Electron capture by an electric dipole in two dimensions

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The question of the existence of a nonzero minimum dipole moment D_0 that can sustain an electron bound state for an electric dipole in two dimensions is examined both classically and quantum mechanically. The results suggest that in the latter case, $D_0 \lesssim 0.209$ compared to the Fermi-Teller value 0.904 for three dimensions (in atomic units).

I. INTRODUCTION

The question of the existence of a bound state for an electron in the field of an electric dipole, in three dimensions, has an interesting history. In 1955, G. Handler [1] pointed out that the electron bound states for a finite dipole, consisting of equal and opposite point charges $\pm e$ separated by a distance R and thus having dipole moment $D = eR$ could be treated by separating the Schrödinger equation in prolate spheroidal coordinates as suggested by Jaffé and Baber and Hassé [2,3]. For the units used here, $\hbar = 1$, $e^2 = 2$, $m_e = 1$, the unit dipole moment is 2.52 debye, the energy unit is the Rydberg, and distances are measured in Bohr radii. Handler estimated the binding energy E for $D = 0.424, 0.707, 0.990$ and pointed out that E depends on D and not separately on R. Although he did not indicate this explicitly, the consequence is that $E(D)$ is the same for a finite and a point dipole. Stimulated by this work and sensing its usefulness for studying defects in solids, a few years later Wallis, Herman, and Milnes [4] carried out a much more extensive numerical analysis for the ground state and several excited states with $1.188 < D < 42.426$. At the lower limit their procedure became unstable and they raised, but left open, the question as to whether there is a minimum value $D_0 > 0$ which can support a bound state.

In the 1960's there was renewed interest in explaining the large electron cross sections observed in Townsend scattering [5] for molecules possessing large dipole moments (e.g., $D_{\mathrm{H_2O}} = 0.990$), but not for less polar molecules (e.g., $D_{\mathrm{H_2S}} = 0.566$). This led back to the question raised in [4] and resulted in an explosion of papers treating the problem (most of these are listed in [6]). The conclusion is that [7] $D_0 = 0.904\,128$.

In 1968, after a seminar by one of the authors of [7], a participant mentioned that in 1950 Wightman [8] had quoted a paper by Fermi and Teller [9] on μ-meson scattering containing the line "… when the mesotron approaches the [hydrogen] nucleus to a distance of 0.639 Bohr radii, the binding energy of the electron becomes zero." This paper contains no indication of how this value was obtained. However, we can infer from [8] that the question was presented to Wightman as a thesis project by John Wheeler; the derivation is summarized in [8]. Historical research by Turner [6] showed that Fermi's notebooks contain several pages de-

voted to the calculation, but that he stopped short of arriving at the critical value. Turner also reports that in a private communication Teller told him that he probably worked out the value. This is likely the case, since Teller had much earlier carried out a very similar calculation for the ground state of the hydrogen molecular ion [10].

In this paper we present an investigation of D_0 in two dimensions, which from phase space considerations, one expects to be less than its value in three dimensions. Since semiconductor quantum wells can be engineered to contain a low density two-dimensional electron gas, the trapping of electrons in a dipole potential set up by a distribution of ionized donors and acceptors could have profound effects on the properties of these systems. It is surprising that this elementary problem has not been examined previously.

Our note is organized as follows: In Sec. II the problem is examined by classical mechanics and we conclude that $D_0 = 0$, i.e., any dipole can support a bound state. In Sec. III a simple quantum mechanical variational estimate is made to obtain an upper bound for D_0. In Sec. IV the Schrödinger equation is set up and separated in elliptic cylindrical coordinates. In Sec. V numerical results are presented for the ground state and we conclude with a brief discussion.

II. CLASSICAL CALCULATION

In the (x, y) plane let charge e be located at $(-R/2, 0)$ and $-e$ be located at $(R/2, 0)$ and let r_1 be the distance of an electron at (x, y) from the first and r_2 be its distance from the second charge. In confocal elliptic coordinates defined by $\xi = (r_1 + r_2)/R$, $\eta = (r_1 - r_2)/R$,

$$x = \frac{R}{2}\xi\eta \quad \text{and} \quad y = \pm \frac{1}{2}R\sqrt{(\xi^2 - 1)(1 - \eta^2)}. \quad (1)$$

Therefore, the kinetic energy is, in atomic units,

$$K = \frac{1}{4}(\dot{x}^2 + \dot{y}^2) = \frac{R^2}{16}(\xi^2 - \eta^2)\left[\frac{\dot{\xi}^2}{\xi^2 - 1} + \frac{\dot{\eta}^2}{1 - \eta^2}\right], \quad (2)$$

and the potential energy is

$$V = 2\left(\frac{1}{r_2} - \frac{1}{r_1}\right) = \frac{8\eta}{R(\xi^2 - \eta^2)}. \quad (3)$$

The canonical momenta are

$$p_1 = \frac{\partial K}{\partial \dot{\xi}} = \frac{\partial W}{\partial \xi} = \frac{R^2}{8}(\xi^2 - \eta^2)\frac{\dot{\xi}}{\xi^2 - 1}, \tag{4}$$

$$p_2 = \frac{\partial K}{\partial \dot{\eta}} = \frac{\partial W}{\partial \eta} = \frac{R^2}{8}(\xi^2 - \eta^2)\frac{\dot{\eta}}{1 - \eta^2}, \tag{5}$$

where $W(\xi, \eta)$ is the transformation function. The Hamilton-Jacobi equation

$$(\xi^2 - 1)\left(\frac{\partial W}{\partial \xi}\right)^2 + p^2\xi^2 + (1 - \eta^2)\left(\frac{\partial W}{\partial \eta}\right)^2 - p^2\eta^2 + 2R\eta = 0, \tag{6}$$

with $p^2 = -1/4R^2E$, where $E < 0$ is the (bound state) energy, is clearly separable by $W(\xi, \eta) = W_1(\xi) + W_2(\eta)$. Writing the separation constant A^2, we have

$$(\xi^2 - 1)p_1^2 + p^2\xi^2 - A^2 = 0, \tag{7}$$

or

$$p_1 = \pm \sqrt{\frac{A^2 - p^2\xi^2}{\xi^2 - 1}}. \tag{8}$$

Since the momentum must be real and $\xi \geq 1$, we have $1 \leq \xi \leq A/p$. Thus for all $E < 0$, the ξ coordinate is bounded, which means that no matter how small R is, there is a bounded orbit. Thus classically $D_0 = 0$.

III. QUANTUM MECHANICAL CALCULATION: VARIATIONAL APPROXIMATION

Let the polar coordinates of the electron be r and ϕ. In atomic units the electron Hamiltonian is

$$H = -\partial_r^2 - \frac{1}{r}\partial_r - \frac{1}{r^2}\partial_\phi^2 - \frac{2}{\sqrt{(R/2)^2 + r^2 + rR\cos\phi}}$$

$$+ \frac{2}{\sqrt{(R/2)^2 + r^2 - rR\cos\phi}}. \tag{9}$$

A simple, but reasonable, trial wave function is

$$\psi(r, \phi) = e^{-ar}(1 - br\cos\phi), \tag{10}$$

with variational parameters $a, b > 0$. One obtains for the energy functional

$$E(R, a, b) = \frac{a^2}{2\pi(a^2 + 3b^2/4)}\left[a^2 + \frac{3\pi^2}{2}b^2 + 32a^2bF(R, a)\right], \tag{11}$$

where, in terms of the complete elliptic integrals **K** and **E**,

$$F(a, R) = R^2\left[\int_0^1 ue^{-aRu}[\mathbf{E}(u) - \mathbf{K}(u)]du\right.$$

$$\left. + \int_1^\infty u^2e^{-aRu}[\mathbf{E}(1/u) - \mathbf{K}(1/u)]du\right]. \tag{12}$$

By exploring this numerically we found that on varying a the minimum value for small fixed R occurs for b near 0.5 and by plotting

$$E(R, a, 1/2) = \frac{a^2}{2\pi(a^2 + 3/16)}\left[a^2 + \frac{3\pi^2}{8} + 16a^2F(R, a)\right] \tag{13}$$

against a for fixed R, we obtained the values

$$a = 1.5, \quad b = 1/2, \quad \text{and} \quad R_{min} = 0.35, \tag{14}$$

where R_{min} is the separation at which the energy minimum vanishes. Hence we obtain the variational upper bound $D_0 \leq 0.495$. As we shall see, this is too large by about a factor of 2, but does confirm that it is less than the three-dimensional value.

IV. PLANAR TWO CENTER SCHRöDINGER EQUATION

Again, let charges Z_1e and Z_2e be located at $x = -R/2$ and $x = R/2$, respectively. The Hamiltonian for an electron is

$$\mathcal{H} = -\nabla^2 - 2\left(\frac{Z_1}{r_1} + \frac{Z_2}{r_2}\right). \tag{15}$$

The electronic energy is $E + 2Z_1Z_2/R$. In the confocal elliptic coordinates $1 \leq \xi = (r_1 + r_2)/R < \infty$, $-1 \leq \eta = (r_1 - r_2)/R \leq 1$, $z = 0$, the Laplacian is

$$\nabla^2 = \frac{4}{R^2(\xi^2 - \eta^2)}\left[\sqrt{\xi^2 - 1}\frac{\partial}{\partial \xi}\left(\sqrt{\xi^2 - 1}\frac{\partial}{\partial \xi}\right)\right.$$

$$\left. + \sqrt{1 - \eta^2}\frac{\partial}{\partial \eta}\left(\sqrt{1 - \eta^2}\frac{\partial}{\partial \eta}\right)\right]. \tag{16}$$

One finds that the Schrödinger equation separates, with $\Psi(\xi, \eta) = X(\xi)S(\eta)$, into

$$\sqrt{\xi^2 - 1}[\sqrt{\xi^2 - 1}X']' + [A - p^2\xi^2 + R(Z_1 + Z_2)\xi]X(\xi) = 0, \tag{17}$$

and

$$\sqrt{1 - \eta^2}[\sqrt{1 - \eta^2}S']' - [A - p^2\eta^2 + R(Z_1 - Z_2)\eta]S(\eta) = 0. \tag{18}$$

We have introduced a separation constant A and the energy parameter $p^2 = -R^2E/4$. To specify boundary conditions, we note that $\xi = 1$, $\eta = -1, 1$ are regular singular points, at which the respective functions must be finite, and $\xi = \infty$ is an irregular singular point at which the wave function must vanish. The initial conditions are, from a series analysis, $X(1) = 1$, $X'(1) = -[A - p^2 + R(Z_1 + Z_2)]$, $S(-1) = 1$, and $S'(-1) = A - p^2 - R(Z_1 - Z_2)$.

Recently, Bondar, Hnatich, and Lazur [11] have carried out the separation of the Schrödinger equation for the two-Coulomb centers problem in $d \geq 2$ spatial dimensions in hyperspheroidal coordinates. For small intercenter separation in $d = 2$ they find it convenient to introduce a new set of functions, the angular Coulomb elliptic functions, which are closely related to the Mathieu functions, for which they present a number of formal expansions. For the case they

study, the hydrogen molecular ion, they find that these are useful for obtaining the excited states ($n \geqslant 5$), but that for the ground state, as we suggest here, numerical integration is more efficient.

To illustrate our numerical procedure, we first examine the two-dimensional hydrogen molecular ion $Z_1 = Z_2 = 1$ for which the ground state has been studied by Zhu and Xiong [12]. This gives us the equations

$$(1 - \eta^2)S'' - \eta S' - [A - p^2 \eta^2]S(\eta) = 0, \qquad (19a)$$

$$(\xi^2 - 1)X'' + \xi X' + [A - p^2 \xi^2 + 2R\xi]X(\xi) = 0. \qquad (19b)$$

Note that if one introduces new variables by $\xi = \cosh u$, $\eta = \cos t$ one obtains a pair of Mathieu equations

$$S''(t) - (A - p^2 \cos^2 t)S(t) = 0, \qquad (20a)$$

$$X''(u) + (2R \cosh u + A - p^2 \cosh^2 u)X(u) = 0. \qquad (20b)$$

Although we make no use of them here, in principle the system (20) can be solved in terms of the 2π-periodic Mathieu functions $ce_{0,1}$, where $A(p^2)$ is to be determined as a characteristic constant following the procedure outlined in [13], but this is difficult to deal with numerically and it is simpler to proceed as follows: Choose p^2 and integrate Eq. (19a) from $\eta = -t_0$ varying A to obtain $S'(0) = 0$ (for the ground state S is even) with no intervening nodes. Here, since $\eta = -1$ is a singular point, we start from $t_0 = -1 + 10^{-8}$ computing the values at this point from the first two terms of the series expansion. This gives us a table of pairs (p^2, A). Next introduce each pair into Eq. (19) and integrate numerically from $\xi = 1 + 10^{-8}$ while varying R to obtain $X(a) = 0$ for a sufficiently large value of $a > 0$ to ensure numerical stability. Although A vanishes with p^2, the behavior is singular and it does not appear possible to find this limiting solution simply by setting A and p^2 in Eq. (19) [as well as in Eq. (21) below]. The solution was carried out by the short interactive MATHEMATICA procedure in the Appendix. Some results are shown in Table I.

The relation between the electronic energy $E + 2/R$ and R is sketched in Fig. 1. We find that the energy minimum $E_0 = -5.645$ occurs for $R = 0.513$ in close agreement with the corresponding values from [11]: $E_0 = -5.646$ at $R = 0.511$.

V. QUANTUM CALCULATION OF THE PLANAR DIPOLE GROUND STATE

In this case, we have $Z_1 = -Z_2 = 1$, so our equations become

$$(\xi^2 - 1)X'' + \xi X' + (A - p^2 \xi^2)X(\xi) = 0, \qquad (21a)$$

$$(1 - \eta^2)S'' - \eta S' - (A - p^2 \eta^2 + \sqrt{2}D\eta)S(\eta) = 0, \qquad (21b)$$

subject to $X(1) = 1$, $X'(1) = -A + p^2$, $S(-1) = 1$, and $S'(-1) = A - p^2 - \sqrt{2}D$. We ignore the electrostatic term $2/R$. The system is essentially a two-dimensional hydrogen atom located at $(-R/2, 0)$ perturbed by an "electron" at $(R/2, 0)$, so the ground state wave function has no symmetry about the ori-

TABLE I. Hydrogen molecular ion binding energies in Rydbergs, with their corresponding values of the parameters p^2, A, and R in Bohr radii.

p^2	A	R	$E + 2/R$
0.01	0.005003	0.0509	23.8519
0.05	0.025078	0.1185	2.63098
0.10	0.050312	0.1731	−1.79551
0.20	0.101250	0.2569	−4.33972
0.30	0.152811	0.3262	−5.14127
0.40	0.204994	0.3881	−5.47099
0.50	0.257799	0.4451	−5.60182
0.60	0.311222	0.4986	−5.64276
0.62	0.321981	0.5090	−5.64464
0.63	0.327370	0.5141	−5.64466
0.64	0.332764	0.5192	−5.64457
0.70	0.365261	0.5494	−5.63718
0.80	0.419913	0.5980	−5.60421
0.90	0.475174	0.6447	−5.56137

gin, except for $y \rightarrow -y$, nor can it have any nodes. Once again, Eq. (21a) is Mathieu's equation [13]. As a quantizing condition we require that $X(\xi)$ vanish for large $\xi > a$, where a was initially set at 200 and then doubled as necessary to check stability in determining A (reaching $a = 128\,000$ at one point). The wave function magnitude is reduced in the vicinity of the negative charge, and therefore has a minimum at $\eta = 1$, so we use as a second condition $S'(1) = 0$. Again, since only the dipole moment D occurs in the equations and the boundary conditions, the energy does not depend separately on R, so it must be the same for a point dipole (directed along the x axis) and a finite dipole.

By numerical integration using the MATHEMATICA procedure in the Appendix we find the results displayed in Fig. 2. Selected values are given in Table II.

At very small values of D it becomes necessary to integrate over such a large range of ξ that we felt values obtained for $p^2 < 3 \times 10^{-6}$ would not be reliable.

At large values of D, the ground state energy approaches $E = -4$, which is that for a two-dimensional (2D) hydrogen
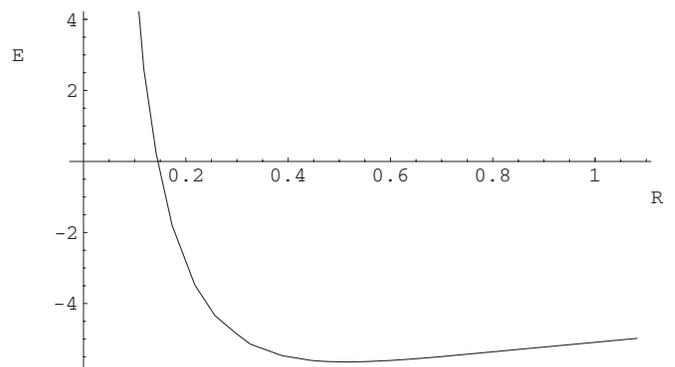
FIG. 1. Energy in Rydberg vs R in Bohr radii for a planar hydrogen molecular ion.
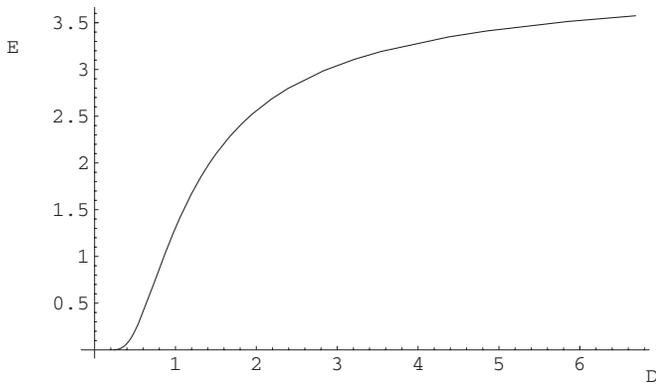
FIG. 2. Ground state energy in Rydberg vs D in debye for a finite dipole.

atom, as expected physically. By linear interpolation of the lowest values in Table II we estimate that $D_0 l 0.209$.

VI. DISCUSSION

We have examined, from various points of view, the existence of a positive minimum dipole moment D_0 that will bind an electron in two dimensions and estimate that for a finite dipole the quantum mechanical value is at most 0.209 in atomic units. This is smaller than the three-dimensional value 0.904 found by Fermi and Teller as is to be expected from phase space considerations. By arguing that the energy depends only on D the curve of binding energy must be the same for a finite as for a point dipole. However, our result has not been proven rigorously and there is, for example, the

TABLE II. Finite dipole ground state energies E in Rydbergs, with their corresponding values of the parameters p^2, and A in Bohr radii, and the dipole values D in Debye.

p^2	A	D	$-E$
3×10^{-6}	0.047781	0.2231	0.00048
4×10^{-6}	0.049742	0.2278	0.00062
5×10^{-6}	0.051349	0.2316	0.00074
6×10^{-6}	0.052718	0.2348	0.00087
1×10^{-5}	0.056861	0.2443	0.00134
1×10^{-4}	0.083236	0.2987	0.00897
5×10^{-4}	0.114230	0.3539	0.03194
0.001	0.133156	0.3845	0.05411
0.002	0.157205	0.4209	0.09091
0.003	0.174424	0.4455	0.12049
0.004	0.188418	0.4648	0.14811
0.005	0.200467	0.4810	0.17287
0.01	0.246265	0.5387	0.27564
0.10	0.592531	0.8762	1.04195
0.50	1.409073	1.4167	1.99296
1.00	2.211411	1.8187	2.41890
5.00	7.464567	3.5396	3.19177
10.00	13.39605	4.8420	3.41116

remote possibility that the ground state energy might have nonanalytic behavior such as e^{-c/D^2} for $D \rightarrow 0$, which would lie "below the radar" of our numerical procedure. This could be settled by solving the Schrödinger equation for a point dipole. We have found that the latter separates in polar coordinates to give a Bessel function of r times a Mathieu function of ϕ, but have not yet succeeded in working out the ground state.

Note added in proof. Recently, the paper [16] appeared in which the two-dimensional Schrödinger equation is solved for the critical case ($E=0$) and shows that $D_0=0$. Therefore the ground state energy in the range $0 < D < 0.2231$ remains to be examined. In conclusion we merely note that an electron is more easily trapped by an ionized impurity complex in two dimensions than in three, but defer specific applications until other effects, such as screening [14,15], are accounted for; this will be dealt with elsewhere.

APPENDIX: MATHEMATICA ROUTINES

The MATHEMATICA routine used to generate Fig. 1 and Table I is the following:

```
p^2=37; A=0.04943042775949;
NDsolve[{(1−t^2)S'[t]−t S'[t]−
        (A−p^2 t^2)S[t]==0,
        S[−1+10^{−8}]==1+(A−p^2) 10^(−8),
        S'[−1+10^(−8)]==A−p^2},
        S[t],{t,−1+10^(−8),0.99999999}]
s[t_]:= Evaluate[S[t]/.%]; s'[0]
R=0.34937
NDsolve[{(x^2−1)X''[x]+x X'[x]+
        (A−p^2 x^2+2 R x)X[x]==0,
    X[1+10^(−8)]==1−(A−p^2+2R)10^(−8),
    X'[1+10^(−8)]==−A+p^2−2 R},
    X[x],{x,1+10^(−8),200}]
g[x_]:= Evaluate[X[x]/.%]; g'[200]
E=−4 p^2/R^2
```

The MATHEMATICA routine for Fig. 2 and Table II is

```
p^2=20; A=24.7100590
NDSolve[{(x^2−1) X''[x]+x X'[x]+
        (A−p^2 x^2)X[x]==0,
        X[1+10^(−8)]==1−(A−p^2)10^(−8),
        X'[1+10^(−8)]==−(A−p^2)},
        X[x],{x,1+10^(−8),200}]
```

```
g[x_] := Evaluate[X[x]/. %]; g′[200]
R = 4.73090;
NDSolve[{(1−t^2)S″[t]−t S′[t]−
     (A−p^2 t^2+2 R t) S[t]==0,
     S[−1+10^(−8)]==1+(A−p^2−2 R)10^(−8),
```

```
     S′[−1+10^(−8)]==A−p^2−2 R},
     S[t],{t,−1+10^(−8),0.999999999}];
s[t_] := Evaluate[S[t]/. %]; s′[0.999999999]
d = Sqrt[2] R
En = −4p^2/R^2
```

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