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$\mathbf{A}^{\perp}\cdot\mathbf{p}$ versus Φ for coupling electrons to interface optical phonons in quantum wells

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The interface optical-phonon modes and their interaction with electrons in layered semiconductor structures are considered. In a canonical theory where retardation effects are retained from the outset, the theory leads naturally to the quantization of the free interface oscillations in the radiation gauge for which the scalar potential is zero and the vector potential is transverse ($\phi=0$, $\nabla\cdot\mathbf{A}=0$). The description is thus entirely in terms of a *transverse* vector potential $\mathbf{A}^{\perp}$ which satisfies $\nabla\cdot\mathbf{A}^{\perp}=0$ everywhere, except at the interfaces where, as usual, only boundary conditions apply. The interaction between the two subsystems (electrons and interface modes) is the well-known minimal-coupling Hamiltonian which is in the form $e\,\mathbf{A}^{\perp}\cdot\mathbf{p}/m^*$. The main aspects of the quantization of such retarded modes are summarized. It is then shown that for a double heterostructure the nonretarded vector potential can be expressed in terms of the gradient of a unique field operator Λ which enters a unitary transformation $e^{i\Lambda}$. We demonstrate that the result of applying this transformation on the total minimal-coupling Hamiltonian is the unitary-equivalent Hamiltonian in which the coupling to electrons is in the form $e\Phi$. This Φ is identical to that given by Mori and Ando. The matrix elements using the $e\Phi$ form of coupling are then compared with those using the $e\,\mathbf{A}^{\perp}\cdot\mathbf{p}/m^*$ coupling and seen to be clearly different. However, when the emission rates are evaluated using the two coupling Hamiltonians, interesting and nontrivial manipulations are required to prove that the same results emerge for the total emission rate from any given initial electronic state of the double heterostructure. The reasons for the agreement of the two sets of results for first-order transitions are pointed out and discussed.

I. INTRODUCTION

There are a number of excitations in solids, such as the vibrational modes of polar crystals, which involve an electric field, and for those excitations which propagate at speeds well below that of light it is usual to associate the field with a scalar potential. While this procedure is correct for truly longitudinally polarized modes, it is, strictly speaking, incorrect for purely transversely polarized modes, i.e., those (normally identified as polaritons) whose fields are associated with a transverse vector potential. Nevertheless, in the unretarded limit, the field associated with a transversely polarized mode is commonly associated with a scalar potential. The idea behind this is that the frequency is much lower than it would be for light at the same wavelength, and an electrostatic approximation, embodied by $\nabla\times\mathbf{E}^{\perp}\approx\mathbf{0}$, is therefore valid. This looks as if the transverse mode has been endowed with a longitudinal character, therefore allowing the use of a scalar potential. In fact, of course, a transverse wave remains transverse with $\nabla\times\mathbf{E}^{\perp}$ always finite, though small, and it retains thereby its vector potential. Nevertheless, the physical argument for employing a scalar potential is very plausible. If this is accepted, it then remains to be shown that the interaction with an electron is as well described by the $e\Phi$ interaction as by the $e\,\mathbf{A}^{\perp}\cdot\mathbf{p}/m^*$ interaction (here $\mathbf{A}^{\perp}$ and Φ are the transverse vector potential and the scalar potential, m^* is the electronic effective mass, and $\mathbf{p}$ is its momentum operator). The very different forms of the two interactions make their equivalence in this respect by no means obvious. As far as we are aware, this matter has not been resolved, though its existence has been highlighted before.[1]

A resolution of the issue of which coupling Hamiltonian should be employed in actual calculations is needed, particularly in view of the importance in layered structures of the interaction between interface polaritons (Fuchs and Kliewer interface modes) and an electron, which has been treated using $e\Phi$ by a number of authors[2–5] and using $\mathbf{A}^{\perp}\cdot\mathbf{p}$ by others.[6] Scattering by the AlAs interface modes of electrons in GaAs wells in a GaAs/AlAs superlattice is predicted to be the dominant mechanism in narrow quantum wells[5–7] (a conclusion, incidentally, indifferent to whether $e\Phi$ or $\mathbf{A}^{\perp}\cdot\mathbf{p}$ is used). The importance of the AlAs interface modes has recently been confirmed by the experimental work of Tsen *et al.*[8]

In this paper we analyze how, in the unretarded limit, the theory with the $e\,\mathbf{A}^{\perp}\cdot\mathbf{p}/m^*$ coupling can be transformed to another, where the coupling is $e\Phi$, using a unitary transformation, and conclude that the two approaches give very different differential rates between individual states, but these differences disappear if the transition is on the energy shell. Surprisingly, considering the difference in the form of the two interactions, the same scattering rate is obtained, but a self-energy term appears in the Hamiltonian where $e\Phi$ is used and further differences are envisaged when higher-order transitions are considered. The equivalence of the first-order scattering rates for both inter- and intrasubband processes is illustrated in detail for the case of an electron in an infinitely deep well.

The paper is organized as follows. In Sec. II we discuss the formalism for the polaritons in a system of layered media and single out the interface polaritons in their fully retarded forms for quantization and for coupling to electrons. In Sec. III we discuss the unretarded limit of the theory and the unitary transformation that is needed to cast the old Hamiltonian in a new form, emphasizing its scalar potential coupling. In Sec. IV we compare and contrast the predictive powers of the two Hamiltonians by considering explicit evaluations of the lowest-order process involving interface polariton emission by electrons. In Sec. V we comment on the results and discuss their implications with regard to gauge transformations and unitary equivalence.

II. FORMALISM

A theory of interaction of electrons with transverse electromagnetic fields in polar semiconductor media can be straightforwardly constructed once three physically motivated approximations are made. First, we assume that we are dealing with isotropic media, and second, that a continuum approximation is valid. These, when taken together, amount to being able to define a single dielectric function $\epsilon(\omega)$ for the medium. The third assumption involves the effective-mass approximation for the electrons near the Γ minimum of, e.g., III-V compounds. The Hamiltonian that is consistent with such a physical situation is written as follows:

$$H=\frac{1}{2m^*}[\mathbf{p}-e\,\mathbf{A}(\mathbf{x})]^2+V_c(z)+\int d\mathbf{r}\,\mathcal{H}_{\text{field}}\ , \tag{1}$$

where $V_c(z)$ stands for the Coulomb potential in which the electrons move, $\mathbf{x}$ and $\mathbf{p}$ are the position and momentum vectors of the electron, and m^* is its effective mass. The Hamiltonian density $\mathcal{H}_{\text{field}}$ accounts for the free transverse electromagnetic fields coupled to the polarization fields of the medium and can be written succinctly in the form[9,10]

$$\mathcal{H}_{\text{field}}=\tfrac{1}{2}\epsilon_0\sum_{\omega}\left[\left[\frac{\partial(\omega\epsilon)}{\partial\omega}\right]\mathbf{E}^{\perp 2}(\omega,\mathbf{r})+c^2\mathbf{B}^2(\omega,\mathbf{r})\right]\ , \tag{2}$$

where the sum symbolizes a spectral sum over all the allowed transverse electromagnetic fields of the medium, henceforth referred to as polaritons, satisfying

$$\epsilon(\omega)\neq 0\ . \tag{3}$$

The strategy while using perturbation theory is to divide H into a zero-order part, describing the two noninteracting systems (electrons and polaritons) plus the interaction. The zero-order Hamiltonian for the electrons is

$$H_e^0=\frac{p^2}{2m^*}+V_c\ . \tag{4}$$

With the Coulomb aspects of the problem separated out, as contained in V_c, we have only the free fields to consider. The appropriate gauge to choose is that for which

$$\nabla\cdot\mathbf{A}=0,\quad \phi=0\ . \tag{5}$$

Writing $\phi=0$ for the polaritons merely asserts that all Coulomb aspects associated with the presence of real charges (as opposed to polarization charges) have already been taken into account in V_c. Equation (5) describes a version of the Coulomb gauge, which is normally referred to as the radiation[11] or transverse gauge. The transverse gauge, Eq. (5), provides the natural conditions to impose for the purpose of quantizing the photon fields.[12,13] It has also been adopted in the context of lattice dynamics by Chu and Chang.[14] The theory can therefore be described entirely in terms of a transverse vector potential which can be shown to satisfy

$$\nabla\cdot\mathbf{A}^{\perp}=0,\quad \nabla^2\mathbf{A}^{\perp}+\frac{\omega^2\epsilon}{c^2}\mathbf{A}^{\perp}=0\ . \tag{6}$$

$\mathbf{A}^{\perp}$ is the transverse vector potential associated with the polaritons and $\mathbf{E}$ and $\mathbf{B}$ are the field vectors such that

$$\mathbf{E}^{\perp}=-\dot{\mathbf{A}}^{\perp},\quad \mathbf{B}=\nabla\times\mathbf{A}^{\perp}\ . \tag{7}$$

We should emphasize that, for convenience, we have chosen to work in the transverse gauge in which the free fields have no scalar potential. Gauge transformations that preserve $\mathbf{E}^{\perp}$ and $\mathbf{B}$ can be legitimately made, but these will have to involve adding to our transverse vector potential a longitudinal component $\mathbf{A}^L$ and there will then have to exist a scalar potential ϕ to account for the presence of the additional component $\mathbf{A}^L$. The additional potentials are connected by gauge conditions that are different from Eqs. (5). Clearly, the resulting formalism, albeit legitimately correct, would be cumbersome to use. We therefore continue to employ the transverse gauge given by Eqs. (5).

The next steps of the theory in the case of the infinite bulk can be straightforwardly developed. The main ingredients involve the quantization of the modes and the use of perturbation theory to calculate relevant attributes of their interaction with the electrons through various emission and absorption processes. Such a treatment has been previously considered in detail,[13,15] so we do not discuss the case of the bulk any further here.

Our concern in this paper is primarily with the interface modes that are known to exist when such polar materials are joined at smooth interfaces to other polar materials, forming a heterostructure.[5] The corresponding theory is formally the same as that given above, except that the vector potential $\mathbf{A}^{\perp}$ is that satisfying the boundary conditions at the heterostructure interfaces.

We are interested in the case of a double heterostructure, for example GaAs/AlAs. A layer of width d of GaAs is sandwiched between two much-thicker layers of AlAs. We use the labels 1 and 2 to refer, respectively, to AlAs (occupying the region $|z|>d/2$) and GaAs (occupying the region $|z|<d/2$). The dielectric functions appropriate for the two types of material are given by

$$\epsilon_i(\omega)=\epsilon_i^{\infty}\left[\frac{\omega_{Li}^2-\omega^2}{\omega_{Ti}^2-\omega^2}\right],\quad i=1,2\ , \tag{8}$$

where, for material i, we have ϵ_i^{∞} as the high-frequency dielectric constant, and ω_{Li} and ω_{Ti} as the zone-center LO and TO phonon frequencies. The field equation is

$$\nabla^2\mathbf{A}^{\perp}+\frac{\epsilon(\omega,z)\omega^2}{c^2}\mathbf{A}^{\perp}=0\ , \tag{9}$$

where $\epsilon(\omega,z)$ describes the abrupt changes of ϵ at the two interfaces separating the three regions of the heterostructure. The required interface modes emerge from the procedure of applying the standard electromagnetic boundary conditions at the two interfaces at $z=\pm d/2$ and seeking solutions that decay on either side of the interfaces. The mode frequencies conform with the well-known dispersion relations

$$\frac{\epsilon_2 q_1}{\epsilon_1 q_2}=-\coth(q_2 d/2)\quad (S\text{ modes}) \tag{10}$$

and

$$\frac{\epsilon_2 q_1}{\epsilon_1 q_2}=-\tanh(q_2 d/2)\quad (A\text{ modes})\ , \tag{11}$$

where S and A stand for symmetric and antisymmetric solutions, respectively. The symmetry refers to that of the in-plane component of the electric-field vector. The wave vectors q_1 and q_2 are given by

$$q_i^2=q_\parallel^2-\frac{\omega^2\epsilon_i}{c^2},\quad i=1,2\ . \tag{12}$$

The quantized transverse vector potential $\mathbf{A}^\perp$ associated with the interface modes can then be written as

$$\mathbf{A}^\perp(\mathbf{r},t)=\sum_\alpha \int d^2\mathbf{q}_\parallel[\,\tilde{\mathbf{A}}_\alpha(\mathbf{q}_\parallel,z)e^{i(\mathbf{q}_\parallel\cdot\mathbf{r}_\parallel-\omega t)}a_\alpha(\mathbf{q}_\parallel)+\text{H.c.}\,]\ , \tag{13}$$

where we have written $\mathbf{r}=(\mathbf{r}_\parallel,z)$. The vector coefficients $\tilde{\mathbf{A}}_\alpha(\mathbf{q}_\parallel,z)$ are the mode vector functions associated with branch α and are found to be given explicitly by

$$\tilde{\mathbf{A}}_\alpha=C_\alpha[\hat{\mathbf{r}}_\parallel F_\alpha(z)+\hat{\mathbf{z}}G_\alpha]e^{i(\mathbf{q}_\parallel\cdot\mathbf{r}_\parallel-\omega t)}\ , \tag{14}$$

where the carets denote unit vectors. The functions F_α and G_α for $\alpha=S$ and A are given explicitly by

$$F_S=-i\left[e^{q_1 z}\left\{\frac{e^{-q_1 d/2}\cosh(q_2 z)}{\cosh(q_2 d/2)}\right|e^{-q_1 z}\right]\ , \tag{15}$$

$$F_A=-i\left[-e^{q_1 z}\left|\frac{e^{-q_1 d/2}\sinh(q_2 z)}{\sinh(q_2 d/2)}\right|e^{-q_1 z}\right]\ , \tag{16}$$

$$G_S=-\frac{q_\parallel}{q_1}\left[-e^{q_1 z}\left|\frac{q_1 e^{-q_1 d/2}\sinh(q_2 z)}{q_2\cosh(q_2 d/2)}\right|e^{-q_1 z}\right]\ , \tag{17}$$

$$G_A=\frac{q_\parallel}{q_1}\left[-e^{q_1 z}\left|\frac{q_1 e^{-q_1 d/2}\cosh(q_2 z)}{q_2\sinh(q_2 d/2)}\right|-e^{-q_1 z}\right]\ , \tag{18}$$

where the vertical bars represent the left (at $z=-d/2$) and right (at $z=+d/2$) boundaries of the double heterostructure. Finally, the quantities C_α appearing in Eq. (14) are the mode coefficients and are given by

$$C_\alpha=\left[\frac{\hbar\omega_\alpha}{(2\pi)^2\epsilon_0(D_E^\alpha+2D_B^\alpha)}\right]^{1/2}\ . \tag{19}$$

D_E^α and D_B^α arise from the canonical quantization procedure and are described as follows. For D_E^α we obtain

$$D_E^\alpha=\omega_\alpha^3 e^{-q_1 d}\left[\frac{q_\parallel^2+q_1^2}{q_1^3}\frac{\partial\epsilon_1}{\partial\omega}+\xi_\alpha\frac{\partial\epsilon_2}{\partial\omega}\right]\ , \tag{20}$$

with

$$\xi_S=\frac{(q_\parallel^2+q_2^2)\sinh(q_2 d)-q_2 d(q_\parallel^2-q_2^2)}{2q_2^3\cosh^2(q_2 d/2)} \tag{21}$$

and

$$\xi_A=\frac{(q_\parallel^2+q_2^2)\sinh(q_2 d)+q_2 d(q_\parallel^2-q_2^2)}{2q_2^3\sinh^2(q_2 d/2)}\ . \tag{22}$$

For D_B^α we have

$$D_B^\alpha=\frac{\omega_\alpha^4 q_\parallel\epsilon_1 e^{-q_1 d}}{2q_1 c^2}\left[\frac{\epsilon_1-\epsilon_2}{q_1^2 q_2^2}+\frac{g_\alpha\epsilon_2 d}{q_2\sinh(q_2 d)}\right]\ , \tag{23}$$

with $g_S=1$ and $g_A=-1$.

The above equations (13)–(23) define the quantized transverse vector potential associated with the interface polaritons in the double heterostructure. The mode operators $a_\alpha(\mathbf{q}_\parallel)$ and $a_\alpha^\dagger(\mathbf{q}_\parallel)$ are boson operators satisfying the commutation relation

$$[a_\alpha(\mathbf{q}_\parallel),a_\beta^\dagger(\mathbf{q}_\parallel')]=\delta_{\alpha\beta}\delta(\mathbf{q}_\parallel-\mathbf{q}_\parallel')\ , \tag{24}$$

and the procedure is carried out in such a way that the field Hamiltonian given by the last term of Eq. (2) reduces to the canonical form. The total Hamiltonian of the electron in interaction with the interface polaritons is thus given by

$$H=\frac{1}{2m^*}(\mathbf{p}-e\,\mathbf{A}^\perp)^2+V_c(z)+H_{\text{field}}\ , \tag{25}$$

where H_{field} is given by

$$H_{\text{field}}=\tfrac{1}{2}\sum_\alpha\int d^2\mathbf{q}_\parallel\hbar\omega_\alpha[a_\alpha(\mathbf{q}_\parallel)a_\alpha^\dagger(\mathbf{q}_\parallel)+a_\alpha^\dagger(\mathbf{q}_\parallel)a_\alpha(\mathbf{q}_\parallel)]\ . \tag{26}$$

The above Hamiltonian will be referred to as the minimal-coupling Hamiltonian. It is the basis for the calculations of transition rates due to emission of interface polaritons by quantum-well electrons reported recently by Al-Dossary, Babiker, and Constantinou.[6]

III. UNITARY TRANSFORMATION

We have seen that in a fully retarded canonical theory it is natural that the interface modes be quantized only in terms of their transverse vector potential $\mathbf{A}^\perp$. The total Hamiltonian of the electrons in interaction with the interface optical modes in the double heterostructure is given by Eqs. (25) and (26) and the mode operators satisfy the commutation relations given by Eq. (24). The mode frequencies of the different branches satisfy the fully retarded dispersion relations given in Eqs. (10) and (11). Our concern in the rest of this paper is with the large-$q_\parallel$ limit of the theory. The large-$q_\parallel$ limit, in fact, corresponds to the regime in which one deals with calculations of electron-phonon interactions and in fact corresponds to the unretarded limit of the theory. It is not too difficult to check that when this limit is applied to expressions (13)–(23) they amount to the result that the transverse vector potential $\mathbf{A}^{\perp}$ can be conveniently written in terms of the gradient of a field operator Λ as follows:

$$\mathbf{A}^{\perp}_{\text{retarded}} \rightarrow \mathbf{A}^{\perp}_{\text{unretarded}} = -\frac{\hbar}{e}\nabla\Lambda \ , \tag{27}$$

where Λ is given by

$$\Lambda = \frac{ie}{\hbar}\sum_{\alpha}\int d\mathbf{q}_{\parallel}\frac{1}{\omega}(a_{\alpha}\widetilde{\phi}_{\alpha}+a^{\dagger}_{\alpha}\widetilde{\phi}^{*}_{\alpha}) \ . \tag{28}$$

The corresponding unretarded forms of the dispersion relations are as follows: for the symmetric branches ($\alpha=S$) we have

$$\frac{\epsilon_2}{\epsilon_1} = -\coth(q_{\parallel}d/2) \ , \tag{29}$$

and for the antisymmetric ones ($\alpha=A$) we have

$$\frac{\epsilon_2}{\epsilon_1} = -\tanh(q_{\parallel}d/2) \ . \tag{30}$$

In Eq. (28) we have, for convenience, omitted the $\mathbf{q}_{\parallel}$ labels in the mode operators a_{α} and $a^{\dagger}_{\alpha}$. The functions $\widetilde{\phi}_{\alpha}$ are the mode functions pertaining to branch α at wave vector $\mathbf{q}_{\parallel}$. Each $\widetilde{\phi}_{\alpha}$ corresponds to the unretarded versions of F_{α} and G_{α}, obtainable from the full expressions given earlier in Eqs. (15)–(18). We have for the symmetric functions ($\alpha=S$)

$$\widetilde{\phi}_{S} = \left[\frac{\hbar\epsilon_2}{2(2\pi)^2\epsilon_0 q_{\parallel}D}\right]^{1/2} \times \left[\begin{array}{c|c|c} e^{q_{\parallel}(z+d/2)} & \dfrac{\cosh(q_{\parallel}z)}{\cosh(q_{\parallel}d/2)} & e^{-q_{\parallel}(z-d/2)} \end{array}\right] \times e^{i(\mathbf{q}_{\parallel}\cdot\mathbf{r}_{\parallel}-\omega t)} \ , \tag{31}$$

where the vertical bars represent the left (at $z=-d/2$) and right (at $z=+d/2$) boundaries of the double heterostructure. Similarly, for the antisymmetric functions ($\alpha=A$) we have

$$\widetilde{\phi}_{A} = \left[\frac{\hbar\epsilon_2}{2(2\pi)^2\epsilon_0 q_{\parallel}D}\right]^{1/2} \times \left[\begin{array}{c|c|c} -e^{q_{\parallel}(z+d/2)} & \dfrac{\sinh(q_{\parallel}z)}{\sinh(q_{\parallel}d/2)} & e^{-q_{\parallel}(z-d/2)} \end{array}\right] \times e^{i(\mathbf{q}_{\parallel}\cdot\mathbf{r}_{\parallel}-\omega t)} \ . \tag{32}$$

In the above the quantity D appearing in the denominators of the mode coefficients is given by

$$D = \epsilon_2\frac{\partial\epsilon_1}{\partial\omega} - \epsilon_1\frac{\partial\epsilon_2}{\partial\omega} \ . \tag{33}$$

The nonretarded minimal-coupling Hamiltonian is obtainable simply by substituting from Eq. (27) into Eqs. (25) and (26). We have

$$H = \frac{(\mathbf{p}+\hbar\nabla\Lambda)^2}{2m^*} + V_c(z) + \tfrac{1}{2}\sum_{\alpha}\int d\mathbf{q}_{\parallel}\hbar\omega(\mathbf{q}_{\parallel},\alpha)[\alpha^{\dagger}_{\alpha}(\mathbf{q}_{\parallel})a_{\alpha}(\mathbf{q}_{\parallel}) + a_{\alpha}(\mathbf{q}_{\parallel})a^{\dagger}_{\alpha}(\mathbf{q}_{\parallel})] \ . \tag{34}$$

Equation (34) is the unretarded Hamiltonian that can be used for the evaluation of the matrix elements and the transition rates of electrons in GaAs/AlAs quantum wells, leading to approximate results compared to those that have already emerged from the fully retarded theory described in our earlier work.[6] We have verified that the results thus obtained are excellent approximations of those given earlier.

Consider now the unitary transformation that is generated by the operator U, given by

$$U = e^{-i\Lambda} \ , \tag{35}$$

where Λ is as defined by Eqs. (27) and (28) and is thus strictly dictated by the expressions correctly emerging from the procedure of taking the unretarded limit of the fully retarded transverse vector potential. When the unitary transformation is applied to the theory corresponding to the Hamiltonian in Eq. (34), it amounts to the transformation of the relevant operators, represented generically by O, via the well-known expansion

$$O' = e^{i\Lambda}Oe^{-i\Lambda} = O + i[\Lambda,O] + \frac{i^2}{2!}[\Lambda,[\Lambda,O]] + \cdots \ . \tag{36}$$

Thus, although H' will formally have the same appearance as H in Eq. (34) but with primed quantities, i.e.,

$$H' = \frac{(\mathbf{p}'+\hbar\nabla\Lambda)^2}{2m^*} + V_c(z) + \tfrac{1}{2}\sum_{\alpha}\int d\mathbf{q}_{\parallel}\hbar\omega(\mathbf{q}_{\parallel},\alpha)[a'^{\dagger}_{\alpha}(\mathbf{q}_{\parallel})a'_{\alpha}(\mathbf{q}_{\parallel}) + a'_{\alpha}(\mathbf{q}_{\parallel})a'^{\dagger}_{\alpha}(\mathbf{q}_{\parallel})] \ , \tag{37}$$

the evaluation of the right-hand side of Eq. (36) leads to expressing H' in terms of the old (unprimed) operators. With the square involving $\mathbf{p}'$ expanded, the Hamiltonian H' can be evaluated by transforming it term by term using Eq. (36). Alternatively, and much more conveniently, we can proceed without expanding the square as follows. Consider first the transformed $\mathbf{p}'$. We have, using $\mathbf{p}=-i\hbar\nabla$,

$$\mathbf{p}' = \mathbf{p} + i[\Lambda,\mathbf{p}] = \mathbf{p} - \hbar\nabla\Lambda \ , \tag{38}$$

where, for $O\equiv\mathbf{p}$, the series in Eq. (36) terminates at the first commutator. Since $\nabla\Lambda$ commutes with Λ, the only other operator transformations required to complete the evaluation of the new Hamiltonian are those of a'_{α} and $a'^{\dagger}_{\alpha}$. We have for a'_{α}

$$a'_{\alpha} = a_{\alpha} + i[\Lambda,a_{\alpha}] \ , \tag{39}$$

and the commutator gives

$$i[\Lambda,a_\alpha]=i\frac{(ie)}{\hbar}\sum_{\alpha'}\int d\mathbf{q}'_\parallel\frac{1}{\omega'}[a^\dagger_{\alpha'},a_\alpha]\tilde{\phi}^*_\alpha=\frac{e}{\hbar\omega}\tilde{\phi}^*_\alpha \ . \tag{40}$$

We therefore have

$$a'_\alpha=a_\alpha+\frac{e}{\hbar\omega}\tilde{\phi}^*_\alpha \ , \tag{41}$$

and similarly

$$a'^\dagger_\alpha=a^\dagger_\alpha-\frac{e}{\hbar\omega}\tilde{\phi}_\alpha \ . \tag{42}$$

Denoting the H'_{field} the field part of the Hamiltonians in Eq. (37), we have on substituting for a'_α and $a'^\dagger_\alpha$ using Eqs. (41) and (42)

$$H'_{\text{field}}=\tfrac{1}{2}\sum_\alpha\int d\mathbf{q}_\parallel\hbar\omega \times\left[\left[a^\dagger_\alpha-\frac{e}{\hbar\omega}\tilde{\phi}_\alpha\right]\left[a_\alpha+\frac{e}{\hbar\omega}\tilde{\phi}^*_\alpha\right]+\left[a_\alpha+\frac{e}{\hbar\omega}\tilde{\phi}^*_\alpha\right]\left[a^\dagger_\alpha-\frac{e}{\hbar\omega}\tilde{\phi}_\alpha\right]\right] . \tag{43}$$

On multiplying out the brackets, we find that the result can be written in the form

$$H'_{\text{field}}=H_{\text{field}}-e\Phi+\Delta_{\text{self}} \ , \tag{44}$$

where H_{field} is exactly the field part of the old Hamiltonian. The second term $e\Phi$ emerges from the expansion such that

$$\Phi=\sum_\alpha\int d\mathbf{q}_\parallel(a_\alpha\tilde{\phi}_\alpha-a^\dagger_\alpha\tilde{\phi}^*_\alpha) \ . \tag{45}$$

We are thus naturally led to define a new operator Φ, which turns out to be exactly the scalar potential for the interface modes. With $\tilde{\phi}_\alpha$ given by Eqs. (31) and (32), the above scalar potential, given by Eq. (45), is in fact the scalar potential given by Mori and Ando.[5] The last term, denoted by Δ_{self}, is formally identified as a self-energy term contributing to the mass of the electron due to its coupling to the interface modes. It is given by

$$\Delta_{\text{self}}=-e^2\sum_\alpha\int d\mathbf{q}_\parallel\frac{\tilde{\phi}^*_\alpha\tilde{\phi}_\alpha}{\hbar\omega} \ . \tag{46}$$

Substituting for $\mathbf{p}'$ and H'_{field} using the above results and after cancellation of the terms involving $\nabla\Lambda$ within the square of the first term, the transformed Hamiltonian Eq. (37) can be written as follows:

$$\begin{aligned}H'&=e^{i\Lambda}He^{-i\Lambda}\\&=\frac{\mathbf{p}^2}{2m^*}+V_c-e\Phi\\&\quad+\tfrac{1}{2}\sum_\alpha\int d\mathbf{q}_\parallel\hbar\omega(a^\dagger_\alpha a_\alpha+a_\alpha a^\dagger_\alpha)+\Delta_{\text{self}} \ .\end{aligned} \tag{47}$$

The Hamiltonian H' given by Eq. (47) is the unitary equivalent of the "old" unretarded Hamiltonian H given in Eq. (34).

IV. COMPARISON OF $\mathbf{A}^\perp\cdot\mathbf{p}$ AND Φ COUPLINGS

In Sec. II we derived the quantized vector potential $\mathbf{A}^\perp$. From $\mathbf{A}^\perp$ we were able, in Sec. III, to deduce a specific scalar potential Φ associated with it in the unretarded limit, and we saw that this Φ is precisely that given by Mori and Ando.[5]

In this section we consider the relaxation processes mediated by the interface modes that can arise for electrons confined in a double-heterostructure quantum well. We distinguish intersubband and intrasubband processes and aim to compare and contrast the predictive powers of the two theories using both the minimal-coupling version and its unitary equivalent.

The two alternative interaction Hamiltonians appropriate for the emission processes referred to above are

$$H_{\text{int}}(\mathbf{A}^\perp)=-\frac{e}{m^*}\mathbf{A}^\perp\cdot\mathbf{p} \tag{48}$$

and

$$H_{\text{int}}(\Phi)=-e\Phi \ . \tag{49}$$

The first-order processes we are interested in occur between an initial state, denoted by $|i\rangle$, and a final state, denoted by $|f\rangle$. These are defined as follows:

$$|i\rangle=|\Psi_i,(0)\rangle, \quad |f\rangle=|\Psi_f,(\mathbf{q}_\parallel,\alpha)\rangle \ , \tag{50}$$

where $|\Psi_i\rangle$ and $|\Psi_f\rangle$ are electronic stationary states corresponding to the Hamiltonian H^0_e given by Eq. (4). $|(\mathbf{q}_\parallel,\alpha)\rangle$ is the single interface polariton state of wave vector $\mathbf{q}_\parallel$ and branch α, while $|(0)\rangle$ is the vacuum state.

A. Intrasubband transitions

The electron states and their energies associated with the *intrasubband* scattering within the first subband are given by

$$|\Psi_i\rangle=\frac{1}{2\pi}\left[\frac{2}{d}\right]^{1/2}e^{i\mathbf{k}^i_\parallel\cdot\mathbf{r}_\parallel}\cos\left[\frac{\pi z}{d}\right] , \tag{51}$$

$$E_i=\mathcal{E}_1+\frac{\hbar^2(k^i_\parallel)^2}{2m^*} \tag{52}$$

and

$$|\Psi_f\rangle=\frac{1}{2\pi}\left[\frac{2}{d}\right]^{1/2}e^{i\mathbf{k}^f_\parallel\cdot\mathbf{r}_\parallel}\cos\left[\frac{\pi z}{d}\right] , \tag{53}$$

$$E_f=\mathcal{E}_1+\frac{\hbar^2(k^f_\parallel)^2}{2m^*} \ , \tag{54}$$

where, for simplicity, we have assumed an infinite confining quantum-well potential V_c. $\mathcal{E}_n$ are the lowest-energy eigenvalues corresponding to the Hamiltonian in Eq. (4) and are given by

$$\mathcal{E}_n=\frac{\hbar^2\pi^2n^2}{2m^*d^2}, \quad n=1,2,3,\ldots , \tag{55}$$

with d the quantum-well width.

From symmetry considerations, only the symmetric interface modes contribute to intrasubband processes. The first matrix element can now be written down using the original minimally coupled version in unretarded form. We have

$$\mathcal{M}(\mathbf{A}^{\perp})=\left\langle f\left|\frac{e}{m^*}\mathbf{A}^{\perp}\cdot\mathbf{p}\right|i\right\rangle , \tag{56}$$

which is

$$\mathcal{M}(\mathbf{A}^{\perp})=-\frac{2(2\pi)^2 e\hbar}{m^* d^3}f(q_{\parallel})[k_{\parallel}^{i}\cos(\theta)-\tfrac{1}{2}q_{\parallel}]\times\delta(\mathbf{k}_{\parallel}^{i}-\mathbf{k}_{\parallel}^{f}-\mathbf{q}_{\parallel}) , \tag{57}$$

with θ the angle between the vectors $\mathbf{k}_{\parallel}^{i}$ and $\mathbf{q}_{\parallel}$. The second matrix element emerges when the transformed Hamiltonian is employed. It is

$$\mathcal{M}(\Phi)=-\langle f|e\Phi|i\rangle , \tag{58}$$

which yields

$$\mathcal{M}(\Phi)=-\frac{2(2\pi)^2 e\omega(q_{\parallel})}{q_{\parallel}d^3}f(q_{\parallel})\delta(\mathbf{k}_{\parallel}^{i}-\mathbf{k}_{\parallel}^{f}-\mathbf{q}_{\parallel}) . \tag{59}$$

In Eqs. (57) and (59) the function $f(q_{\parallel})$ is given by

$$f(q_{\parallel})=C(q_{\parallel})e^{-q_{\parallel}d/2}\left[\frac{\tanh(q_{\parallel}d/2)}{q_{\parallel}^2+(2\pi/d)^2}\right] , \tag{60}$$

where $C(q_{\parallel})$ is given by

$$C(q_{\parallel})=\left[\frac{\hbar\epsilon_2}{2(2\pi)^2\epsilon_0 q_{\parallel}\omega^2(q_{\parallel})e^{-q_{\parallel}d}D}\right]^{1/2} . \tag{61}$$

It is seen from the above that $\mathcal{M}(\mathbf{A}^{\perp})$ and $\mathcal{M}(\Phi)$ are different. In particular, the former has an angular dependence (θ), while the latter does not.

If, however, one is interested in calculating the emission rate using Fermi's "golden rule" then one would evaluate the following:

$$\Gamma(\mathbf{A}^{\perp})=\frac{2\pi}{\hbar}\int d\mathbf{q}_{\parallel}\int d\mathbf{k}_{\parallel}^{f}|\mathcal{M}(\mathbf{A}^{\perp})|^2\delta(E_i-E_f-\hbar\omega(q_{\parallel})) , \tag{62}$$

and similarly

$$\Gamma(\Phi)=\frac{2\pi}{\hbar}\int d\mathbf{q}_{\parallel}\int d\mathbf{k}_{\parallel}^{f}|\mathcal{M}(\Phi)|^2\delta(E_i-E_f-\hbar\omega(q_{\parallel})) . \tag{63}$$

It is straightforward then to show that we have

$$\Gamma(\mathbf{A}^{\perp})=\Gamma(\Phi)=\frac{16(2\pi)^5 e^2 m^*}{\hbar^3 d^6}\times\int_{q_-}^{q_+}dq_{\parallel}\frac{\omega^2(q_{\parallel})f^2(q_{\parallel})}{q_{\parallel}[4k_{\parallel}^{i\,2}q_{\parallel}^2-(q_{\parallel}^2+q_0^2)^2]^{1/2}} , \tag{64}$$

where

$$q_{\pm}=k_{\parallel}^{i}\pm(k_{\parallel}^{i\,2}-q_0^2)^{1/2} , \tag{65}$$

where q_0 is defined by

$$q_0^2=\frac{2m^*\omega(q_{\parallel})}{\hbar} . \tag{66}$$

It is easy to see that conservation of energy in effect wipes out the differences in the matrix elements and therefore leads to identical intrasubband rates.

B. Intersubband transitions

In the case of intersubband scattering we assume that the electronic initial state is that at the bottom of the second subband and relaxation is by transitions to the lowest subband. The initial electronic state is therefore given by

$$|\Psi_i\rangle=\frac{1}{2\pi}\left[\frac{2}{d}\right]^{1/2}\sin\left[\frac{2\pi z}{d}\right] . \tag{67}$$

The corresponding energy eigenvalue is that conforming with $\mathbf{k}_{\parallel}^{i}=0$:

$$E_i=\mathcal{E}_2 , \tag{68}$$

and the appropriate final state is

$$|\Psi_f\rangle=\frac{1}{2\pi}\left[\frac{2}{d}\right]^{1/2}e^{i\mathbf{k}_{\parallel}^{f}\cdot\mathbf{r}_{\parallel}}\cos\left[\frac{\pi z}{d}\right] , \tag{69}$$

with the corresponding energy eigenvalue

$$E_f=\mathcal{E}_1+\frac{\hbar^2(k_{\parallel}^{f})^2}{2m^*} . \tag{70}$$

From symmetry, only the antisymmetric modes contribute and it is straightforward to show that the corresponding matrix elements are as follows:

$$\mathcal{M}(\mathbf{A}^{\perp})=\left\langle f\left|\frac{e}{m^*}\mathbf{A}^{\perp}\cdot\mathbf{p}\right|i\right\rangle , \tag{71}$$

giving

$$\mathcal{M}(\mathbf{A}^{\perp})=-\tfrac{8}{3}e\omega_0 dC(q_{\parallel})e^{-q_{\parallel}d/2}\coth(q_{\parallel}d/2)\times\left[\frac{1}{(q_{\parallel}d)^2+\pi^2}-\frac{3}{(q_{\parallel}d)^2+9\pi^2}\right]\delta(\mathbf{q}_{\parallel}+\mathbf{k}_{\parallel}^{f}) , \tag{72}$$

where ω_0 is given by

$$\omega_0=\frac{\mathcal{E}_2-\mathcal{E}_1}{\hbar}=\frac{3\pi^2\hbar}{2m^*d^2} , \tag{73}$$

and finally we have

$$\mathcal{M}(\Phi)=-2e\omega(q_{\parallel})dC(q_{\parallel})e^{-q_{\parallel}d/2}\coth(q_{\parallel}d/2)\times\left[\frac{1}{(q_{\parallel}d)^2+\pi^2}-\frac{1}{(q_{\parallel}d)^2+9\pi^2}\right]\delta(\mathbf{q}_{\parallel}+\mathbf{k}_{\parallel}^{f}) . \tag{74}$$

Again it is evident that the two matrix elements are quite different for the same transition. It is, however, straightforward to proceed to the calculation of the corresponding transition rates, and we obtain the simple result

$$\frac{\Gamma(\mathbf{A}^{\perp})}{\Gamma(\Phi)}=\left[\frac{\omega_0}{\omega(q_{\parallel})}\right]^2\left[1-\frac{(q_{\parallel}d)^2}{3\pi^2}\right]^2 . \qquad (75)$$

It can now be verified that the right-hand side reduces to unity once we make use of the relation of conservation of energy embodied in the δ function

$$\delta(E_i-E_f-\hbar\omega(\mathbf{q}_{\parallel}))=\delta\left[\hbar\omega_0-\hbar\omega(q_{\parallel})-\frac{\hbar^2q_{\parallel}^2}{2m^*}\right] . \qquad (76)$$

The above conclusions are consistent with the situation in which two canonically connected theories are used to describe the first-order interactions involved in the transitions between stationary states of the total zero-order Hamiltonian.[12] For real transitions, involving matrix elements *on the energy shell,* the two theories yield exactly the same results. This is one of the main conclusions of this paper and confirms the validity of the methods used by Al-Dossary, Babiker, and Constantinou[6] in their calculations of the electron-interface optical-phonon interactions. For virtual transitions, however, energy need not be conserved and the interaction Hamiltonians yield different matrix elements. The appearance of the self-energy term Δ_{self} in the transformed Hamiltonian, Eq. (47), is indicative of the fact that the transformation has resulted in the explicit appearance of contributions that would otherwise have arisen from virtual self-energy transitions. Similar aspects would arise if the two theories were to be employed in calculations of scattering profiles and spectroscopic line shapes. Then the scattering cross section determining the profile $P(\omega)$ would be proportional to the square of the transition matrix element, which is *not on the energy shell.*[12] As a result, when the relevant predictions of the two theories are compared, one would expect a relative shift of the center of the line profile and, in principle, perceivable differences in the line shape.

Higher-order processes, too, are expected to involve different calculational details arising from the use of the old or new Hamiltonians. We defer further comments on the relative calculational merits of the two theories to the last section.

V. COMMENTS AND CONCLUSIONS

In this paper we have discussed the theory of interaction between interface polaritons and electrons in semiconductor low-dimensional structures. The main issues have concerned the calculational frameworks that may be used for the evaluation of dynamical attributes of the interaction involving the emission and absorption of the interface modes by the electrons. We have shown that a theory developed from first principles would involve quantizing the fields in the transverse gauge (radiation gauge) for which $\phi=0$ and the vector potential is pure transverse. This leads to the minimal coupling of electrons to the interface modes in their fully retarded form, described only via a transverse vector potential. Calculations using the minimal-coupling form are therefore likely to give the desired results whether retardation is retained or ignored at an intermediate or later stage of the calculations. The unretarded limit of the theory has been shown, by application of a unitary transformation, to lead to a version of the theory in which the coupling is in terms of a scalar potential. Thus the connection between the complete theory and its nonretarded scalar potential version is established, clarifying a recent controversy about the appropriate coupling between the modes and electrons.[16–18]

The transformation is not a gauge transformation, as it may appear at first sight. Gauge transformations change the longitudinal part of a vector potential, leaving the electric and magnetic fields unchanged.[19] In the present case we have chosen to work in the radiation gauge for which $\phi=0$ and $\nabla\cdot\mathbf{A}^{\perp}=0$, so there is neither a longitudinal field $\mathbf{A}^L$ nor a scalar field ϕ to begin with, i.e., before the unretarded limit is taken. However, when the unretarded limit is taken, we find that the longitudinal part introduced is the limit of a unique transverse vector potential, not an addition to it. This is apparently a peculiarity of interface polaritons which, in the unretarded approximation, acquire a longitudinal character, in addition to their normal transverse character, i.e., the modes appear to be both divergence free and curl free simultaneously. If retardation is retained throughout, this apparent anomaly would be absent and there is no question of applying any transformation. When the unretarded limit is found, the vector potential merely takes the shape of the gradient of a scalar function: taking the unretarded limit is not tantamount to applying a gauge transformation. When the unitary transformation is applied, the theory is equivalent in full to the unretarded polariton theory. However, we have demonstrated here that the predictive ability of the transformed version depends on the way it is utilized in conjunction with perturbation theory.

We have seen that, for all first-order interactions involving real transitions, the two theories lead to exactly the same results. In contrast, the manifest differences in the transition matrix elements are indicative of differences in predictions whenever virtual transitions come into play, as one would expect in principle to be the case, for example, in calculations of electron-energy-loss spectroscopy involving such interface modes. Furthermore, the appearance of the self-energy term in the transformed Hamiltonian is a clear indication of the role of such virtual transitions in exhibiting differences in calculational details using the two Hamiltonians. In the context of III-V semiconductor heterostructures such as GaAs/AlAs systems, clearly we have established that use of the two coupling Hamiltonians $e\,\mathbf{A}^{\perp}\cdot\mathbf{p}/m^*$ and $e\Phi$ would lead to the same results for intersubband as well as intrasubband emission rates, since these involve first-order matrix elements that are on the energy shell.

We now discuss the implications of this work for the different models employed to describe the electron-phonon interaction in layered structures. We emphasize that the use of a scalar potential in the unretarded limit to evaluate the interface optical-phonon scattering rates in III-V quantum-well systems is justified. Any previous criticism of the scalar potential approach[1] and the suggestion that the interface modes couple to electrons weakly[20] turn out to be not applicable in the unretarded limit. A brief mention of the appropriateness of a scalar interaction for interface modes emerging from the minimal-coupling form of the interaction was in fact made in Ref. 21, but the point was not pursued any further there. Finally, we address briefly the question of which model is appropriate for the description of the confined modes in the GaAs/AlAs system. Recent complex lattice-dynamical calculations[7] and more-involved continuum models[22,23] have shown that the simple dielectric continuum (DC) model (e.g., Ref. 7) and the related continuum model of Huang and Zhu (HZ) (Ref. 24) give good agreement with the scattering rates found via lattice-dynamical calculations,[7] in contrast to the hydrodynamical model,[1,21] which gives lower rates.[25] Despite their success in yielding rates that are in agreement with microscopic calculations for GaAs/AlAs systems, the DC and HZ models are found to be inadequate (as is the hydrodynamic model) in explaining the angular anisotropy of the zone-center optical modes[26,27] in these systems. In this case, microscopic models[7,28,29] or macroscopic models which include bulk dispersion[22,23,30] are required.

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