Hydrogenic impurities in a quantum well wire in intense, high-frequency laser fields

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Calculation of the binding energy of an axial donor hydrogenic impurity in an ideal, infinite, cylindrical quantum wire placed in an intense, high-frequency laser field is reported. By making use of a nonperturbative theory that ''dresses'' both the potential of the impurity and the confinement potential in the quantum wire, and the variational approach a rapid decrease of the binding energy for different values of the wire radius with increasing field intensity is predicted. [S0163-1829(96)08548-7]

The study of the interaction of intense laser fields with bulk solid-state materials has been considered on several occasions.[1–9] In particular the changes induced by an intense, high-frequency radiation field on the binding energy of a hydrogenic impurity in a bulk semiconductor was considered in Ref. 9. It was found, by making use of a nonperturbative method[10] and the variational approach, that the binding energy of the bound electron decreases with increasing laser intensity. As is well known, the binding energy of an impurity is a signature of its location in a given structure and it is also related to the electronic states of the bound system, which has important consequences for both the electronic mobility and the optical properties of the structure. With the advent of artificial semiconductor structures such as quantum wells, quantum wires, and quantum dots, a new channel for the investigation of the interaction of intense fields with such structures was opened. The effect of an intense laser field on the binding energy of the bound states of a shallow hydrogenic impurity placed in a two-dimensional quantum-well semiconductor[11] structure was recently considered[12] and it was found that for an on-center hydrogenic impurity in the given quantum well the binding energy for different well widths decreases rapidly with increasing laser field amplitude.

The importance of electron confinement in quasi-two-dimensional problems suggests that more dramatic effects should occur when the impurity is placed in a quasi-one-dimensional environment.[13,14] In fact, as shown in Ref. 13, the binding energy of a hydrogenic donor placed on the axis of a cylindrical quantum-well wire is enhanced over its bulk value. Moreover, it has been shown that the effective strength of the Coulomb interaction depends on the dimensionality of the problem and that it is greatly enhanced when the dimensionality is reduced by varying the quantum wire radius.[14]

In this paper we report the effect of an intense, high-frequency laser field on the binding energy of a hydrogenic impurity placed in a cylindrical quantum-well wire of radius d taking into account the laser ''dressing'' effects of Refs. 9 and 12 on both the impurity Coulomb potential and the confinement potential, respectively. In the latter, because the quantum-wall wires have well-defined shapes (either cylindrical or rectangular) it is expected that the ''dressed'' confining potential should also affect the impurity binding energy.

We have thus considered a single point charge donor impurity in a quantum-well wire embedded in an intense, high-frequency laser field in a nonrelativistic dipole approximation. Since our main goal here is to bring about a new intense field effect on the physical properties of impurities in quantum wires we assume, for the sake of simplicity, that the impurity binding energy will be determined using an ideal, infinite cylindrical confining potential and that the wire is sufficiently long (ideal) that motion along the wire's axis of symmetry is free; i.e., the confining potential is a function only of a radial coordinate. As far as the electrons are concerned, the effective-mass approximation is used in constructing the Hamiltonian. The variational approach is employed here to determine the ''laser-dressed'' ground-state binding energy of the impurity. The variational wave function will incorporate a field-modulated hydrogenic part and, to confine the electrons in the wire, the appropriate Bessel functions.

The approach used in the present calculation is based upon a nonperturbative theory that has been developed to describe the atomic behavior in intense high-frequency laser fields[10] and it is briefly introduced as follows. We assume that the radiation can be represented by a monochromatic plane wave (frequency ω), linearly polarized (real polarization vector $\boldsymbol{\epsilon}$), and take the electrodynamic potentials in the dipole approximation $\mathbf{A}(\mathbf{t})=A_0\boldsymbol{\epsilon}\cos(\omega t)$, $\Phi=0$. The semiclassical Schrödinger equation in the momentum gauge, describing the interaction dynamics in the laboratory frame of reference, was transformed by Kramers (see also Henneberger and other people)[15] into the form[16]

$$\{(1/2m)\mathbf{P}^2+V[\mathbf{r}+\boldsymbol{\alpha}(t)]\}\psi=i\hbar\,\partial\psi/\partial t \tag{1}$$

by applying the time-dependent translation $\mathbf{r}\rightarrow\mathbf{r}+\boldsymbol{\alpha}(t)$. Here $V(\boldsymbol{r})$ is the atomic binding potential and

$$\boldsymbol{\alpha}(\mathbf{t})=\boldsymbol{\epsilon}\alpha_0\,\sin(\omega t),\quad \alpha_0=-(eA_0/mc\omega), \tag{2}$$

represents the quiver motion of a classical electron in the laser field and $V[\mathbf{r}+\boldsymbol{\alpha}(t)]$ is the ''dressed'' potential energy. In terms of the (time-averaged) laser beam intensity I we write

$$\alpha_0=(I^{1/2}/\omega^2)(e/m)(8\pi/c)^{1/2}. \tag{3}$$

Equation (1) characterizes, in fact, the dynamics in a moving frame of reference, which follows the quiver motion of the classical electron (''Kramers reference frame'').

By application of the Floquet method of solution,[10] Eq. (1) was cast into a system of coupled differential equations in coordinate space for the Floquet components of the wave function Ψ, containing a (in general complex) quasienergy parameter E. An iterative method of solution was devised, proceeding essentially in inverse powers of ω. To lowest order in the iteration (i.e., in the high-frequency limit), the set of coupled equations reduces to a single one,[9,10,12]

$$[(1/2m)\mathrm{P}^2+V_0(\alpha_0,\mathbf{r})]\psi_0=E\psi_0, \tag{4}$$

for the zeroth Floquet component ψ_0. Equation (4) contains the ''dressed'' potential $V_0(\alpha_0,\mathbf{r})$, which depends on I and ω only through α_0.[17] The frequency condition under which this should hold was shown to be $\boldsymbol{\omega}\gg|E_0^m(\alpha_0)|$, where $E_0^m(\alpha_0)$ is the lowest eigenvalue having the same quantum number m as the initial state of the atom in the field.[10]

For the Coulomb case $V(\mathbf{r})=-e^2/|\mathbf{r}|$, the ''dressed'' potential has the form[18]

$$V_0(\boldsymbol{\alpha}_0,\mathbf{r})=-(e^2/2)\left[\frac{1}{|\mathbf{r}+\boldsymbol{\alpha}_0|}+\frac{1}{\mathbf{r}|-\boldsymbol{\alpha}_0|}\right]. \tag{5}$$

Equations (4) and (5) were obtained earlier by other people, albeit using different approaches.[15]

We may well expect that for a single hydrogenic donor impurity in a quantum-well wire (QWW) in the presence of the laser-dressed Coulomb potential, Eq. (5), and also in the presence of a laser-dressed confining $V_{\mathrm{conf}}(\boldsymbol{\rho},\boldsymbol{\alpha}_0)$ potential, respectively, we can choose for an order of magnitude estimate the Hamiltonian (laser field polarized along the x axis)

$$H=\frac{\hat{P}^2}{2m}+V_0(\boldsymbol{\rho},z,\boldsymbol{\alpha}_0)+V_{\mathrm{conf}}(\boldsymbol{\rho},\boldsymbol{\alpha}_0), \tag{6}$$

where

$$V_0(\boldsymbol{\rho},z,\boldsymbol{\alpha}_0)=-\frac{e^2}{2\kappa}\left\{\frac{1}{[(\boldsymbol{\rho}-\boldsymbol{\rho}_0+\boldsymbol{\alpha}_0)^2+z^2]^{1/2}}+\frac{1}{[(\boldsymbol{\rho}-\boldsymbol{\rho}_0-\boldsymbol{\alpha}_0)^2+z^2]^{1/2}}\right\}, \tag{7}$$

and

$$V_{\mathrm{conf}}(\boldsymbol{\rho},\boldsymbol{\alpha}_0)=\tfrac{1}{2}[V_{\mathrm{conf}}(\boldsymbol{\rho}+\boldsymbol{\alpha}_0)+V_{\mathrm{conf}}(\boldsymbol{\rho}-\boldsymbol{\alpha}_0)]. \tag{8}$$

In Eqs. (6) and (7), for instance, m is the electron's effective mass and κ the dielectric constant of the wire material. The $\boldsymbol{\epsilon}_\rho$ direction is perpendicular to the axis of the wire, $\boldsymbol{\rho}_0$ gives the impurity's location along this direction, the z direction is along the axis of the wire, and $V_{\mathrm{conf}}(\boldsymbol{\rho})$ is the bare confinement potential[13] of the QWW. With d the radius of the wire, $V_{\mathrm{conf}}(\boldsymbol{\rho},\boldsymbol{\alpha}_0)$ is zero for $\rho\leqslant d_{\mathrm{eff}}$ and infinite otherwise, where d_{eff} is to be given below.

In what follows we shall give briefly the main results of the calculation for the binding energy of our impurity-quantum wire system in the presence of the ''dressing'' laser field. Details of this calculation are given elsewhere.[19]

Taking account of both the cylindrical confining geometry and the hydrogenic ''dressed'' impurity potential, a field-modulated trial wave function

$$\Psi(\mathbf{r})=NJ_0[k_{10}(\rho+d-d_{\mathrm{eff}})]\exp\left\{-\frac{\lambda}{2}(|\mathbf{r}_1|+|\mathbf{r}_2|)\right\},\quad \rho\leqslant d_{\mathrm{eff}},$$
$$\Psi(\mathbf{r})=0,\quad \rho\geqslant d_{\mathrm{eff}}, \tag{9}$$

where

$$[|\mathbf{r}_1|=[(\boldsymbol{\rho}-\boldsymbol{\rho}_0+\boldsymbol{\alpha}_0)^2+z^2]^{1/2}, \tag{10}$$

$$|\mathbf{r}_2|=[(\boldsymbol{\rho}-\boldsymbol{\rho}_0-\boldsymbol{\alpha}_0)^2+z^2]^{1/2}, \tag{11}$$

and

$$d_{\mathrm{eff}}=[(d^2-\alpha_0^2\sin^2\theta)^{1/2}-\alpha_0\cos\theta] \tag{12}$$

is assumed as the ground-state wave function in the laser ''dressed'' impurity plus laser ''dressed'' confining potential, where N is the normalization constant of the wave function and λ the variational parameter. Because of the dressing effect on the confining potential, an ''effective'' region of confinement for the impurity and the unidimensional electrons in the quantum wire appears (see, for instance, Fig. 3 and a discussion following it below). In this case Eq. (9) is seen to satisfy the boundary condition that $\Psi(\rho=d_{\mathrm{eff}}=0$ provided $J_0(k_{10}d)=0$. In Eq. (12), θ is the angle between $\boldsymbol{\rho}$ and $\boldsymbol{\alpha}_0$.

Proceeding further, for the sake of simplicity we choose the situation in which the impurity is on center (i.e., $\rho_0=0$). The laser ''dressed'' binding energy $E_b(d,\alpha_0)$ of the hydrogenic impurity is defined as the ground-state energy of the system without the impurity present, less the ground-state energy $\epsilon(d,\alpha_0)$ with the impurity; i.e.,

$$E_b(d,\alpha_0)=\frac{\hbar^2k_{10}^2}{2m}-\epsilon(d,\alpha_0). \tag{13}$$

where $\hbar^2k_{10}^2/2m$ is the unperturbed kinetic energy.[13] The binding energy, when defined in this manner, is a positive quantity. Calculating $\epsilon(d,\alpha_0)=\langle T\rangle+\langle V_0(\boldsymbol{\rho},z,\alpha_0)+V_{\mathrm{conf}}(\boldsymbol{\rho},\boldsymbol{\alpha}_0)\rangle$, it is found that $E_b(d,\alpha_0)$, normalized to effective Rydberg units $R_d^*=e^2/a_B^*\kappa$, where $a_B^*=\kappa\hbar^2/me^2$, is given by

$$E_b=-(\lambda a_B^*)^2+\frac{2}{y}\frac{\pi K_0(2\lambda a_B^*y\alpha_0')F+2C}{\pi\alpha_0'K_1(2\lambda a_B^*y\alpha_0')F+2D}, \tag{14}$$

with

$$C=\int_0^{\pi/2}\int_{\alpha_0'}^{d_{\mathrm{eff}}'}tJ_0^2[x(t+1-d_{\mathrm{eff}}')]K_0(2\lambda a_B^*yt)dt\,d\theta, \tag{15}$$

$$D=\int_0^{\pi/2}\int_{\alpha_0'}^{d_{\mathrm{eff}}'}t^2J_0^2[x(t+1-d_{\mathrm{eff}}')]K_1(2\lambda a_B^*yt)dt\,d\theta, \tag{16}$$

and

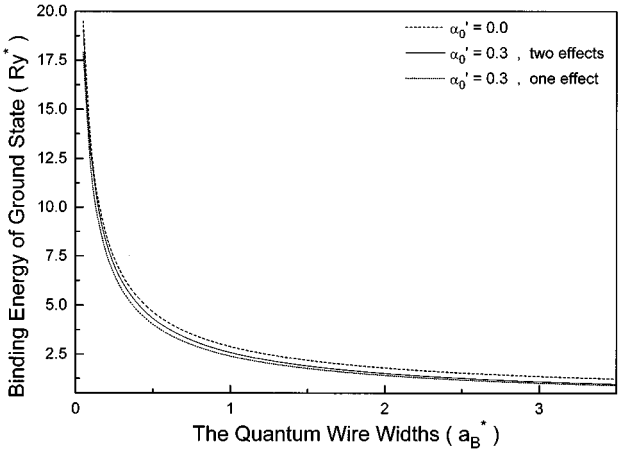

FIG. 1. Binding energies of the impurity as a function of the radii of the wire in units of a_B^* in the absence of the laser field ($\alpha_0'=0$), for the impurity ''laser-dressed'' potential (one effect) and for the two ''laser-dressed'' potentials (two effects), respectively. Here $\alpha_0'\equiv\alpha_0/d$.

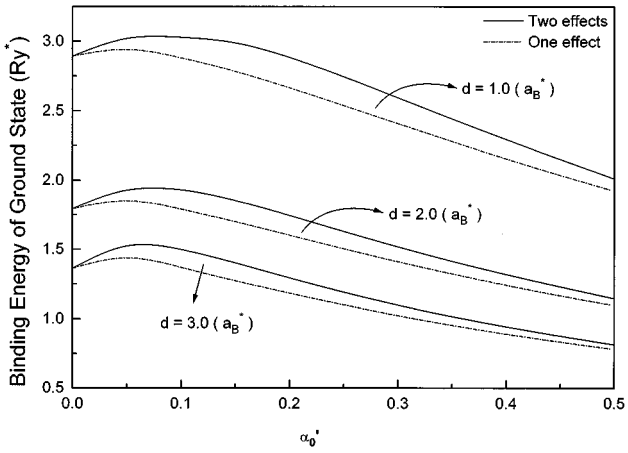

FIG. 2. Binding energies of the impurity as a function of the laser field amplitude for different values of the wire radius considering both the ''laser-dressed'' impurity potential (one effect) and the two ''laser-dressed'' potentials (two effects), respectively. Here $\alpha_0'=\alpha_0/d$.

$$F=\int_0^{\alpha_0'} tJ_0^2[x(t+1-d_{\rm eff}')]dt. \tag{17}$$

For $GaAs/Al_xGa_{1-x}As$ quantum wire Ry*=5.7 meV and $a_B^*=9.87$ nm. In Eqs. (15)–(17) K_0 and K_1 are the modified Bessel functions of the second kind, $t=\rho/d$, $\alpha_0'=\alpha 0/d$, $d_{\rm eff}'=d_{\rm eff}/d$, $x=k_{10}d=2.4048,\ldots$, which is the first zero of $J_0(x)$, and $y=d/a_B^*$. The remaining radial integrations must be performed numerically, as no analytical method for completing the integration is known.

In the case of $\alpha_0'=0$ (i.e., no laser field present) Eq. (14) reproduces the well-known result for hydrogenic impurities in quantum-well wires [Eq. (13) of Ref. 13]. A plot of Eq. (14) for $\alpha_0'=0$ is given in Fig. 1, which shows the same dependence on the radius of the QWW as that of Eq. (13) in Ref. 13 as expected. Figure 1 also shows the ''dressed'' binding energy counterpart for a fixed value of α_0' for the two dressing cases, namely, the one that is presently considered (two effects) and the other case, that in which only the impurity potential is dressed by the field, the confining potential being the bare potential (one effect).[20] We see from this plot that the behavior of the three curves are similar in shape, the only difference between them being the relative values of the binding energy as the field amplitude is varied. In examining the result, Eq. (14), for the $\alpha_0'\neq 0$ case, we first notice that the binding energy increases to very high values very quickly for $y\to 0$ ($d\to 0$) in agreement with the zero-field result.[13] This is a result that is a consequence of the simple model of an ideal infinite potential well we are considering here. Taking into account the ''real'' barrier depth will lead to a finite value for the binding energy as shown, for instance, in the second part of the calculation in Ref. 13. Nevertheless, bringing this effect into consideration definitely changes the result quantitatively, but does not alter the qualitative prediction as the one found above in regard to the physical behavior of our system in the presence of the ''dressing'' laser field based on the simple model for our quantum wire. Proceeding further, in Fig. 2 we show the behavior of the ground-state binding energy of the impurity attached to the ground subband of the QWW as a function of α_0' for three different radii of the QWW system. In this plot, besides considering the realistic case (two effects), we also show the one-effect result for comparison. It tells us that in the intense field regime (α_0' large), the binding energies decrease as α_0' increases, in perfect agreement with the quasi-two-dimensional case.[12] By increasing and decreasing α_0' we mean the increasing and decreasing of the laser intensity through Eq. (3) keeping the laser frequency ω fixed. Figure 2 clearly shows us that the joint action of the two ''dressed'' potential (two effects) makes the impurity binding energy larger as compared with the one-effect case. Because of the ''quiver motion'' of the confining potential at $\pm\boldsymbol{\alpha}_0$ imposed by the laser field the ''dressing'' field acts in a way to change the region of confinement of the impurity and the one-dimensional electrons in the QWW. This new region, which we have denoted as the effective confinement region (or the effective quantum-wire shape), is shown schematically in Fig. 3 and it is given by the crossed area. It thus follows that because of the reduced confinement region we may say that the ''effective dimensionality'' of the system is reduced and the electron states become more localized. As a consequence of this we have an increase of the binding energy for the two-effects curve as shown in Fig. 2. It is also shown in Fig. 2 that by increasing the radius of the QWW from $d=1a_B^*$ to $3a_B^*$ there is a decreasing of the strength of the binding energy in agreement with the two-dimensional case[12] *and* it is a signature of these low-dimension systems independent of whether the laser field is on or off.[11,13] A last point concerning Fig. 2 is the presence of a very broad maximum in the binding energy as we go from large to small values of α_0'. Since this maximum also appears in the curves for $d=2a_B^*$ and $d=3a_B^*$ we believe this is associated with the numerical solution of the integrals Eqs. (15)–(17), as we see no physical argument for its existence at all. Finally, we should like to make some comments regarding the range of laser intensities within which the nonperturbative theory is valid. A lower limit can be established in that the laser intensity I is such that the amplitude of the electron oscillation is of the

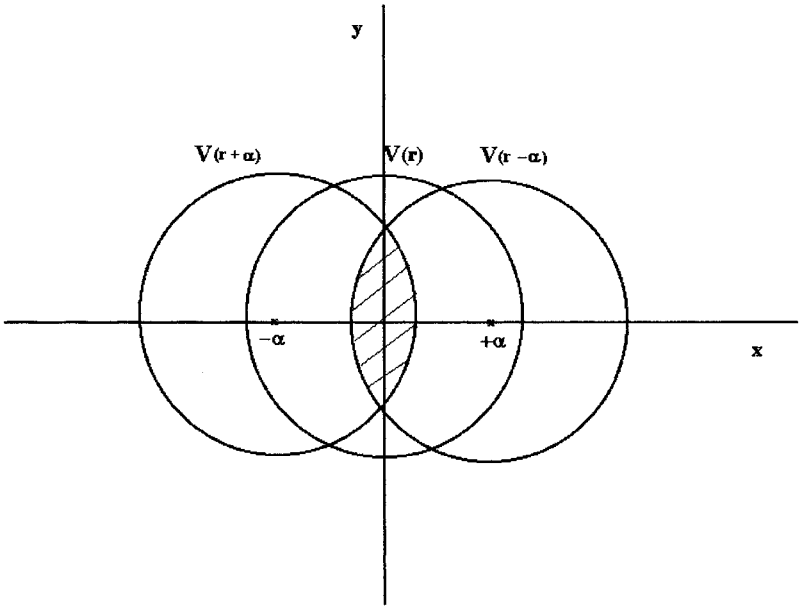

FIG. 3. Cross sections of the shapes of the bare $V(\boldsymbol{\rho})$ and ''dressed'' $V(\boldsymbol{\rho}\pm\alpha_0)$ quantum wire confinement potentials. The crossed area indicates the ''effective'' confinement region in the wire.

order of or greater than the size of the bound system a_B^*. That is, $I>I_c=m^{*2}ca_B^{*2}\omega^4/4\pi e^2$. We call this intensity range the intense field regime. For a typical quantum-wire nanostructure made of GaAs material for which $a_B^*=9.87$ nm we find $I_c\sim10^{-42}$ W/cm^2. For lasers of practical interest, for instance, in the case of a CO_2 laser ($\omega=2.0\times10^{14}$ s^{-1}) our model is applicable for $I>10^7$ W/cm^2, readily available in practice.

The above prediction, namely, the decreasing of the binding energy with increasing laser field amplitude should, we believe, have important consequences for optical studies on QWW's. This effect should be apparent, for instance, in the optical spectra of donors in quantum-well wires[21] if one considers the additional presence of an intense laser field. The above findings make the result of great utility in the fabrication of electronic sensors using these low-dimensional semiconductor materials.

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