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# LoSurdo-Stark effect for a hydrogenic impurity in a thin layer: Two-dimensional model

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The LoSurdo-Stark effect for a bound electron in a two-dimensional hydrogenic atom has been studied as a tractable model for impurity states in a thin layer, such as in superlattices, with an external electric field applied parallel to the layer. Energy shifts and splittings, obtained via perturbation theory, and field-induced ionization are discussed. The model calculation predicts a reduced dependence on the electric field of an electron in an impurity state in a two-dimensional layer when compared with the field dependence of an electron in a corresponding three-dimensional hydrogenic state.

The science and technology of superlattices, first proposed by Esaki and Tsu,[1] has received much attention with a view to the development of new classes of electronic devices. Several theoretical studies have been made of the binding energies of hydrogenic impurity states in quantum well systems, which model superlattices such as in the GaAs-$\mathrm{Ga}_{1-x}\mathrm{Al}_x\mathrm{As}$ system.[2-5] Dependence of the impurity energy levels on an electric field, or LoSurdo-Stark effect, applied in the direction of the growth axis of the superlattice has also been studied[6,7] to explain the strong decrease of photoluminescence intensity and the red shift of its peak position as the field strength is increased.[8] In addition, the high mobility of conduction carriers parallel to the planes of a superlattice, generated by modulation doping,[9] is of particular interest for application to high electron mobility transistor (HEMT) devices, and so forth. The LoSurdo-Stark effect for electrons bound to impurities in a thin layer, with the external electric field parallel to the layer, is a phenomenon fundamental to the analysis of electronic properties of thin-layer systems as well as of two-dimensional systems in general.[10]

In this Rapid Communication we discuss the LoSurdo-Stark effect for a two-dimensional (2D) hydrogenic atom as a model of an impurity state localized in a thin layer. We derive the splitting and shift of the energy levels by Rayleigh-Schrödinger perturbation theory (RSPT), which for the 2D atom can be obtained directly from appropriate RSPT formulas for the 3D case. We obtain the 2D tunneling-ionization rate also from the corresponding 3D formula. The main differences between the 2D and 3D cases have to do with the values of quantum numbers, degeneracies, and how the electric field dependence of the energy shifts and ionization rates is affected by the various quantum numbers.

The Hamiltonian for an electron of effective mass $\mu^*$ moving in the fields of an ion of charge $Z|e|$ and of a constant uniform electric field $F$ pointing in the $x$ direction in a planar medium with dielectric constant $\kappa$ is given by

$$H=H^{(0)}+|e|Fx \;, \tag{1}$$

$$H^{(0)}=-\frac{\hbar^2}{2\mu^*}\left[\frac{d^2}{dx^2}+\frac{d^2}{dy^2}\right]-\frac{Ze^2}{\kappa r} \;, \tag{2}$$

where $r=(x^2+y^2)^{1/2}$, the distance of the electron from the impurity site. Toward simplification, we use atomic units. The constants $\hbar$, $\mu^*$, $\kappa$, $e$, and $Z$ are dropped from the above Hamiltonians. The units for energy, length, and field strength are then $\mu^*e^4Z^2/\hbar^2\kappa^2$, $a=\hbar^2\kappa/\mu^*e^2Z$, and $Z|e|/\kappa a^2$, respectively.

The Schrödinger equation for the unperturbed Hamiltonian $H^{(0)}$ was solved 32 years ago by Kohn and Luttinger[11] in a paper on donor states in $n$-type Si by separation in polar coordinates. The solution has some similarity with hydrogen in three dimensions, which we exploit notationally:

$$E_n=-\tfrac{1}{2}n^{-2} \;, \tag{3}$$

$$\Psi_{n,m}(r,\phi)=N_{n,m}(2r/n)^{|m|}\times e^{-r/n}L_{n-|m|-1/2}^{(2|m|)}(2r/n)e^{im\phi} \;. \tag{4}$$

Here $N_{n,m}$ denotes a normalization constant, and $L_j^{(i)}$ denotes a generalized Laguerre polynomial.[12] An important difference between the 2D and 3D case is that the analog of the 3D principal quantum number $n$ here takes on integer-plus-one-half values (rather than integer values). The magnetic quantum number $m$ takes on integral values from $n-\frac{1}{2}$ to $\frac{1}{2}-n$:

$$n=\tfrac{1}{2},\tfrac{3}{2},\tfrac{5}{2},\ldots, \tag{5}$$

$$m=n-\tfrac{1}{2},n-\tfrac{3}{2},\ldots,-n+\tfrac{1}{2} \;. \tag{6}$$

Although $n+\frac{1}{2}$ could have been used above, so that the symbol $n$ could take on only integer values, the half-integer-value usage has the advantage of preserving many relevant formulas of the 3D hydrogenic atom [such as Eq. (3) for $E_n$]. Note that because $n$ starts with the value $\frac{1}{2}$ in the 2D case (versus 1 in the 3D case), the energy of the ground state is four times what it would be in the 3D case, and the maximum in the radial probability density occurs at $\frac{1}{4}$ the corresponding 3D radius. The degeneracy of the "$n$"th level is the odd number $2n$. These $2n$ states in a sense arise from the "planar" 3D states for which the $l$ and 3D $|m|$ quantum numbers are equal. The levels for which $l$ is greater than the 3D $|m|$ are in that same sense pushed (in energy) to infinity as the domain for the $z$ coordinate of the 3D atom is shrunk from $(-\infty,+\infty)$ to $[0,0]$.

Both the perturbed and unperturbed Schrödinger equations are separable in parabolic coordinates, the natural coordinate system for the Hamiltonian (1):

$$\xi=(r+x),\ \eta=(r-x)\ . \tag{7}$$

The separated equations, moreover, are identical with the corresponding separated equations in three dimensions [see, in particular, Eqs. (8) and (9) of Ref. 13], except that the 3D $|m|$ quantum number is replaced by the values $\pm\frac{1}{2}$. To aid in comparing the resulting 2D and 3D equations (and also to avoid confusion in that there is no "$m$" quantum number in 2D in the parabolic separation), we replace $|m|$ in the 3D equations by $m_{3D}$. Then if the equation pertains explicitly to a 3D state, $m_{3D}$ means $|m|$, while for a 2D state it means $\pm\frac{1}{2}$. The parabolic quantum numbers $n_1$ and $n_2$ take on the same set of values $0, 1, 2, \dots,$ and the relation to $n$ is, *mutatis mutandis*, the same as in 3D:[14]

$$n=n_1+n_2+m_{3D}+1=n_1+n_2\pm\tfrac{1}{2}+1\ , \tag{8}$$

$$\Psi_{n_1,n_2,m_{3D}}=N_{n_1,n_2,m_{3D}}(\xi\eta/n)^{m_{3D}/2}e^{-(\xi+\eta)/2n}\times L_{n_1}^{(m_{3D})}(\xi/n)L_{n_2}^{(m_{3D})}(\eta/n)\ . \tag{9}$$

(It is of some interest that the separated 2D parabolic equations are equivalent to the 1D anharmonic oscillator,[15] while the separated 3D parabolic equations are equivalent to the radially symmetric 2D anharmonic oscillator.) The RSPT energy coefficients can be obtained from the earlier solution of the 3D LoSurdo-Stark effect in hydrogen,[14] for which the energy coefficients were given (in Table II of Ref. 14) as polynomials in the quantities $M=\frac{1}{4}(m_{3D}^2-1)$, $k_1=n_1+\frac{1}{2}m_{3D}+\frac{1}{2}$, and $k_2=n_2+\frac{1}{2}\times m_{3D}+\frac{1}{2}$. For instance, for the 2D ground state for which $n=\frac{1}{2}$ and $(n_1,n_2,m_{3D})=(0,0,-\frac{1}{2})$, we have

$$E^{(1)}=\tfrac{3}{2}n(k_1-k_2)=0\ , \tag{10}$$

$$E^{(2)}=\frac{n^4}{16}[-14(k_1^2+k_2^2)-40k_1k_2-10+9(m_{3D}^2-1)] = -\tfrac{21}{256}\ . \tag{11}$$

Similarly, for the three states with $n=\frac{3}{2}$, i.e., $(n_1,n_2,m_{3D})=(1,0,-\frac{1}{2})$, $(0,0,+\frac{1}{2})$, and $(0,1,-\frac{1}{2})$, one finds that

$$E^{(1)}=\tfrac{9}{4},\ E^{(2)}=-\tfrac{1053}{64},\ (n_1,n_2,m_{3D})=(1,0,-\tfrac{1}{2})\ , \tag{12}$$

$$E^{(1)}=0,\ E^{(2)}=-\tfrac{4455}{256},\ (n_1,n_2,m_{3D})=(0,0,+\tfrac{1}{2})\ , \tag{13}$$

$$E^{(1)}=-\tfrac{9}{4},\ E^{(2)}=-\tfrac{1053}{64},\ (n_1,n_2,m_{3D})=(0,1,-\tfrac{1}{2})\ . \tag{14}$$

The energy change due to the 2D and the 3D LoSurdo-Stark effects is depicted in Fig. 1 for the sake of comparison.

The field-induced tunneling-ionization rate of the 2D hydrogen atom is related to $-(2/\hbar)$ times the imaginary part of the complex resonance eigenvalue. As for the case of the RSPT expansion, the 2D result follows from the 3D

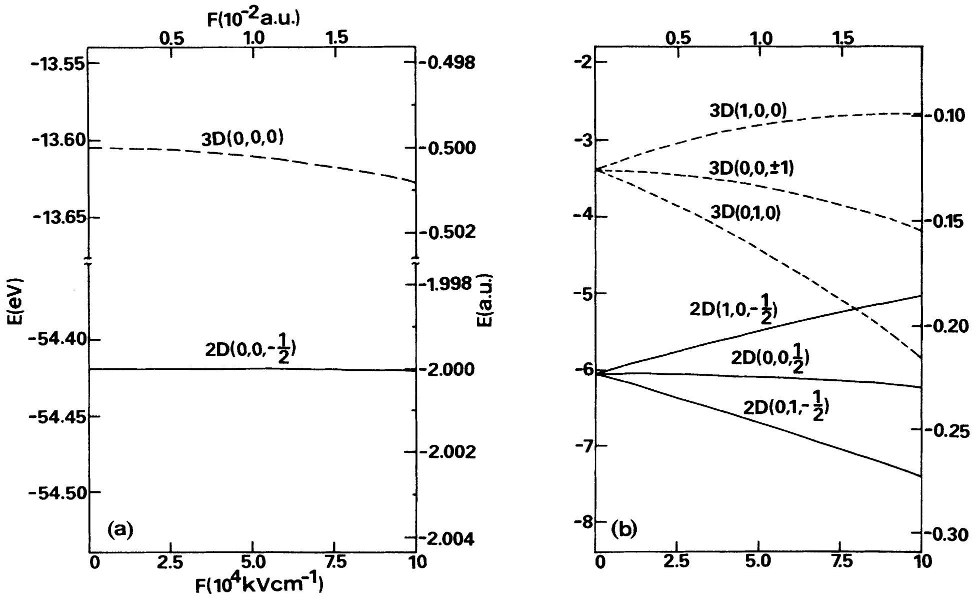

FIG. 1. $E=E^{(0)}+E^{(1)}F+E^{(2)}F^2$ for the (a) ground and (b) first excited states of the 2D and 3D hydrogenic atoms with $\mu^*$, $\kappa$, and $Z$ being unity. For easy visualization the plots have been taken to very high $F$ to exaggerate the differences between the 2D and 3D states. The units of variables in (b) are the same as those in (a).

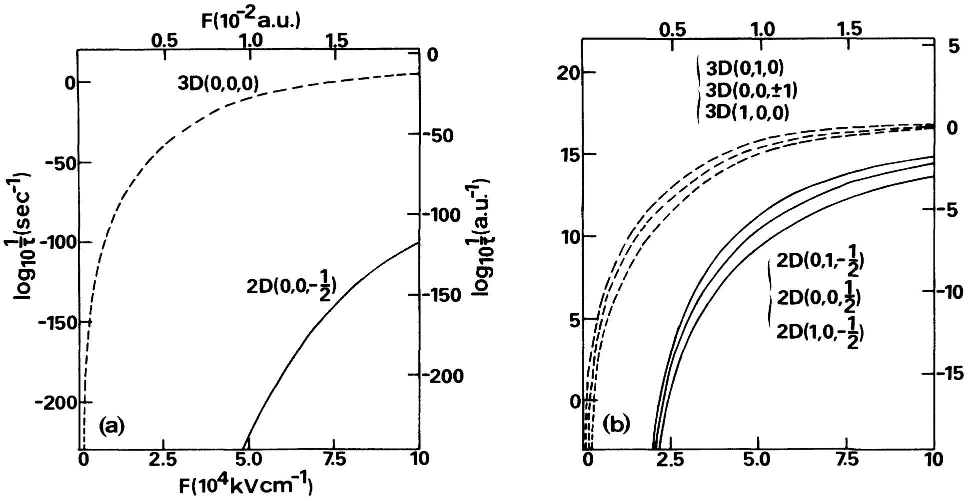

FIG. 2. Field-induced tunneling-ionization rate $1/\tau$ for the (a) ground and (b) first excited states of the 2D and 3D hydrogenic atoms with $\mu^*$, $\kappa$, and $Z$ being unity. Note the substantial difference in the values of the 2D and 3D cases. The units of variables in (b) are the same as those in (a).

result[13] by substituting $\pm\frac{1}{2}$ for the $m_{3D}$ quantum number $|m|$. (Compare Ref. 15, where this aspect of the 1D anharmonic oscillator is treated in detail.) Although one can easily derive the full asymptotic series for Im$E$,[15,16] we shall be content here with the leading term

$$-\mathrm{Im}E \sim [2n^3 n_2!\Gamma(n_2+m_{3D}+1)]^{-1}(\tfrac{1}{4}n^3F)^{-(2n_2+m_{3D}+1)}e^{[3(n_1-n_2)-2/(3n^3F)]} \quad (15)$$

For the ground and lowest excited levels, $-$Im$E$ has the explicit asymptotic forms

$$-\mathrm{Im}E \sim 4\pi^{-1/2}(F/32)^{-1/2}e^{-16/3F},\quad (n_1,n_2,m_{3D})=(0,0,-\tfrac{1}{2})\ , \quad (16)$$

$$\sim \tfrac{4}{27}\pi^{-1/2}(27F/32)^{-1/2}e^{3}e^{-16/81F},\quad (n_1,n_2,m_{3D})=(1,0,-\tfrac{1}{2})\ , \quad (17)$$

$$\sim \tfrac{8}{27}\pi^{-1/2}(27F/32)^{-3/2}e^{-16/81F},\quad (n_1,n_2,m_{3D})=(0,0,+\tfrac{1}{2})\ , \quad (18)$$

$$\sim \tfrac{8}{27}\pi^{-1/2}(27F/32)^{-5/2}e^{-3}e^{-16/81F},\quad (n_1,n_2,m_{3D})=(0,1,-\tfrac{1}{2})\ . \quad (19)$$

Let us now compare $E^{(1)}$, $E^{(2)}$, and Im$E$ for the 2D case with the 3D case.

For the ground state both cases have $E^{(1)}=0$, while $E^{(2)}_{2D}=-\frac{21}{256}$ compared with $E^{(2)}_{3D}=-\frac{9}{4}$. Thus the 2D ground-state polarizability is $\sim\frac{1}{28}$ times the 3D value. The ratio of the 2D Im$E$ to the 3D Im$E[=(-2/F)e^{-2/3F}]$ is $(128/\pi)^{1/2}F^{1/2}e^{-14/3F}$. Thus, ionization in the 2D case is greatly suppressed over the 3D case (for small $F$). The ionization rate $1/\tau$ in the 2D and the 3D cases is shown in Fig. 2.

For the first excited states ($n=\frac{3}{2}$) of the 2D case, the linear splitting ($E^{(1)}_{2D}=+\frac{9}{4},0,-\frac{9}{4}$) is reduced by a factor $\frac{3}{4}$ over the first excited states ($n=2$) of the 3D case ($E^{(1)}_{3D}=+3,0,-3$). Similarly, the ionization rates for the 2D states are suppressed for small $F$ by the factors $k(8F/\pi)^{1/2}e^{-37/324F}$, where $k=\frac{1}{2}(\frac{64}{27})^{3/2}$, $(\frac{64}{27})^{5/2}$, or $(\frac{64}{27})^{7/2}$, depending whether $(n_1,n_2)=(1,0)$, $(0,0)$, or $(0,1)$.

In summary, the 2D hydrogenic atom has, in general, a smaller response to an external electrostatic field than does a 3D atom, with the greatest contrast between 2D and 3D occurring with the ground state. These results for the 2D model represent a limiting case—that of zero thickness—of an electron bound to an impurity in a thin layer, and as such they suggest a behavior for the electric field dependence of thin-layer systems of practical interest.

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