frac{\partial U}{\partial x}-\frac{e}{mc}H_z\mathcal{P}_y+\frac{e}{mc}H_y\mathcal{P}_z\ .\end{aligned} \tag{2}$$

Calculating the matrix elements of (2) and taking into account that

$$\left[\frac{d\mathcal{P}}{dt}\right]_{fi}=i\omega_{fi}\mathcal{P}_{fi}\quad[\omega_{fi}=(\varepsilon_f-\varepsilon_i)/\hbar]\ ,$$

we obtain

$$i\omega_{fi}(\mathcal{P}_x)_{fi}=(F_x)_{fi}-\omega_z(\mathcal{P}_y)_{fi}+\omega_y(\mathcal{P}_z)_{fi}\ , \tag{3}$$

where $\omega_\alpha=eH_\alpha/mc$ and the effective force

$$\mathbf{F}=-\nabla U+e\mathbf{E}\ . \tag{4}$$

Two similar expressions can be obtained from (3) by a cyclic permutation of x,y,z. Solution of this linear system gives the eventual formula for $(\mathcal{P}_\alpha)_{fi}$:

$$(\mathcal{P}_\alpha)_{fi}=\frac{(F_\alpha)_{fi}(\omega_{fi}^2-\omega_\alpha^2)-\sum\limits_{\beta,\gamma}(F_\beta)_{fi}[(1-\delta_{\alpha\beta})\omega_\alpha\omega_\beta+ie_{\alpha\gamma\beta}\omega_{fi}\omega_\gamma]}{i\omega_{fi}(\omega_{fi}^2-\omega_c^2)}\ . \tag{5}$$

0163-1829/93/48(16)/11883(7)/$06.00

Here, $\omega_c=(\omega_x^2+\omega_y^2+\omega_z^2)^{1/2}$ is the cyclotron frequency and $e_{\alpha\beta\gamma}$ is the antisymmetric tensor, equal to ± 1 if all three indices are different and vanishing in other cases.

Strictly speaking, in the presence of electric field $\mathbf{E}$, the electronic states in QW are nonstationary and our formulas are incorrect. In fact, however, they are also adequate for not very strong $\mathbf{E}$, until the characteristic time of tunneling decay for the initial state Ψ_i exceeds considerably the period of classical oscillations $\hbar/\varepsilon_i$.

We have managed to express optical matrix elements through the energy spectrum of the system ω_{fi} and the matrix elements of another physical quantity: the effective force $\mathbf{F}$. There is a wide range of physical objects where this procedure considerably simplifies the calculation. These are step-shaped rectangular and triangular QW's corresponding to the situation when the whole space can be divided into regions with constant (but different) values of potential energy. The most attention will be paid to one-dimensional wells with the potential

$$U(x)=\sum_j \Delta U_j \Theta(x-x_j) \ , \tag{6}$$

where

$$\Delta U_j = U(x_j+0)-U(x_j-0)$$

are the band offsets at heterointerfaces $x=x_j$, which can be both positive and negative, and $\Theta(x)$ is the unit step function. In this case the term ∇U in the effective force (4) is the sum of several δ functions, and the corresponding matrix elements do not require integration over the entire space and contain only the values of wave functions at the interfaces. The matrix elements also do not contain the uniform electric field $\mathbf{E}$ since the wave functions Ψ_i and Ψ_f^* are orthogonal. As a result,

$$(F_\alpha)_{fi}=-\sum_j \Delta U_j \Psi_i(x_j)\Psi_f^*(x_j) \ . \tag{7}$$

If at some interface the potential step is very high ($\Delta U_j \to \infty$), then $\Psi(x_j)\to 0$ and Eq. (7) contains an uncertainty. To resolve it, we note that in this limit the wave function in the barrier has the form

$$\Psi(x)=\Psi(x_j)\exp[-\sqrt{2\Delta U_j m}\,(x-x_j)/\hbar]$$

and, hence, its derivative at the interface is

$$\Psi'(x_j)=-\sqrt{2\Delta U_j m}\,\Psi(x_j)/\hbar \ .$$

For $\Delta U\to\infty$, the penetration depth of the wave function tends to zero, so we may neglect the coordinate dependence of the potential caused by electric and magnetic fields. As a result, the wave functions in (7) are to be replaced by their derivatives:

$$\lim_{\Delta U_j\to\infty} \Delta U_j \Psi_i(x_j)\Psi_f^*(x_j)=\frac{\hbar^2}{2m}\Psi_i'(x_j)\Psi_f^{*\prime}(x_j) \ . \tag{8}$$

At extremely high magnetic fields, the wave functions are localized in the area with the width $\sim\lambda=(c\hbar/eH)^{1/2}$ much less than the QW width a. The energy of the ground state depends on the momentum parallel to the QW plane (see Sec. VII) and has its minimal value for the state localized far from the interfaces. As a result, the wave function of the ground state has an exponentially small value at the interfaces which means that, according to Eq. (7), $(F_\alpha)_{fi}\to 0$. In this case, $(\mathcal{P}_\alpha)_{fi}$ will have a nonzero value only if the denominator in Eq. (5) tends to zero and we obtain the well-known selection rules for free electrons in a quantizing magnetic field: $\omega_{fi}=\pm\omega_c$.

Formulas (5), (7), and (8) give the final solution of the problem of optical matrix elements for various QW in uniform electric and magnetic fields. Note that we have not assumed both the initial (i) and the final (f) state to be localized in QW and, hence, our formulas can describe not only interlevel transitions but also optical ionization of QW, that is, the light-induced electron transitions from the bound state in QW to the delocalized states above QW. If the photon energy $\hbar\omega$ exceeds considerably the QW depth, then the final state corresponds to that of an almost free electron with $|\Psi_f(x)|=L^{-1/2}$ (L is the normalizing length) which is independent of ω. In this case Eq. (5) gives that for $\omega\to\infty$, $(\mathcal{P}_\alpha)_{fi}\sim\omega^{-1}$. The total electron-photon matrix element

$$M=\left[\frac{2\pi\hbar e}{\omega m^2}N\right]^{1/2}(\mathcal{P}_\alpha)_{fi}\sim\omega^{-3/2}$$

(N is the photon density). The absorption coefficient $\alpha(\omega)$ is proportional to $|M|^2$ times the number of possible final states for a given value of ω. Since y- and z-momentum components are conserved in optical transitions, the latter factor is equal to the one-dimensional density of states describing x motion, which is $\sim\omega^{-1/2}$ in the absence of magnetic field. So we obtain the asymptotic behavior of the QW photoionization spectrum: $\alpha(\omega)\sim\omega^{-7/2}$. For the particular case of rectangular QW this result has been known before,[2] but we see that it is of general character and takes place for any QW shape. Now we shall apply the general expressions (5)–(8) to some particular low-dimensional systems.

III. TRIANGULAR QUANTUM WELL WITH THE INFINITE WALL

Let us consider first a triangular QW, $U=-Fx$ ($x<0$), with the infinite potential wall at $x=0$. The wave functions of the well-known problem are the Airy functions

$$\Psi_i=C_i\mathrm{Ai}[-(x+\varepsilon_i/F)/l_F] \ ,$$

where $l_F=(\hbar^2/2mF)^{1/3}$ and the normalizing constant

$$C_i=[\sqrt{l_F}\mathrm{Ai}'(-\varepsilon_i/Fl_F)]^{-1} \ .$$

The integral

$$\int_{-\infty}^{0}\mathrm{Ai}[-(x+\varepsilon_i/F)/l_F]\mathrm{Ai}'[-(x+\varepsilon_f/F)/l_F]dx$$

representing the optical matrix element has no analytical representation and usually is calculated either numerically or in the quasiclassical approximation.[3] Our approach allows us to obtain the exact and very simple expression for this element.

According to (5), (7), and (8),

$$(\mathcal{P}_x)_{fi}=i\frac{\hbar^2}{2m\omega_{fi}}\Psi_i'(0)\Psi_f'(0)$$

$$=i\frac{\hbar^2}{2m\omega_{fi}l_F^3}=i\frac{(2e\hbar mF)^{1/3}}{\alpha_{f+1}-\alpha_{i+1}}\ , \tag{9}$$

where $-\alpha_i$ is the $(i+1)$th zero for the Airy function ($\alpha_0 \simeq 2.24$; $\alpha_1 \simeq 4.09$).

IV. ASYMMETRIC RECTANGULAR WELL

The next model to be considered is the QW with different wall heights [Fig. 1(a)] used in some cases in photovoltaic detectors.[4-6] According to Eq. (3), the diagonal elements $(F_x)_{ii}=0$. In our case this means that $U_2\Psi_i^2(0)=U_1\Psi_i^2(a)$. The wave function of the ith bound state has i nodes in the interval $0<x<a$ and, hence,

$$\Psi_i(0)=(-1)^i\sqrt{U_1/U_2}\,\Psi_i(a)\ , \tag{10}$$

which, after substituting into Eqs. (5) and (7), gives

$$(\mathcal{P}_x)_{fi}=\begin{cases}2i\omega_{fi}^{-1}U_2\Psi_i(0)\Psi_f(0)\ , & \text{for odd } i+f\\ 0\ , & \text{for even } i+f\ .\end{cases} \tag{11}$$

So the selection rule resulting from the parity considerations in symmetric QW appears to take place for this particular type of asymmetric QW also.

To calculate the exact value of nonzero matrix elements, we need the value of $\Psi(0)$. The simplest way to find it is to use the virial theorem:[7]

$$\frac{1}{2}\left\langle x\frac{dU}{dx}\right\rangle_i=\varepsilon_i-\langle U\rangle_i\ , \tag{12}$$

where $\langle\ \rangle_i$ means the averaging over the state i. $\langle U\rangle$ contains integration only over barrier regions where $U\neq 0$. Since for $x<0$,

$$\Psi_i(x)=\Psi_i(0)\exp[\sqrt{2m(U_1-\varepsilon_1)}\,x/\hbar]\ ,$$

and similarly for $x>a$, Eq. (12) gives the relation between $\Psi_i(0)$ and $\Psi_i(a)$ which, together with Eq. (10), can be used to determine both of these values and, finally, to calculate optical matrix elements:

$$(\mathcal{P}_x)_{fi}=4i\omega_{fi}^{-1}(\varepsilon_i\varepsilon_f)^{1/2}(a+\kappa_{i1}^{-1}+\kappa_{i2}^{-1})^{-1/2}$$

$$\times(a+\kappa_{f1}^{-1}+\kappa_{f2}^{-1})^{-1/2}\ , \tag{13}$$

where

$$\kappa_{ik}=\hbar^{-1}\sqrt{2m(U_k-\varepsilon_i)}\ ,\quad k=1,2\ .$$

V. DOUBLE QUANTUM-WELL STRUCTURE

Now we consider the system of two QW separated by a tunnel barrier with the energy spectrum representing a series of doublets [Fig. 1(b)]. In this system there is a principal possibility of an inverse population inside the upper doublet under the optical pumping from the lower doublet states.[8] Therefore, the probabilities of both intradoublet and interdoublet optical transitions are of considerable interest. We shall consider the situation when the tunnel transparence

$$T\simeq\exp(-2a\kappa_a)[\kappa_{a,b}=\sqrt{2m(U_{a,b}-\varepsilon_i)}/\hbar]$$

of the central barrier is not large so that the doublet splitting is much less than the interdoublet energy separation. In this case, while considering the interdoublet transitions, we may neglect T and use the results of Sec. IV. So, only the intradoublet transitions require special treatment, which will be given below. Our approximation allows us to neglect the difference between ε_i and ε_f and consider κ_a and κ_b to be the same for both states of interest.

By means of (5) and (7), we obtain

$$(\mathcal{P}_x)_{fi}=\frac{2i}{\omega_{fi}}[U_b|\Psi_i(b)\Psi_f(b)|-U_a|\Psi_i(a)\Psi_f(a)|]$$

$$=\frac{2i}{\omega_{fi}}[(\beta_i\beta_f)^{1/2}-(\alpha_i\alpha_f)^{1/2}]\ ,$$

$$\alpha_{i,f}=U_a|\Psi_{i,f}(a)|^2=U_a|\Psi_{i,f}(-a)|^2\ ,$$

$$\beta_{i,f}=U_b|\Psi_{i,f}(b)|^2=U_b|\Psi_{i,f}(-b)|^2\ , \tag{14}$$

where i and f belong to the same doublet and, hence, have different parity.

For $T\rightarrow 0$, $\alpha_{i,f}\rightarrow\beta_{i,f}$ [see (11)] and, at the same time, $\omega_{fi}\rightarrow 0$. To the first order in T, there are no corrections to $\Psi_i(\pm b)$ and $\beta_i\simeq\beta_i^0/2$, where the index "0" means characteristics found in Sec. V for a single asymmetric QW. To obtain corrections to $\Psi_i(\pm a)$ and find α_i, we shall use again the virial theorem. Since for $x>b$,

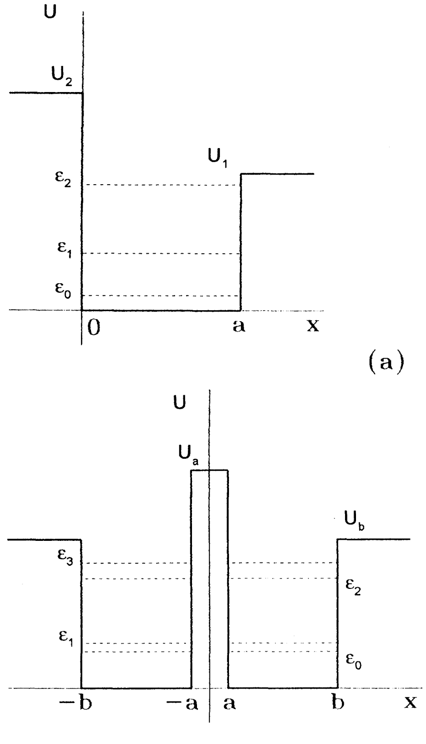

FIG. 1. Energy-band diagram of (a) a single asymmetric QW and of (b) a double QW structure.

$$\Psi_i = \Psi_i(b)\exp[-\kappa_b(x-b)] ,$$

and for $|x|<a$,

$$\Psi_i = \Psi_i(a)\frac{\exp(\kappa_a x)\pm\exp(-\kappa_a x)}{\exp(\kappa_a a)\pm\exp(-\kappa_a a)}$$

(the + and − signs correspond to the symmetric and antisymmetric states), then Eq. (12) gives the relation determining α_i:

$$\varepsilon_i - \beta_i^0[b+(\kappa_b)^{-1}]/2 = \alpha_i\{-a[1\mp 4\exp(-2a\kappa_a)] + \kappa_a^{-1}[1\mp 2\exp(-2a\kappa_a)]\} . \tag{15}$$

In the same way

$$\begin{aligned} \varepsilon_{i,f} &= [(b-a)+(\kappa_a)^{-1}+(\kappa_b)^{-1}]\beta_i^0/2 \mp \hbar\omega_{fi}/2 , \\ \hbar\omega_{fi} &= 4a\beta_i^0\exp(-2a\kappa_a) , \end{aligned} \tag{16}$$

which, after substitution into (14), gives

$$(\mathcal{P}_x)_{fi} = \frac{i\hbar}{4}\frac{\exp(-2a\kappa_a)}{(a-\kappa_a^{-1})} = \frac{i\hbar^2\omega_{fi}(b-a+\kappa_a^{-1}+\kappa_b^{-1})}{32a\varepsilon_i(a-\kappa_a^{-1})} . \tag{17}$$

VI. EFFECTIVE-MASS MISMATCH

So far, we have considered the problem assuming the effective mass m to be the same across the whole structure. But generally this is not the case and at the interfaces $x=x_j$ not only the potential energy but also the effective mass may be discontinuous. In this situation our calculations (2) are incorrect, but they can be generalized to take into account the effective-mass mismatch.

A system with the one-dimensional potential $U(x)$ and the effective-mass profile $m(x)$ is characterized by the Hamiltonian[9]

$$\mathcal{H} = -\frac{\hbar^2}{2}\frac{\partial}{\partial x}m^{-1}(x)\frac{\partial}{\partial x} + U(x) + \frac{p^2}{2m(x)} , \tag{18}$$

where **p** is the momentum in the yz plane. Contrary to all previous results, the variables in the corresponding Schrödinger equation do not separate even in the absence of magnetic field.

If the effective mass is coordinate dependent, then the optical transitions will be caused by the symmetrized Hermitian operator $\{\mathcal{P},m^{-1}(x)\}$ [where $\{\hat{A},\hat{B}\}\equiv(\hat{A}\hat{B}+\hat{B}\hat{A})/2$] rather than $\mathcal{P}$. Therefore, instead of $(\mathcal{P}_x)_{fi}$, we shall calculate matrix elements of the operator $\mathfrak{B}\equiv m_0\{\mathcal{P},m^{-1}(x)\}$, where m_0 is some constant value, say, the free-electron mass.

Using Eq. (18), one can prove the identities

$$\begin{aligned} i\omega_{fi}(\mathfrak{B}_x)_{fi} &= \frac{i}{\hbar}[\mathcal{H},\mathfrak{B}_x]_{fi} \\ &= m_0\left\{\left[\frac{dm^{-1}}{dx}\right],\left[\mathcal{H}-U(x)-\frac{p^2}{2m}\right]\right\}_{fi} \\ &\quad -\frac{m_0}{m}\left[\frac{dU}{dx}\right]_{fi} , \\ i\omega_{fi}(\mathfrak{B}_y)_{fi} &= \frac{i}{\hbar}[\mathcal{H},\mathfrak{B}_y]_{fi} \\ &= -\frac{\hbar}{2}pm_0\left[m^{-1}\frac{d}{dx}\left[\frac{dm^{-1}}{dx}\right] + \left[\frac{dm^{-1}}{dx}\right]\frac{d}{dx}m^{-1}\right]_{fi} , \end{aligned} \tag{19}$$

which allows us to calculate the matrix elements

$$(\mathfrak{B}_x)_{fi} = \frac{im_0}{\omega_{fi}}\sum_j \Psi_i(x_j)\Psi_f^*(x_j) \times\left[\Delta U_j\tilde{m}_j^{-1} + \Delta m_j^{-1}\left[\tilde{U}_j - \frac{\varepsilon_f+\varepsilon_i}{2} + p^2\tilde{m}_j^{-1}\right]\right] , \tag{20}$$

$$(\mathfrak{B}_y)_{fi} = \sum_j \frac{\hbar p m_0}{2\omega_{fi}}\Delta m_j^{-1}\left[\frac{\Psi_i'}{m}(x_j)\Psi_f^*(x_j) - \frac{\Psi_f^{*\prime}}{m}(x_j)\Psi_i(x_j)\right] , \tag{21}$$

generalizing (7) to the case of nonconstant effective mass. Here

$$\begin{aligned} \tilde{U}_j &= [U(x_j+0)+U(x_j-0)]/2 , \\ \tilde{m}_j^{-1} &= [m^{-1}(x_j+0)+m^{-1}(x_j-0)]/2 , \\ \Delta m_j^{-1} &= m^{-1}(x_j+0)-m^{-1}(x_j-0) . \end{aligned}$$

Note that both Ψ and (Ψ'/m) are continuous at the interfaces.

We see that the effective-mass mismatch causes an additional term in the optical matrix element $(\mathfrak{B}_x)_{fi}$. It can be considered as some renormalization of the band offsets ΔU_j and for the light polarization normal to the QW plane does not cause any quantitatively new effect. In particular, the asymptotic behavior of the QW photoionization spectrum $\alpha(\omega)\sim\omega^{-7/2}$ remains the same.

For the parallel light, polarization transitions between different quantum size levels become possible only due to effective-mass mismatch at the heterointerfaces[10] and are described by the matrix element $(\mathfrak{B}_y)_{fi}$ which is proportional to the electron momentum parallel to the interface. Note that here, contrary to the case of x polarization, optical transitions in a symmetric QW will occur between states of the same parity.

Comparing Eqs. (20) and (21), we see that $(\mathfrak{B}_y)_{fi}$ contains the products of one wave function with its derivative rather than those of two wave functions. For delocalized states above QW this derivative is proportional to the wave vector, or to the square root of the energy of these states. In the case of the QW photoionization by high-energy photons, this means that $\Psi_f'/\Psi_f \sim \omega^{1/2}$. As a result, the absorption coefficient will have an additional factor ω compared to the case of x polarization, which results in the QW photoionization spectrum having the high-frequency asymptotics $\alpha(\omega) \sim \omega^{-5/2}$.

VII. OPTICAL TRANSITIONS IN PARALLEL MAGNETIC FIELD

The next problem to be calculated is the interlevel light absorption in the magnetic field parallel to the QW plane ($\mathbf{H} \| \mathbf{z}$). For simplicity we consider a QW with infinite walls at $x = \pm a/2$. We restrict ourselves to the case of not very high fields:

$$\varepsilon_0 \equiv \frac{\pi^2 \hbar^2}{2ma^2} > \hbar\omega_c \ . \tag{22}$$

In this case the energy spectrum of the system can be determined by considering the magnetic field as a perturbation:[11]

$$\varepsilon(n,p_y,p_z) = n^2\varepsilon_0 + \frac{m\omega_c^2 a^2}{24}\left[1 - \frac{6}{\pi^2 n^2}\right] + \frac{p_y^2}{2m}\left[1 + \frac{m\omega_c^2 a^2}{n^2\varepsilon_0}\left[\frac{1}{3} - \frac{5}{\pi^2 n^2}\right]\right] + \frac{p_z^2}{2m} \ . \tag{23}$$

One can see two effects of magnetic field on the energy spectrum: (i) a quadratic level shift and (ii) anisotropic dispersion in the y-z plane due to the effective-mass change along the y axis (note that the effective mass increases for the ground subband and decreases for the excited subbands).

For an infinite QW where Eq. (8) takes place, the matrix elements given by Eqs. (5) and (7) can be written in the following form:

$$\begin{aligned} (\mathcal{P}_x)_{fi} &= -i\frac{\hbar^2\omega_{fi}}{2m(\omega_{fi}^2 - \omega_c^2)}\Psi_i'(x_j)\Psi_f^{*\prime}(x_j) \ , \\ (\mathcal{P}_y)_{fi} &= i\frac{\omega_c}{\omega_{fi}}(\mathcal{P}_x)_{fi} \ . \end{aligned} \tag{24}$$

This means that any transition can be caused either by x- or by y-polarized light, but the ratio of the absorption intensities for these two polarizations is equal to $(\omega_{fi}/\omega_c)^2$.

To calculate the matrix elements, one determines the wave-function derivatives at the interfaces. As in Sec. IV, the most convenient way to do it is connected with the virial theorem. This theorem in its standard form (12) is not valid in magnetic field, but we can reformulate it to include the effect of the field. In so doing, we introduce the notation

$$\begin{aligned} \tilde{U}(x) &= U(x) + m\omega_c^2(x - x_0)^2/2 \ , \\ \tilde{\varepsilon}_i &= \varepsilon_i - (p_z)^2/2m \ , \\ x_0 &= cp_y/(eH) \ , \end{aligned}$$

which allows us to reduce the Schrödinger equation to the standard form with kinetic and potential energies:

$$-\frac{\hbar^2}{2m}\Psi_i'' + \tilde{U}\Psi_i = \tilde{\varepsilon}_i\Psi_i$$

and to apply the virial theorem to this transformed equation:

$$\frac{1}{2}\left\langle (x \pm a/2)\frac{d\tilde{U}}{dx}\right\rangle_i = \tilde{\varepsilon}_i - \langle \tilde{U} \rangle_i \ . \tag{25}$$

With the help of Eq. (8), the last formula can be transformed to the following expression:

$$\frac{\hbar^2 a}{4m}|\Psi_i'(\pm a/2)|^2 = \varepsilon_i - \frac{p_y^2 + p_z^2}{2m} + \frac{m\omega_c^2}{2}[x_0(3\langle x \rangle_i \pm 1) - 2\langle x^2 \rangle_i \mp a\langle x \rangle_i/2] \ . \tag{26}$$

Comparing Eqs. (24) and (26), we conclude that the matrix element we are interested in can be expressed in terms of average values of x and x^2. In the case of relatively low magnetic field (22), $\langle x^2 \rangle_i$ can be calculated assuming $H = 0$, which gives

$$\langle x^2 \rangle_i = \frac{a}{12}\left[1 - \frac{6}{\pi^2 n^2}\right] \ .$$

As to $\langle x \rangle$, in this limit it vanishes, whereas in the next order in H, $\langle x \rangle_i \sim a^4 p_y/\hbar\lambda^2$, where λ is the magnetic length. In our further calculations we shall assume the electron concentration n_s to be not very high so that only one quantum subband is occupied and $|p_y|a < \hbar$. In this case the exact value of a numerical factor in $\langle x \rangle_i$ is of no importance since for the condition (22) the terms $\sim \langle x \rangle_i$ appear to be negligibly small.

Substituting the expressions for $\langle x \rangle$ and $\langle x^2 \rangle$ into (24) and (26), we obtain the expressions for the matrix elements describing the transitions between the lowest quantum levels $n = 1,2,3$:

$$(\mathcal{P}_x)_{21} \simeq i\frac{8}{3}\frac{\hbar}{a} \ , \tag{27}$$

$$(\mathcal{P}_x)_{31} \simeq i\frac{5}{12\pi^2}\frac{eHp_y a^2}{\hbar c} \ . \tag{28}$$

The latter matrix element is seen to have a small numerical factor. As a result, all corrections proportional to $m\omega_c^2 a^2/\varepsilon_0$ appear to be very small and can be neglected even on condition (22) without the requirement of a strong inequality $\hbar\omega_c \ll \varepsilon_0$.

We use Eqs. (27) and (28) to calculate the interlevel absorption spectra:

$$\alpha(\omega)=\frac{\pi^2e^2}{cn_\omega m^2\omega a\hbar^2}\times\int dp_y\int dp_z|\mathcal{P}_{fi}|^2\delta(\varepsilon_f-\varepsilon_i-\hbar\omega)f(\varepsilon_i)\ . \qquad (29)$$

Here, n_ω is the refraction index and $f(\varepsilon_i)$ is the Fermi function. The spectra will have a finite width since the energy versus p_y dependences are different in different subbands [see Eq. (23)]. We shall consider $\alpha(\omega)$ for x-polarized light. As we have already mentioned, the spectra for y polarization will differ only by a constant factor $(\omega_{fi}/\omega_c)^2$.

For transitions $1\rightarrow n$ in the degenerate electron gas, the absorption band is characterized by the low-frequency edge

$$(\hbar\omega)_{\min}=\varepsilon_0(n^2-1)+\frac{m\omega_c^2a^2}{4\pi^2}\frac{(n^2-1)}{n^2} \qquad (30)$$

and the bandwidth

$$\Delta(\hbar\omega)\equiv\hbar(\omega_{\max}-\omega_{\min})=\frac{\pi}{4}\eta n_s a^4 m\omega_c^2\ , \qquad (31)$$

where

$$\eta=\frac{5}{\pi}2(1-n^{-4})-\tfrac{1}{3}(1-n^{-2})$$

is the numerical factor equal to 0.22 for $1\rightarrow 2$ transitions and 0.20 for $1\rightarrow 3$ transitions. In our calculations we have used the relation between electron concentration n_s and Fermi energy E_F valid for the limiting case $\hbar\omega_c\ll\varepsilon_0$: $E_F=\varepsilon_0+\pi\hbar^2n_s/m$.

The $\alpha(\omega)$ dependence inside the absorption band is considerably different for allowed (n even) and forbidden (n odd) transitions. In the first case,

$$\alpha(\omega)=\frac{1024\pi^4c\hbar^2}{9\eta n_\omega H^2a^7\omega m}\left[\frac{\omega_{\max}-\omega}{\omega-\omega_{\min}}\right]^{1/2}. \qquad (32)$$

The integral absorption in the band $\int d\omega\,\alpha(\omega)$ is proportional to n_s, which seems quite natural for intraband transitions. In the second case,

$$\alpha(\omega)=\frac{100\pi^2c\hbar}{9\eta^2n_\omega a^5H^2\omega}[(\omega_{\max}-\omega)(\omega-\omega_{\min})]^{1/2}\ . \qquad (33)$$

For this case the integral absorption is proportional to n_s^2 rather than to n_s. This is caused by the fact that absorption in the parallel polarization is possible only for electrons with nonzero p_y and, therefore, has an additional proportionality to E_F, that is, to the electron concentration. The ratio of total allowed and forbidden absorption is of order $\lambda^4/(n_sa^6)$ and depends dramatically on the QW width a since the matrix element $(\mathcal{P}_x)_{21}$ decreases, whereas $(\mathcal{P}_x)_{31}$ increases with a [see Eqs. (27) and (28)].

The $\alpha(\omega)$ dependences are shown schematically in Fig. 2. One can see that the band of allowed transitions is strongly asymmetric, having a divergence at the low-frequency edge. The band of forbidden transitions has a symmetric, ellipselike shape.

VIII. QUANTUM WIRES AND DOTS

In conclusion, we consider optical transitions in electron systems confined in more than one direction. The general expression (5) is valid for any dimensionality of the system, and the only problem is to calculate matrix elements of $\mathbf{F}$. Let the surface S_{lj} be the boundary between domains with different potential energies V_l and V_j. Then the matrix element $(\mathbf{F})_{fi}$ is determined by integration only over S_{lj} where ∇U differs from zero:

$$(\mathbf{F})_{fi}=-\sum_{l,j}\int_{S_{lj}}d\mathbf{S}(V_l-V_j)\Psi_i(\mathbf{r})\Psi_f^*(\mathbf{r})\ . \qquad (34)$$

Here, the sum is taken over all interfaces, and $d\mathbf{S}$ is the vector of elementary area oriented along the normal to the interface.

If some potential step is extremely high ($V_l\rightarrow\infty$), then, by analogy with Eq. (8),

$$\int d\mathbf{S}(V_l-V_j)\Psi_i(\mathbf{r})\Psi_f^*(\mathbf{r})=\frac{\hbar^2}{2m}\int d\mathbf{S}\frac{\partial\Psi_i(\mathbf{r})}{\partial n}\frac{\partial\Psi_f^*(\mathbf{r})}{\partial n}\ , \qquad (35)$$

where derivatives are taken along the interface normal.

To illustrate this approach, let us calculate optical matrix elements for a cylindrical wire with the radius R and infinitely high potential walls. The wave functions of electron motion normal to the wire axis are

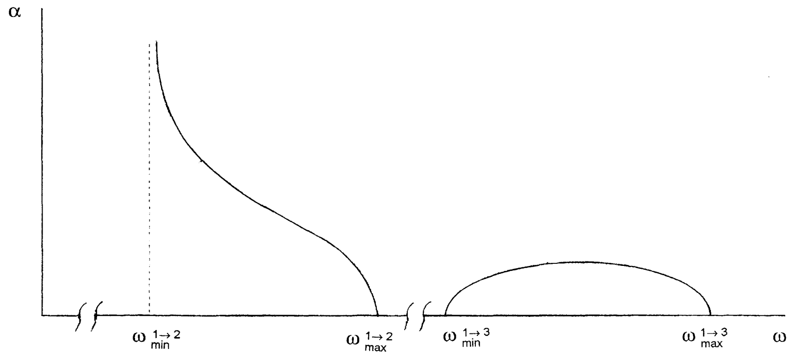

FIG. 2. Schematic view of the interlevel absorption spectra in the parallel magnetic field.

$$\Psi_{nk}(\rho,\phi)=\frac{J_k(\gamma_{kn}\rho/R)\exp(ik\phi)}{\sqrt{\pi}RJ_{k+1}(\gamma_{kn})}\;, \tag{36}$$

where J_k is the kth-order Bessel function and γ_{kn} is its nth zero. The corresponding energy levels

$$\varepsilon_{nk}=\frac{\hbar^2}{2mR^2}\gamma_{kn}^2\;. \tag{37}$$

Using Eqs. (9) and (34)–(37), we obtain the expressions for optical matrix elements between the states $i\equiv(k,n)$ and $f\equiv(k',n')$:

$$(\mathcal{P}_x)_{fi}=\frac{i\hbar}{R}\frac{\gamma_{kn}\gamma_{k'n'}}{\gamma_{k'n'}^2-\gamma_{kn}^2}\delta_{k',k\pm1}\;. \tag{38}$$

One can see that optical transitions are allowed only between quantum states with azimuthal numbers k differing by unity. Our procedure is much simpler than direct calculation of the integrals determining matrix elements.

IX. CONCLUSION

We have presented a general expression for the matrix elements describing interlevel absorption in various size-quantized systems in the presence of uniform electric and magnetic fields. For a wide class of rectangular and triangular confining potentials, this approach considerably simplifies the problem. The method does not require detailed knowledge of the wave functions and, hence, is much simpler than the standard procedure of solving the Schrödinger equation followed by integration of matrix elements. As a result, selection rules and analytical expressions for the matrix elements are obtained for many cases where the standard procedure is much more complicated and/or can be fulfilled only numerically. Our approach is also very convenient for numerical calculations since the Schrödinger equation is to be solved only for several points. As examples, some particular shapes of QW's as well as the problem of interlevel transitions in the magnetic field have been considered.

ACKNOWLEDGMENT

We would like to thank V. I. Perel' and R. A. Suris for valuable discussions.

---

[1] *Intersubband Transitions in Quantum Wells,* edited by E. Rosencher, B. Vinter, and B. Levine (Plenum, New York, 1992).

[2] A. Ya. Shik, *Intersubband Transitions in Quantum Wells* (Ref. 1), p. 319.

[3] H. J. Fischbeck and J. Mertsching, Phys. Status Solidi **31**, 107 (1969).

[4] D. D. Coon and R. P. G. Karunasiri, Appl. Phys. Lett. **45**, 649 (1984).

[5] B. F. Levine, S. D. Gunapala, and M. Hong, Appl. Phys. Lett. **59**, 1969 (1991).

[6] H. Schneider, K. Kheng, F. Fuchs, J. D. Ralston, B. Dischler, and P. Koidl, *Intersubband Transitions in Quantum Wells* (Ref. 1), p. 73.

[7] A. S. Davydov, *Quantum Mechanics* (Pergamon, New York, 1965).

[8] J. W. Bales, K. A. McIntosh, T. C. L. G. Sollner, W. D. Goodhue, E. R. Brown, and B. Lax (unpublished).

[9] D. J. Ben Daniel and C. B. Duke, Phys. Rev. **152**, 683 (1966).

[10] A. Ya. Shik, Fiz. Tekh. Poluprovodn. **22**, 1843 (1988) [Sov. Phys.—Semicond. **22**, 1165 (1988)].

[11] A. I. Lukanin and Z. I. Uritskii, Fiz. Tekh. Poluprovodn. **13**, 2286 (1979) [Sov. Phys.—Semicond. **13**, 1340 (1979)].