Average forces in bound and resonant quantum states

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Average forces in bound and resonant states of simple quantum systems realizable in semiconductor heterostructures are considered theoretically. First, an average electric force in a bound state of electron characterized by a constant effective mass is calculated and shown to be zero. Next, a total force is calculated for a system in which electron effective mass varies in space and it is demonstrated that this force has a component related to the mass variation. Average electric force is then determined from the condition that in a bound state the average total force must vanish. Finally, average electric field is calculated for a system consisting of a quantum well placed in a constant field. A comparison with the density of states shows that the average field is strongly quenched at the energies corresponding to resonant states.

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I. INTRODUCTION

Due to recent advancement in modern semiconductor technology it has become possible to produce handmade quantum systems. The observable quantization in such systems is caused by small values of electron effective masses in most semiconductors. Because the gaps of forbidden energies in different materials may vary considerably, it is possible to create energy barriers at semiconductor interfaces. In systems using alloys one can vary the barrier heights continuously by varying the chemical composition. Since the effective masses of electrons and light holes are to a good approximation proportional to the energy gap in the material, one often deals with carriers' masses having different values in various parts of the system. During the last few years it has become possible to apply external electric fields to semiconductor heterostructures using the so called gated arrangements.

Physical effects produced by the above possibilities are of importance for basic research and industrial applications. Hand-made quantum systems can serve to achieve a better understanding of quantum phenomena since they are more flexible and can be manipulated much more easily than the natural systems like atoms or molecules. In this paper we are concerned with average forces arising from potential and mass discontinuities as well as applied electric fields. Our considerations are limited to one dimension. We encountered the problems of average forces when dealing with a subject of spin splitting due to inversion asymmetry in semiconductor heterostructures, Ref. 1, but clearly the properties of average forces have more general implications. We point out the consequences of general results for semiconductor problems.

Our paper is organized in the following way. In Sec. II we consider an average electric force in bound states of quantum systems characterized by a constant electron mass. Section III treats a similar problem in systems in which the effective mass varies in space. In Sec. IV we go beyond the bound states and treat average electric forces in resonant states created by an application of external electric field.

II. AVERAGE FORCE IN A SYSTEM WITH CONSTANT ELECTRON MASS

We calculate an average value of the time derivative of momentum $\dot{p}_z$ in a bound eigenstate Ψ_n of the Hamiltonian $\hat{H}$. Such a state satisfies the Schrödinger equation

$$\hat{H}\Psi_n = \epsilon_n \Psi_n , \tag{1}$$

where ϵ_n is the eigenenergy. The average value of $\dot{p}_z$ is

$$(\Psi_n, \dot{p}_z \Psi_n) = \frac{1}{i\hbar}[(\Psi_n, \hat{H} p_z \Psi_n) - (\Psi_n, p_z \hat{H} \Psi_n)]$$

$$= \frac{1}{i\hbar}[\epsilon_n(\Psi_n, p_z \Psi_n) - \epsilon_n(\Psi_n, p_z \Psi_n)] = 0 \tag{2}$$

if Ψ_n is square integrable, i.e., if it describes a bound state. To arrive at the result (2) we used the Hermiticity of the Hamiltonian $\hat{H}$.

Now we consider the standard case of a constant electron mass: $m^* = \text{const}$. The Hamiltonian for this case reads

$$\hat{H} = \frac{1}{2m^*} p_z^2 + U(z), \tag{3}$$

where the potential energy $U(z) = qV(z)$, in which $V(z)$ is the electric potential and $q = -e$ for the electron charge. Using the Ehrenfest relation we have

$$\dot{p}_z = \frac{1}{i\hbar}[p_z, \hat{H}] = \frac{1}{i\hbar}[p_z, U] = -\frac{\partial U}{\partial z} = F_{el} . \tag{4}$$

Equation (4) is the well known quantum equivalent of the Newton's second law stating that the time increment of momentum is equal to the force. In case of the Hamiltonian (3) the force is purely electric.

It follows from Eqs. (2) and (4) that the average electric force (or electric field) in a bound state of the Hamiltonian (3) is zero. In symmetric quantum wells the above theorem is manifestly fulfilled, in asymmetric wells it is satisfied less obviously. In this connection we want to discuss a ''tricky''

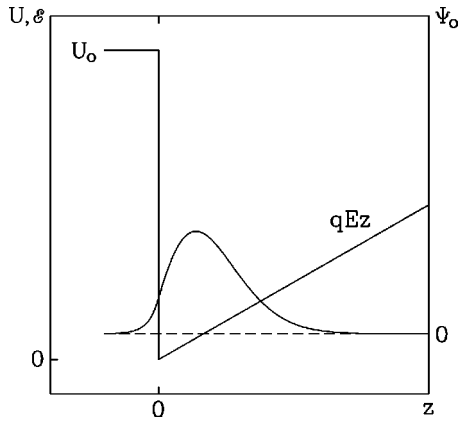

FIG. 1. Triangular quantum well and the wave function of the ground state calculated for the electron mass $m^*=0.066m_0$ and electric field $E=20$ kV/cm.

case for which the theorem is seemingly not satisfied. Let us consider a triangular well with an infinite barrier. This is represented in Fig. 1 if one takes $U_0=\infty$ and $U(z)=qEz$ with constant E. For the infinite barrier the wavefunction vanishes at $z=0$: $\Psi_0(0)=0$. Then the average field appears to be

$$\langle E\rangle=\int_0^\infty \Psi_0^* E\Psi_0 dz=E$$

since Ψ_0 is normalized. Thus the average field appears to be nonzero. The flaw in the above reasoning is that, by taking at the outset $\Psi_0(0)=0$, we have neglected the electric field resulting from the potential drop at the barrier.

A correct treatment of the problem is illustrated in Fig. 1. One should first take a finite barrier U_0. Then the wave function penetrates the barrier into the $z\leqslant 0$ region and the electric force due to the potential drop is $+U_0\delta(z)$, where $\delta(z)$ is the Dirac delta function. This contributes the amount $+U_0|\Psi_0(0)|^2$ to the average electric force, which exactly compensates the positive contribution from the region $z>0$. One can now take higher values of U_0, which increases the electric force due to the potential drop but diminishes the value of $\Psi_0(0)$. The limit of this contribution for $U_0\to\infty$ is nonzero and it compensates exactly the contribution to the average force from the region $z>0$. This compensation is illustrated in Fig. 2. Here F_U is the contribution from the potential drop at $z=0$, and F_E is that from the region $z>0$. At all values of U_0 the two contributions cancel each other, so that the average electric force (or electric field) vanishes. At higher U_0 both contributions saturate.

The electric field component related to the potential drop at the high barrier in MOS structures was overlooked in Refs. 2,3. The fact that in a bound state the average electric field must vanish was remarked by Därr, Kotthaus, and Ando.[4]

III. AVERAGE FORCE IN A SYSTEM WITH VARIABLE ELECTRON MASS

The modern semiconductor technology allows one to create systems in which the effective carrier mass varies with

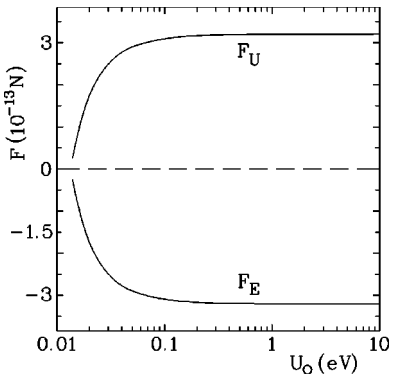

FIG. 2. Two components of average electric force (in newtons) calculated for the well shown in Fig. 1 ($m^*=0.066m_0$, $E=20$ kV/cm). At all values of U_0 the barrier component F_U compensates the constant field component F_E, so the total average force vanishes.

position continuously or abruptly. In classical physics one encounters a similar case considering, for example, a rocket burning fuel during its motion, so that its total mass changes. The initial Hamiltonian for this case is

$$\hat{H}=-\frac{\hbar^2}{2}\frac{\partial}{\partial z}\frac{1}{m^*(z)}\frac{\partial}{\partial z}+U(z). \tag{5}$$

It is easy to verify that in the above form the Hamiltonian is Hermitian.

We want to calculate an average electric force (or field) in bound eigenstates of the Hamiltonian (5). The reasoning presented in Eq. (2) still holds, which means that the average value of $\dot{p}_z$ vanishes. On the other hand the calculation presented in Eq. (4) should now be replaced by

$$\begin{aligned}\dot{p}_z=&\frac{1}{i\hbar}\frac{\hbar}{i}\left[\frac{\partial}{\partial z}\left(-\frac{\hbar^2}{2}\frac{\partial}{\partial z}\frac{1}{m^*}\frac{\partial}{\partial z}+U\right)\right.\\&\left.-\left(-\frac{\hbar^2}{2}\frac{\partial}{\partial z}\frac{1}{m^*}\frac{\partial}{\partial z}+U\right)\frac{\partial}{\partial z}\right]\\=&-\frac{\partial U}{\partial z}+\frac{\hbar^2}{2}\frac{\partial}{\partial z}\left[\left(\frac{\partial}{\partial z}\frac{1}{m^*}\right)\frac{\partial}{\partial z}\right].\end{aligned} \tag{6}$$

Thus the total force has now an electric component related to the potential gradient and a ''mass'' component related to the mass gradient. Since the average total force in a bound state must still be zero, the average electric force is

$$\begin{aligned}\langle F_{el}\rangle=&\int \Psi_n^*\left(-\frac{\partial U}{\partial z}\right)\Psi_n dz=-\langle F_M\rangle\\=&\frac{\hbar^2}{2}\int\left|\frac{\partial\Psi_n}{\partial z}\right|^2\left(\frac{\partial}{\partial z}\frac{1}{m^*}\right)dz.\end{aligned} \tag{7}$$

For a real wave function Ψ_n this agrees with the result of Lommer *et al.*[5] It follows then that, if in a system the mass depends on the position, the average electric force (or field) in a bound state is nonzero.

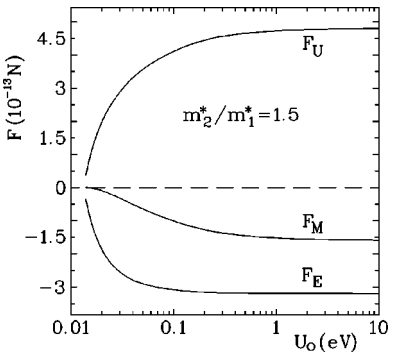

FIG. 3. Two components of the average electric force and the average ''mass'' force (related to the mass change at $z=0$), calculated for the quantum well shown in Fig. 1 as functions of barrier height U_0 for the electron mass $m_1^*=0.066m_0$ and $E=20$ kV/cm. At all values of U_0 the average electric force $\langle F_{el}\rangle=F_E+F_U$ compensates the average ''mass'' force $\langle F_M\rangle$, so the total average force vanishes.

Next we consider a practical situation in which the mass has a constant value in one region of space and another constant value in the neighboring region. This case is often realized in semiconductor heterostructures composed of two different materials. Since the effective mass in each material is proportional to its energy gap, the abrupt changes of the mass and of the potential occur at the same point, that is at the interface. We take $m^*=m_2^*$ for $z<0$, and $m^*=m_1^*$ for $z>0$ (see Fig. 1). It is well known that in this case the boundary conditions for the wave functions at the interface are

$$\Psi_n|_{0^-}=\Psi_n|_{0^+} \quad \text{and} \quad \frac{1}{m_2^*}\frac{\partial\Psi_n}{\partial z}\bigg|_{0^-}=\frac{1}{m_1^*}\frac{\partial\Psi_n}{\partial z}\bigg|_{0^+}. \quad (8)$$

These conditions result from the continuity of the probability current across the interface. For the mass variation assumed above, one has $\partial m^*/\partial z=(m_1^*-m_2^*)\delta(z)$, and Eq. (7) gives

$$\langle F_M\rangle=\frac{\hbar^2}{2}(m_1^*-m_2^*)\left|\frac{1}{m^*}\frac{\partial\Psi_n}{\partial z}\right|^2_{z=0} \quad (9)$$

in which the value at $z=0$ can be taken either using m_2^* and the limit 0^-, or m_1^* and the limit 0^+, since according to Eq. (8) they coincide.

Figure 3 illustrates three contributions to the average total force calculated numerically for $m_2^*/m_1^*=1.5$ as functions of the barrier height U_0. The average electric force (or field) is given by the sum of contributions F_U of the potential drop U_0 and the constant field F_E from the region $z>0$. This sum is now nonzero since it compensates the contribution from the mass gradient at the interface, as given by Eq. (9). The result shown in Fig. 3 may appear paradoxical since it indicates that at high values of the barrier U_0 the force related to the mass gradient does not vanish but saturates, although the wavefunction penetrates less and less the region of $z<0$ and the mass difference $m_2^*-m_1^*$ is constant. We cannot offer an intuitive argument justifying this result, but observe that the

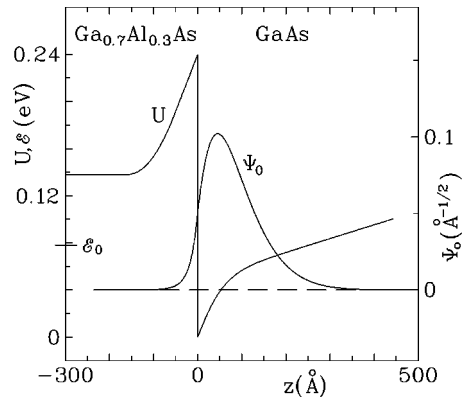

FIG. 4. Real quantum well and the ground state wave function in a modulation doped heterojunction $Ga_{0.7}Al_{0.3}As/GaAs$. The average electric force $\langle F_{el}\rangle=F_L+F_R+F_U$ compensates the average ''mass'' force $\langle F_M\rangle$, so the total average force vanishes (see text).

''mass'' force, as given by Eq. (9), is related to the slope $\partial\Psi_n/\partial z$ at $z=0$ and this slope reaches a constant value as the barrier increases. Within the effective mass approximation the jumps of the potential and the mass occur simultaneously, so that the assumed model, although idealized, is quite realistic.

According to Eq. (9), for $m_1^*<m_2^*$ the average ''mass'' force is negative, for $m_1^*>m_2^*$ it is positive. This means that the average electric force (or field) must also have opposite signs in the two cases in order to keep the average total force equal to zero. This is indeed the case since the relative magnitude of the two masses influences the F_U component of the electric force via the boundary conditions (8). In a three-dimensional system with two different effective masses a free electron motion parallel to the interface results in the so called kinetic barrier, which leads to new effects (see Kubisa and Zawadzki[6]).

Finally, Fig. 4 shows a real potential well in $Ga_{0.7}Al_{0.3}As/GaAs$ heterojunction doped with Si donors in the GaAlAs barrier. The wave function and the potential are computed self-consistently using the Schrödinger and the Poisson equations according to the procedure described by Bastard.[7] The subband energy ϵ_0 is found by requiring that the wave function goes to zero at high positive z values. The electron effective mass in the $Ga_{0.7}Al_{0.3}As$ barrier is $m_2^*=0.088m_0$, while the mass in the GaAs well is $m_1^*=0.066m_0$. The barrier value is 0.24 eV. The average electric force consists of three parts: $F_L=-3.22\times10^{-14}N$ (from the region $z<0$), $F_R=-7.48\times10^{-13}N$ (the region $z>0$), and $F_U=9.53\times10^{-13}N$ (the offset drop). The average ''mass'' force is calculated according to Eq. (9): $\langle F_M\rangle=-1.728\times10^{-13}N$. The electric contributions add up to $\langle F_{el}\rangle=1.728\times10^{-13}N$, so that the average total force vanishes, as it should.

IV. AVERAGE ELECTRIC FIELD IN RESONANT STATES

Now we go beyond the bound states and consider an average electric field (or force) for quantum wells placed in an external electric field. This situation can be realized now in

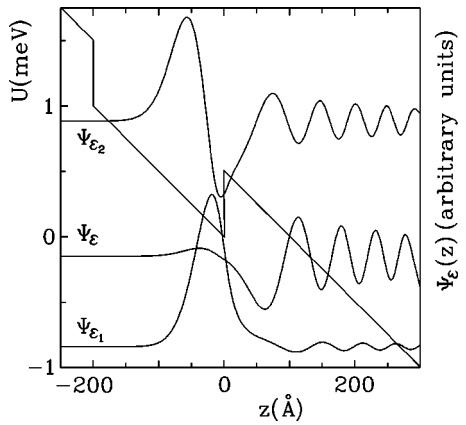

FIG. 5. Rectangular quantum well with a superimposed linear potential and the electron wave functions calculated with the use of a constant electron mass $m^*=0.066m_0$ and $E=-500$ kV/cm for three electron energies: lower resonance ϵ_1, upper resonance ϵ_2, nonresonant energy $\epsilon_1<\epsilon<\epsilon_2$.

so called gated semiconductor heterostructures to which one applies a variable external field by means of the gate (see Nitta *et al.*[8]). To describe the main features of the problem we take the case of a constant effective mass. If after an application of external field the state in the well remains to be bound, the theorem exposed in Sec. II is valid and the average electric field remains zero. However, for a constant electric field the potential energy is $U=qEz$ and, if the well is finite, the resulting situation is shown in Fig. 5. In this case the states in the well are not bound because the electron can tunnel to the region on the right-hand side. Then the above theorem is not valid anymore and the question of average field remains open.

We will characterize the quantum states in the system shown in Fig. 5 by the density of states (DOS) and calculate the wave functions and the average electric field numerically. Since there are no bound states in the system, the spectrum is continuous and the calculation of DOS is not trivial, Refs. 9–11. Since we require the knowledge of the wave functions in order to compute the average field, we will calculate the total DOS in the energy space by means of a local DOS.

A local density of states is defined to treat situations, where the contribution to each state is weighted by the density of its wavefunction at the point in question. The local DOS is (see Davies[12]),

$$\eta(\epsilon,z)=\sum_n |\Psi_n(z)|^2\delta(\epsilon-\epsilon_n), \tag{10}$$

where the sumation is over all quantum numbers. If we consider one dimension and spin degenerate electron states, we can take the continuous energy to be $\epsilon_n=\epsilon'$, the sum in Eq. (10) is replaced by an integral and we obtain $\eta(\epsilon,z)=2|\Psi_\epsilon(z)|^2$, where the factor 2 is due to spin. It can be shown that the total DOS is given by (see Ref. 12),

$$\rho(\epsilon)=\int_{-\infty}^{+\infty}\eta(\epsilon,z)dz=2\int_{-\infty}^{+\infty}|\Psi_\epsilon(z)|^2dz. \tag{11}$$

The wave functions $\Psi_\epsilon(z)$ of the continuous energy spectrum are ortonormalized to the Dirac delta function of energy.

We proceed in the following way. Choosing an energy ϵ within the well we compute numerically a corresponding wavefunction for the potential shown in Fig. 5. For this purpose we employ the method of Runge-Kutta and the boundary conditions requiring the vanishing wave function and its derivative sufficiently far away on the left, but not require its vanishing on the right-hand side (RHS). The calculation of the wave functions is carried out up to 10^6 Å to the right of the well. The computed wave functions are then used to determine the local DOS of Eq. (10) and the total DOS according to the Eq. (11). The same wave function is used to compute the average electric field for the potential shown in Fig. 5 including the vertical potential drops.

The results obtained for $\rho(\epsilon)$ and $\langle E(\epsilon)\rangle$ for the potential shown in Fig. 5 and the electron mass $m^*=0.066m_0$ are shown in Figs. 6(a) and 6(b). It can be seen from Fig. 6(a) that there are two resonant states in the well. It is more

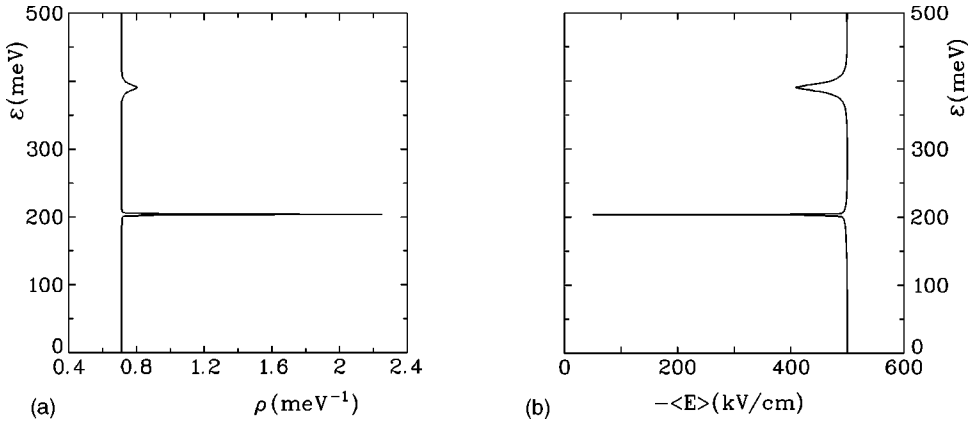

FIG. 6. (a) Total density of electron states for the potential shown in Fig. 5 calculated as a function of electron energy. The peaks correspond to the resonant states. (b) Average electric field as a function of electron energy calculated for the potential shown in Fig. 5 with the use of a constant mass $m^*=0.066m_0$. At nonresonant energies the average field is equal to the external field, at resonant energies the average field is markedly quenched.

difficult to tunnel to the right from the lower state ϵ_1, so the latter is almoust bound, which corresponds to the narrow and high peak in DOS. The wave function for the resonant energy ϵ_1 is shown in Fig. 5. This function is concentrated mostly in the well, but it also has a weak oscillatory component on the RHS which indicates the tunneling probability. If this state were truly bound, there would be no oscillatory component and DOS would have the shape of the Dirac delta function. Figure 6(b) shows that for the resonant energy ϵ_1 the average electric field $\langle E(\epsilon_1)\rangle$ drops as sharply as the DOS increases. For a bound state the average field would be exactly zero in agreement with the above theorem. At nonresonant energies DOS is almost constant, the corresponding wave functions are not concentrated in the well (see Fig. 5) and the average electric field is equal almost exactly to the applied external field. In other words, at nonresonant energies the effect of the well on DOS and on the average field is almost negligible. Around the higher resonant energy ϵ_2 DOS has a smaller and wider peak, the wave function has a sizable oscillatory component and the drop of the average field is less pronounced. As follows from the comparison of Figs. 6(a) and 6(b), $\rho(\epsilon)$ and $\langle E(\epsilon)\rangle$ look almost similar to mirror images of each other. Thus the resonant (or semibound) character of the state markedly quenches the corresponding average electric field.

In our model of the resonant states we assumed a very high value of the constant electric field. In realistic cases of the gated semiconductor heterostructures the applied fields of the order of 10^4 V/cm would result in quasibound resonant states for which the average electric field would be practically zero. Thus, when interpretating experiments on gated semiconductor heterostructures (see, e.g., Ref. 8) one should keep in mind that the application of an external electric field can change asymmetry of the electron wave function and the electron density in the quantum well, but the average electric field in the well remains zero.

V. SUMMARY

We consider theoretically an average electric force acting on the electron in a bound state and show it to vanish, if the electron effective mass is constant. Next we calculate an average force in a system with the effective mass varying with electron position and show that the force has electric and ''mass'' components, the first related to the potential gradient and the second related to the mass gradient. The average total force in a bound state must still vanish. A real case of a quantum well in $Ga_{0.7}Al_{0.3}As/GaAs$ heterostructure is given as an example. Finally, an average electric field is calculated for resonant and nonresonant electron states in a system of a finite rectangular well with a superimposed linear potential (created by a constant electric field). For the same system the total density of states is computed with the use of a local density of states. A comparison of the average field with the total DOS shows that in nonresonant (delocalized) states the average electric field is equal to the applied constant field, while for the resonant states the average field is strongly quenched. This result has important implications for the interpretation of experiments on gated semiconductor heterostructures.

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