Coulomb spectrum in crossed electric and magnetic fields: Eigenstates of motion in double-minimum potential wells

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Two-dimensional electron layers when placed in perpendicular electric and magnetic fields can have a potential well with two minima for the electronic motion normal to the surface. Such double-minimum potential wells also arise for highly excited Rydberg states of atoms in crossed electric and magnetic fields and in certain molecular potential curves. We develop and apply a WKB formalism to such double-minimum wells and calculate the energy splittings that arise when one is near "degeneracy," that is, when either well, considered independently, can support a bound state at the same energy.

I. INTRODUCTION: THE DOUBLE-MINIMUM POTENTIAL

In recent years the study of electron layers on the surface of liquid helium has been actively pursued.[1] Because of the behavior as an almost free two-dimensional gas, they are of interest for a variety of reasons. A major one is that they represent analogs of the three-dimensional gas in a metal but with the added convenience that the number density can be readily varied over many orders or magnitude by changing the value of an external electric field that clamps the electrons to the surface of the liquid. In this manner, for instance, the first experimental observation of Wigner crystallization of an electron gas has been demonstrated in this system.[2] Other recent experiments of "dimples" and lattices formed by these dimples[3] are examples of the interesting phenomena displayed by these electron layers. Our interest in this paper is not in the condensed-matter aspects in the two dimensions of the layer but rather in the atomiclike aspects of this system in the other perpendicular direction normal to the surface. The basic binding provided for motion along this direction (the z direction in what follows) is the image potential seen by an electron.[1] Since liquid He has a permittivity $\tilde{\epsilon}$ which is only very slightly larger than unity, this is a weak attractive image potential, a one-dimensional Coulomb potential

$$V(z)=-Qe^2/z,\quad z>0 \tag{1a}$$

with

$$Q=\tfrac{1}{4}(\tilde{\epsilon}-1)/(\tilde{\epsilon}+1)\simeq 6.955\times 10^{-3}\,, \tag{1b}$$

where $z=0$ marks the surface of the liquid and Q is the effective charge of the one-dimensional Coulomb potential. For $z<0$ the liquid represents a barrier to the electrons and given the other scale of energies set in the problem by Q, the barrier is to a first approximation infinitely high so that the boundary condition can be taken to be that the electronic wave function vanishes at $z=0$. More careful treatments that go beyond this approximation are avail-

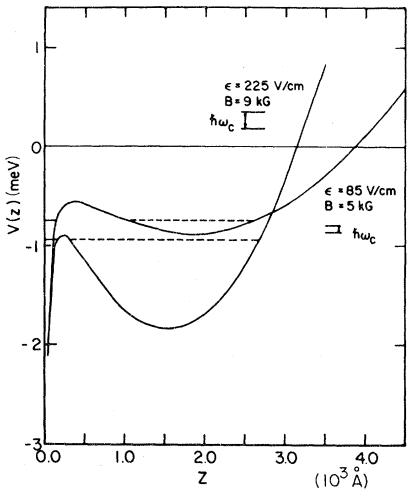

FIG. 1. Potentials $V(z)$ [Eq. (3)] for an electron on the surface of liquid helium in crossed electric and magnetic fields plotted against the distance z from the surface (at $z=0$) for two different values of ϵ and B. ϵ and B values, as well as the cyclotron energies $\hbar\omega_c(=\hbar eB/mc)$, are indicated alongside the appropriate curve. The solid lines in the inner well (near $z=0$) give roughly the positions of the ground-state energy in that well. By "tuning" ϵ and B, this may be made to correspond to an eigenenergy in the outer well, whence a doublet will arise when tunneling lifts this "degeneracy."

able in the literature[4] but we restrict ourselves in this paper to the initial approximation since it is known to be quite accurate in practice. The z motion then is quantized into energy levels $-Q^2me^4/2\hbar^2n^2$, $n=1,2,\ldots$. Note that there is an exact correspondence to the $l=0$ radial problem of the hydrogen atom. In actual experiments, an additional clamping electric field ϵ has been applied in the z direction.[1,2] This added potential $e\epsilon z$ to $V(z)$ in (1) shifts the energy levels and the resulting values are referred to as "electric subbands." The motion parallel to the surface is considered free in the absence of other applied fields so that each of the subbands is infinitely degenerate. Many such subbands have been experimentally observed and their energy positions satisfactorily accounted for.[1] There have also been experiments in which additional magnetic fields tilted at an arbitrary angle to the surface have been applied.[5]

What is of interest to us in this paper is that by a suitable arrangement of tilted magnetic fields and the electric field along z, a novel double-minimum potential well as in Fig. 1 can be formed for the z motion. As the simplest example of such an arrangement consider that the clamping electric field is reversed and a magnetic field B is applied along the surface, say in the x direction. Adopting a gauge $A=(0,-Bz,0)$ to describe this field, the complete Hamiltonian takes the form

$$H=\frac{P_x^2}{2m}+\frac{P_z^2}{2m}+\frac{1}{2m}\left[P_y-\frac{eBz}{c}\right]^2 -\frac{Qe^2}{z}-e\epsilon z,\quad z>0\ . \tag{2}$$

Our interest is in the z motion but some remarks are in order regarding the other dimensions. P_x completely separates from the problem, is a conserved quantum number, and represents a remaining degeneracy of every level. P_y too is conserved because it commutes with H. The problem, therefore, reduces to a one-dimensional one with a combination of an image potential, a linear potential, and a harmonic-oscillator well centered at $z=cP_y/eB$. Such a combination has the generic form of a double-minimum potential. In our calculations, we restrict ourselves to $P_y=0$ when the potential takes the form shown in Fig. 1. We note that upon minimizing the energy with respect to P_y, the minimum lies at $\langle P_y\rangle=m\omega\langle z\rangle$ where $\omega\equiv eB/mc$ is the cyclotron frequency. Since ϵ and B are unspecified our results for $(\langle P_y\rangle=0,\epsilon,B)$ can be mapped on to those where $\langle P_y\rangle$ has been minimized by the replacement $\epsilon-m\omega^2\langle z\rangle/e\rightarrow\epsilon$ and an overall redefinition of the zero of the energy scale by $\frac{1}{2}m\omega^2\langle z\rangle^2$. The problem we consider is, therefore,

$$V(z)=\infty,\quad z<0$$
$$=-\frac{Qe^2}{z}-e\epsilon z+\tfrac{1}{2}m\omega^2z^2,\quad z>0\ . \tag{3}$$

This potential is also relevant to the study of highly excited Rydberg states of atoms in external static fields. In recent years such studies have shown that a particularly interesting regime is the one of "strong mixing" right around the ionization threshold when the external field is on par with the Coulomb field.[6] A characteristic resonance pattern develops which has been partially accounted for[6,7] by considering the motion of the electron in the resulting combined nonseparable potential as composed of coupled motion in perpendicular directions. Some of these directions correspond to bound-state motion, others to escape to infinity, and the combination leads to the resonances. Most studies have dealt with electric or magnetic fields alone though a situation where crossed electric and magnetic fields are present due to a motional Stark effect has been studied experimentally[8] and theoretically.[9] The more general instance of arbitrary ϵ and B leading to double-minimum potentials has only been discussed qualitatively.[7,10] We note that an electric field in the z direction and a magnetic field in the x direction gives a potential for an atom with nulcear charge Q which takes the following form for a certain slice $(x=y=0)$ of the coordinates:

$$V=-\frac{Qe^2}{|z|}-e\epsilon z+\tfrac{1}{2}m\omega^2z^2\ . \tag{4}$$

This potential is, therefore, very similar to (3) except that for $z<0$ it is a steeply rising potential instead of a barrier at $z=0$. Figure 2 gives an example for certain values of ϵ and B. Since it would be of interest to excite atomic levels which fall in the range of energies where there is substantial localization in the outer valley, we present sample calculations applicable to this model as well.

Finally, as an example of double-minimum potentials that have recently been of interest in other areas, we apply our formalism to certain problems[11,12] in molecular physics.

II. WKB CALCULATIONS OF ENERGY LEVELS IN THE DOUBLE-MINIMUM WELL

In this section, we consider bound-state energy levels in the double-minimum potential wells dis-

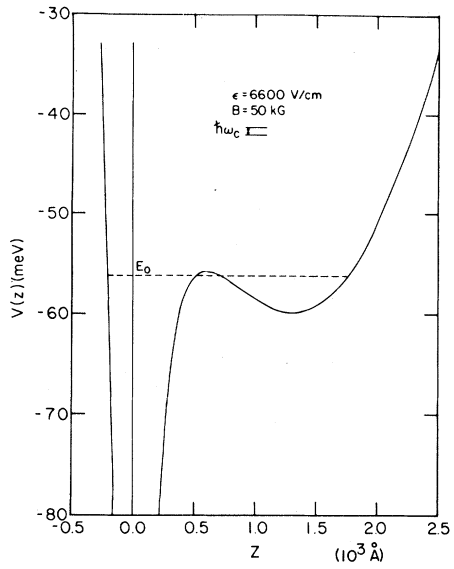

FIG. 2. Plot of a certain slice ($x=0$, $y=0$) of the potential for the hydrogen atom [Eq. (4), $Q=1$] when subjected to crossed electric and magnetic fields applied along $-z$ and x, respectively.

cussed above. A particularly interesting circumstance arises when the two wells, considered independently, can each support a level at the same energy. The fact that the wells are connected will, in fact, lead to a lifting of this degeneracy. The splitting between the two resulting levels will be a measure of the tunneling probability across the barrier separating the wells. Many such examples are familiar in the physics literature when the two wells are identical.[13] The asymmetrical double-well problem has seen less investigation though it is of interest in the molecular-physics literature.[11,12]

We use the WKB method to calculate the energy levels and the splitting. In a situation such as in Fig. 3 and an energy corresponding to the line z_1,z_2,z_3,z_4 it is a straightforward matter to apply the usual WKB connection formulas[14] (based on Airy functions) at the turning points to get the following quantization condition:

$$\cot\lambda\cot\sigma=\tfrac{1}{4}\exp(-2\phi)\ , \tag{5}$$

where

$$\lambda=\int_{z_1}^{z_2}k(z)dz,\quad \sigma=\int_{z_3}^{z_4}k(z)dz\ ,$$
$$\phi=\int_{z_2}^{z_3}\kappa(z)dz \tag{6}$$

and

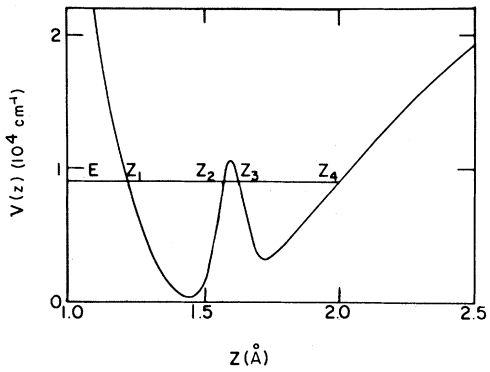

FIG. 3. Example of a double-minimum potential considered in the molecular-physics literature (Ref. 12). This corresponds to a "Morse potential + Gaussian hump." Relevant parameters are given in Ref. 12.

$$k(z)=[2m(E-V)/\hbar^2]^{1/2}=i\kappa(z)\ . \tag{7}$$

The quantization for the individual wells follows, of course, when the tunneling through the barrier is negligible, that is, $\phi\to\infty$, so that

$$\lambda=(n_\lambda+\tfrac{1}{2})\pi,\quad \sigma=(n_\sigma+\tfrac{1}{2})\pi\ . \tag{8}$$

For an energy E_0 when such conditions (8) are satisfied, the resulting doublet of energy levels upon lifting of the degeneracy are at $E_0\pm\delta$ with

$$\delta\simeq\tfrac{1}{2}\exp(-\phi_0)\left[\left[\frac{d\lambda}{dE}\right]_0\left[\frac{d\sigma}{dE}\right]_0\right]^{-1/2}\ . \tag{9}$$

The above expressions suffice for many purposes but can be improved upon, particularly when the barrier width becomes very small, that is when z_2 and z_3 in Fig. 3 gets very close to each other. In that situation, the underlying basis of the above derivation, that WKB solutions across a turning point can be matched through solutions of a linear potential that locally coincides with $V(z)$, becomes inadequate. Instead, the potential in the vicinity of z_2 and z_3 is better described as an inverted harmonic oscillator or parabolic potential. Connection formulas based on Weber functions which now replace Airy functions as the appropriate ones have been established by Miller and Good.[15] Child[16] has used these to develop WKB expressions for a wide variety of situations. For the double-minimum well, the required modifications of (5), (8), and (9) are

$$\cot\tilde{\lambda}\cot\tilde{\sigma}=\frac{[1+\exp(2\phi)]^{1/2}-\exp(\phi)}{[1+\exp(2\phi)]^{1/2}+\exp(\phi)}\ , \tag{10}$$

$$\tilde{\lambda}=(n_\lambda+\tfrac{1}{2})\pi,\quad \tilde{\sigma}=(n_\sigma+\tfrac{1}{2})\pi\ , \tag{11}$$

TABLE I. Doublet splittings $\Delta^{(0)}(=2\delta)$ of the $n_\lambda=0$ level at energy E_0 of a surface state electron on liquid He in crossed ϵ and B fields obtained by the usual WKB method [Eq. (9)]. The potential is given by Eq. (3) with $Q=6.955\times10^{-3}$. For any ϵ and B, E_0 corresponds to the eigenenergy in either well with quantum numbers n_λ and n_σ if tunneling is neglected. $\hbar\omega_c$ is the cyclotron energy ($=\hbar eB/mc$).

ϵ (V/cm)	B (kG)	n_σ	E_0 (meV)	$\hbar\omega_c$ (μeV)	$\Delta^{(0)}$ (μeV)
82.800	4.8281	2	−0.7523	55.89	0.51
82.991	2.9895	42	−0.7546	34.61	1.69
83.876	4.8843	2	−0.7535	56.34	0.57
84.010	3.0165	42	−0.7558	34.92	1.84
84.747	4.7814	3	−0.7547	55.35	0.76
84.993	2.9899	45	−0.7570	34.61	2.01
85.806	4.8337	3	−0.7559	55.96	0.84
86.012	3.0161	45	−0.7582	34.92	2.18
86.859	4.8856	3	−0.7571	56.56	0.93
86.992	2.9913	48	−0.7595	34.63	2.36

$$\delta\simeq\left[\frac{[1+\exp(2\phi_0)]^{1/2}-\exp(\phi_0)}{[1+\exp(2\phi_0)]^{1/2}+\exp(\phi_0)}\right]^{1/2}\times\left[\frac{d\tilde{\lambda}}{dE}\right]_0^{-1/2}\left[\frac{d\tilde{\sigma}}{dE}\right]_0^{-1/2},\tag{12}$$

where

$$\tilde{\lambda}\equiv\lambda-\tfrac{1}{2}\mu(-2\phi/\pi),\quad\tilde{\sigma}\equiv\sigma-\tfrac{1}{2}\mu(-2\phi/\pi)\tag{13}$$

with

$$\mu(x)=\arg\Gamma(\tfrac{1}{2}+\tfrac{1}{2}ix)+\tfrac{1}{2}x\left[1-\ln\left|\frac{x}{2}\right|\right].\tag{14}$$

The above expressions reduce to the earlier ones when $\exp(2\phi)\gg1$. Finally, in cases such as those shown in Fig. 1 where there is an infinite barrier at $z=0$ so that $z_1=0$ and the wave function must vanish there, one has to make the standard modification[17] of replacing λ by $\lambda-\pi/4$, though in our calculation we have replaced λ by $\lambda-\pi/2$ to obtain the well-known hydrogenic energy levels in the inner well in the absence of ϵ and B fields.

For energies above the barrier maximum, if the relation $E-V=0$ has two real roots (z_1,z_4) and two complex-conjugate roots $[z_2^{\pm},\mathrm{Im}(z_2^{+})>0]$, then Eq. (10) is replaced by

$$\cos(\tilde{\lambda}+\tilde{\sigma})=-\frac{\exp(\phi)\cos(\lambda-\sigma+\gamma)}{[1+\exp(2\phi)]^{1/2}},\tag{15}$$

where

$$\phi=-i\int_{z_2^+}^{z_2^-}k\,dz\tag{16}$$

and

$$\gamma=\int_{z_2^+}^{z_0}k\,dz+\int_{z_2^-}^{z_0}k\,dz,\tag{17}$$

z_0 being the point at which the barrier maximum is

TABLE II. Same as in Table I, but now $E_0(=-0.9443$ meV) is kept fixed, and modified WKB values $\Delta^{(m)}$ [Eq. (12)], with $d\mu/dE$ neglected] are also displayed for comparison with $\Delta^{(0)}$ [Eq. (9), evaluated at E_0].

ϵ (V/cm)	B (kG)	n_σ	$\hbar\omega_c$ (μeV)	$\Delta^{(0)}$ (μeV)	$\Delta^{(m)}$ (μeV)
224.84	8.8886	9	102.9	64.21	56.79
225.17	9.1131	8	105.5	64.39	57.09
225.56	9.3655	7	108.4	64.52	57.38
226.04	9.6527	6	111.7	64.58	57.64
226.63	9.9850	5	115.6	64.54	57.82

TABLE III. Similar to Table II, but now the results correspond to the atomic potential [Eq. (4)]. $E_0(=-56.076$ meV) corresponds to the $n_\lambda=17$ Rydberg level in crossed ϵ and B: $\tilde{\lambda}(E_0)=(17-\frac{1}{4}).2\pi$. Note the rapid increase in Δ's with increase in n_σ.

ϵ (V/cm)	B (kG)	n_σ	$\hbar\omega_c$ (meV)	$\Delta^{(0)}$ (μeV)	$\Delta^{(m)}$ (μeV)
6812.9	54.642	0	0.633	4.12	4.13
6662.8	51.329	5	0.594	35.75	35.53
6557.5	48.897	10	0.566	70.84	69.08
6478.1	46.980	15	0.544	100.8	95.54
6415.7	45.408	20	0.526	124.8	114.5

located. The limits z_2,z_3 for the integrals λ,σ are now replaced by z_0. In doing the ϕ integration, that branch of k is chosen which renders ϕ negative. For energies considerably higher than the barrier maximum, both μ and the right-hand side of Eq. (15) vanish and one recovers the usual WKB condition for eigenvalues, viz.,

$$\cos(\lambda+\sigma)=0\ . \tag{18}$$

We have applied the above results to the potential in Eq. (2). E_0 is chosen to be the ground state in the inner well: $n_\lambda=0$. The values of ϵ and B are "tuned" as to bring levels in the outer well to coincide with E_0. Table I gives the values of the doublet spacings $\Delta(=2\delta)$ obtained from Eq. (9) for sample values of small and large n_σ. All the integrals required for presenting the results in Tables I–IV can be expressed in analytical form[18] in terms of complete elliptic integrals of the first, second, and third kind and have been evaluated quite conveniently using a standard algorithm.[19] A representative potential curve is shown in Fig. 1 for which $\epsilon=85$ V/cm and $B=5$ kG. Since the barrier width is quite appreciable here, use of Eq. (9) is justified. The spacings are roughly of the order of μeV and the doublet structure may not be fully resolved in an experimental investigation. Table II presents results for another situation where the parameters are chosen so as to make the barrier at energy E_0 very small (see the curve for $\epsilon=225$ V/cm and $B=9$ kG in Fig. 1). The splittings are, therefore, much larger. The doublet separations now are well within the range of experimental accuracy and the field strengths are quite reasonable for an experimental observation of this phenomenon. It goes without saying that the sensitive dependence on tunneling which is, further, very sensitive to the width of the barrier, makes this phenomenon extremely sensitive to the values of ϵ and B. We also compare in Table II the doublet spacings given by the simpler expression (9) with those obtained from the more accurate Eq. (12) where, however, we have assumed $(d\mu/dE)_0=0$. To our knowledge, these may be the first actual numerical comparison of these alternative expressions. Table III gives sample results for the similar atomic potential problem in Eq. (4). Once again, the values of the electric and magnetic field strengths have been chosen to be those reasonable for such experiments on Rydberg states in external fields.

Finally, we report some results on double-minimum potentials that have been considered in the molecular-physics literature. Table IV displays the first eight eigenvalues corresponding to an

TABLE IV. First eight eigenvalues of a symmetric double-minimum potential (Ref. 20) corresponding to an anharmonic oscillator. 0: usual WKB method [Eqs. (5) and (18)]. m: modified WKB method [Eqs. (10) and (15)]. a: numerically obtained values (Ref. 20).

n	$E^{(0)}$	$E^{(m)}$	$E^{(a)}$	$E^{(a)}-E^{(0)}$	$E^{(a)}-E^{(m)}$
0	−4.3683	−4.4094	−4.4368	−0.0685	−0.0274
1	−4.2833	−4.3282	−4.3498	−0.0665	−0.0216
2	−0.0119	0.0608	0.0242	0.0361	−0.0366
3	1.7587	1.5825	1.5671	−0.1916	−0.0154
4	4.7478	4.8432	4.8312	0.0834	−0.0120
5	8.2573	8.2814	8.2758	0.0185	−0.0056
6	12.181	12.206	12.203	0.022	−0.003
7	16.460	16.479	16.478	0.018	−0.001

TABLE V. Usual and modified WKB results for the eigenenergies of an asymmetric double-minimum potential considered in Ref. 12. 0: usual WKB. m: modified WKB. a: numerically obtained values (Ref. 12). Only those eigenvalues that correspond to four real turning points are shown.

n	$E^{(0)}$ (cm^{-1})	$E^{(m)}$ (cm^{-1})	$E^{(a)}$ (cm^{-1})
1	3207.9	3201.1	3205.3
2	4244.2	4234.9	4227.3
3	5158.9	5147.9	5144.3
4	6140.8	6071.6	6064.2
5	7122.6	7103.2	7092.7
6	7642.7	7625.0	7614.6
7	8960.0	8932.5	8911.5
8	9146.2	9105.7	9095.7
9	10247	10227	10208

anharmonic-oscillator potential calculated using both modified [Eqs. (10) and (15)] and usual [Eqs. (5) and (18)] WKB methods for energies both below and above the barrier height (taken to be zero). The potential used is the same as what is called V_2 in Ref. 11 and was also used by Ezawa *et al.*[20] to compute the eigenvalues employing more accurate numerical methods. A comparison of the WKB results with the values obtained by Ezawa *et al.* clearly shows the marked improvement of the modified WKB values over those due to the usual WKB method. As expected, the WKB results improve with increasing quantum number with the exception of the $n=2$ level. Here, the modified WKB value is at least of the correct sign, unlike the usual one, but is numerically inaccurate, perhaps, due to the very close proximity of two (complex) turning points.

Table V shows the corresponding results for another potential curve shown in Fig. 3, which is a superposition of a Gaussian hump and a Morse potential. We show only those eigenvalues that correspond to four real turning points and compare these with numerically calculated eigenvalues.[12] The required integrals in this case have been evaluated numerically using Gaussian quadrature. Once again, an overall improvement due to the application of the modified WKB formalism may be noted.

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