An electron in a finite-dipole potential

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Some structural properties of the energy eigenfunctions of an electron in a finite-dipole field are analyzed, in particular the asymptotic behavior when the electron is far away, and the coalescence and cusp properties when it is close to the dipole charges. Model wave functions incorporating these properties are developed, which give accurate values for the energies and some other quantities, and a useful insight into the physical structure of the system. Critical radius for the existence of the bound states is obtained from the Wentzel–Kramers–Brillouin approach. These considerations are extended to the description of the system in two dimensions. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1652505]

I. INTRODUCTION

The motion of an electron in the field of a finite-dipole is an important problem in quantum mechanics. In the initial stages, the model was considered by Fermi and Teller,[1] and by Wightman,[2] for analyzing the effect of a slowly moving π^- or μ^- on the binding of an electron. It has been established[1–6] that there is a critical separation between the dipole charges, known as the Fermi–Teller radius, below which there are no bound states of an electron in the dipole field. It has served as a useful model for the description of dipole-bound anions.[7] The dipole potential has also been considered as a model for describing the scattering of an electron by polar molecules,[8–11] and by ion pairs in semiconductors.[12] Here, the dipole tail leads to significant threshold phenomena[13] and appearance of resonances. The bound state energies have been analyzed from different approaches, with continued fractions,[14] variational calculation,[15] WKB approximation,[16] and analytical description.[17] Recently,[18] relativistic effects have been considered by using the Dirac equation. Surprisingly, however, what is missing is an analysis of the structural properties of the basic system of an electron in a finite-dipole field, and the development of simple model wave functions. These are essential for our developing a physical insight into the properties of the system.

Here, we analyze the structural properties of the energy eigenfunctions of an electron in a finite-dipole field, the asymptotic behavior when it is far away from the dipole, and the coalescence and cusp properties when it is close to the dipole charges. We also consider the virial theorem which is very useful in the description of an excited state. Some simple, model wave functions are developed incorporating these properties. These wave functions provide accurate values for the energies and some position variables, and provide a useful insight into their physical structure. We then analyze the critical value of the dipole separation for the bound states to exist, in terms of the WKB approximation. This provides a simple, clear, and accurate description of the domain for the existence of bound states. Finally these considerations are extended to the dynamics of an electron in a finite-dipole potential in two dimensions, which gives a simple illustration of the importance of dimensionality in quantum descriptions, and interdimensional relations.[19] Atomic units $e=m=\hbar=1$ are used throughout.

II. SOME GENERAL PROPERTIES

We begin by describing some general properties of an electron in a finite-dipole potential, in terms of prolate spheroidal coordinates. With the foci of the ellipse at $(0,0,R/2)$ and $(0,0,-R/2)$, these coordinates u,v,ϕ are

$$u=\frac{r_a+r_b}{R}, \quad v=\frac{r_a-r_b}{R}, \quad \phi,$$
$$r_a=|\mathbf{r}-\tfrac{1}{2}\mathbf{R}|, \quad r_b=|\mathbf{r}+\tfrac{1}{2}\mathbf{R}|, \tag{2.1}$$

where $\mathbf{r}$ is the vectorial position of the electron from the origin, and $\mathbf{R}=R\mathbf{k}$ with $\mathbf{k}$ being a unit vector in the z direction.

A. Separable Schrödinger equation

For the finite dipole, we take the positive charge Z at $(0,0,-R/2)$, and the negative charge $-Z$ at $(0,0,R/2)$. Then the potential for the electron in the dipole potential is

$$V=\frac{Z}{r_a}-\frac{Z}{r_b}. \tag{2.2}$$

The corresponding Schrödinger equation in the spheroidal coordinates is

$$-\frac{1}{2}\left(\frac{2}{R}\right)^2\frac{1}{(u^2-v^2)}\left[\frac{\partial}{\partial u}(u^2-1)\frac{\partial}{\partial u}+\frac{\partial}{\partial v}(1-v^2)\frac{\partial}{\partial v}+\left(\frac{1}{u^2-1}+\frac{1}{1-v^2}\right)\frac{\partial^2}{\partial\phi^2}\right]\psi+\frac{2Z}{R}\left(\frac{1}{u+v}-\frac{1}{u-v}\right)\psi=E\psi. \tag{2.3}$$

The equation is separable, and by writing

$$\psi(u,v,\phi)=(u^2-1)^{|m|/2}(1-v^2)^{|m|/2}F(u)G(v)e^{im\phi} \tag{2.4}$$

we get

$$(u^2-1)\frac{d^2F}{du^2}+2(|m|+1)u\frac{dF}{du}+\frac{1}{2}R^2E(u^2-1)F$$
$$=-SF, \quad u\geqslant 1, \tag{2.5}$$

$$(v^2-1)\frac{d^2G}{dv^2}+2(|m|+1)v\frac{dG}{dv}-2ZRvG$$
$$+\frac{1}{2}R^2E(v^2-1)G=-SG, \quad |v|\leqslant 1, \tag{2.6}$$

where S is the separation constant. It may be noted that the states are characterized by the number of nodes in $F(u)$, in $G(v)$, and the value of m, (n_u,n_v,m). We now consider some specific properties of the solutions.

B. Asymptotic behavior

For analyzing the asymptotic behavior of $F(u)$, we first note that

$$\frac{d^2F}{du^2}\to-\frac{1}{2}R^2EF \quad \text{for} \quad u\to\infty \tag{2.7}$$

which implies that

$$F(u)\to e^{-\alpha u}, \quad \alpha=R(-E/2)^{1/2}, \quad \text{for } u\to\infty. \tag{2.8}$$

We therefore consider an asymptotic expansion

$$F=e^{-\alpha u}\sum_{i=0} C_i u^{\eta-i} \quad \text{for } u\to\infty. \tag{2.9}$$

Substituting this in Eq. (2.5) and equating the coefficients of successive power terms in u, we get from the first two terms,

$$F(u)\to u^{\kappa}e^{-\alpha u}, \quad u\to\infty,$$
$$\alpha=R(-E/2)^{1/2}, \tag{2.10}$$
$$\kappa=-(|m|+1).$$

These relations determine the leading behavior for u in the asymptotic region.

It is interesting to consider the asymptotic behavior in terms of spherical coordinates also. Since the dipole potential in Eq. (2.2) has the behavior $\sim 1/r^2$ for large r, we have

$$\frac{d^2}{dr^2}(r\psi)+2E(r\psi)=O(1/r^2) \quad \text{for } r\to\infty. \tag{2.11}$$

This leads to the behavior

$$\psi(\mathbf{r})\to\frac{1}{r}e^{-(-2E)^{1/2}r} \quad \text{for } r\to\infty, \tag{2.12}$$

which is equivalent to the asymptotic behavior in Eq. (2.10). This provides a useful physical understanding of the asymptotic behavior.

C. Coalescence and cusp conditions

When the electron is close to the positive charge at $r_b=0$, one has $u\to 1$ and $v\to 1$. In this limit Eqs. (2.5) and (2.6) lead to

$$2(|m|+1)\frac{1}{F}\frac{dF}{du}\bigg|_{u=1}=-S,$$
$$2(|m|+1)\frac{1}{G}\frac{dG}{dv}\bigg|_{v=1}-2ZR=-S, \tag{2.13}$$

which together imply

$$\frac{1}{F}\frac{dF}{du}\bigg|_{u=1}-\frac{1}{G}\frac{dG}{dv}\bigg|_{v=1}=-\frac{ZR}{|m|+1}. \tag{2.14}$$

Similarly, when the electron approaches the negative charge at $r_a=0$, one has $u\to 1$ and $v\to -1$. Taking these limits, Eqs. (2.5) and (2.6) lead to

$$\frac{1}{F}\frac{dF}{du}\bigg|_{u=1}+\frac{1}{G}\frac{dG}{dv}\bigg|_{v=-1}=\frac{ZR}{|m|+1}. \tag{2.15}$$

The relations in Eqs. (2.14) and (2.15) may be described as the coalescence and cusp conditions[20] when the electron approaches positive or negative charges. Effectively, these relations are the Kato conditions[21] with the angular averaging replaced by the averaging over two angles.[20]

D. Virial theorem

The virial theorem for the energy eigenstates is a very useful relation especially for the excited states. It follows from the property

$$\langle\psi|[H,O]|\psi\rangle=0, \tag{2.16}$$

where $|\psi\rangle$ is an energy eigenstate and O is any operator. Since the interaction of the electron with the positive charge at $r_b=0$ provides the binding force, we take $O=\mathbf{r}_b\cdot\mathbf{p}$ which then leads to

$$\langle\psi|\frac{p^2}{2}|\psi\rangle=\frac{1}{2}\langle\psi|Z\left(\frac{1}{r_b}-\frac{\mathbf{r}_a\cdot\mathbf{r}_b}{r_a^3}\right)|\psi\rangle. \tag{2.17}$$

In terms of the spheroidal coordinates, it takes the form

$$\langle\psi|\frac{p^2}{2}|\psi\rangle=\langle\psi|Z\left(\frac{1}{R(u-v)}-\frac{(u^2+v^2-2)}{R(u+v)^3}\right)|\psi\rangle. \tag{2.18}$$

This relation will be used in developing model wave functions for the excited states.

E. Numerical solutions

Elaborate numerical solutions have been obtained from different approaches.[14,15] Here we describe a simple approach for obtaining numerical solutions to Eqs. (2.5) and (2.6). These equations have two parameters, energy E and separation constant S which are determined by the requirement that the solutions are bounded and nonsingular in the physical domains, $u:(1,\infty)$, and $v:(-1,1)$.

For obtaining the solutions for $F(u)$ and $G(v)$, it is convenient to use the variables

$$u_1=u-1, \quad v_1=v-1 \tag{2.19}$$

in terms of which Eqs. (2.5) and (2.6) lead to

$$u_1(u_1+2)\frac{d^2F}{du_1^2}+2(|m|+1)(u_1+1)\frac{dF}{du_1}+\left[\frac{1}{2}R^2Eu_1(u_1+2)+S\right]F=0, \tag{2.20}$$

$$v_1(v_1+2)\frac{d^2G}{dv_1^2}+2(|m|+1)(v_1+1)\frac{dG}{dv_1}+\left[-2ZR(v_1+1)+\frac{1}{2}R^2Ev_1(v_1+2)+S\right]G=0. \tag{2.21}$$

With the series expansions

$$F=\sum_{i=0} C_i u_1^i, \qquad G=\sum_{i=0} D_i v_1^i, \tag{2.22}$$

we get the recursion relations

$$C_{i+2}=-\frac{[(i+1)(i+2|m|+2)+S]C_{i+1}+R^2EC_i+\frac{1}{2}R^2EC_{i-1}}{2(i+2)(i+|m|+2)}, \tag{2.23}$$

$$D_{i+2}=-\frac{[(i+1)(i+2|m|+2)-2ZR+S]D_{i+1}+(-2ZR+R^2E)D_i+\frac{1}{2}R^2ED_{i-1}}{2(i+2)(i+|m|+2)}. \tag{2.24}$$

Using this expansion in Eq. (2.21) at $v_1=-2$ leads to the condition

$$\sum_{i=0} D_i(-2)^i[(|m|+1)i+2ZR+S]=0. \tag{2.25}$$

This is one constraint on the parameters E and S. For obtaining the bounded solutions for $F(u)$, we first note that

$$C_{i+1}/C_i \to -1/2 \quad \text{for } i\to\infty, \tag{2.26}$$

so the series converges for $u_1<2$. We use the series in Eq. (2.22) to obtain the solutions at $u_1=1/2-\Delta$ and $u_1=1/2$ for small Δ. The solution is continued to higher values of u_1 by converting Eq. (2.20) into a difference equation which leads to

$$F(u_1+\Delta)=\frac{(2h_2-h_0\Delta^2)F(u_1)+(-h_2+h_1\Delta/2)F(u_1-\Delta)}{h_2+h_1\Delta/2} \tag{2.27}$$

with

$$h_0=R^2Eu_1(u_1+2)/2+S, \quad h_1=2(|m|+1)(u_1+1), \quad h_2=u_1(u_1+2). \tag{2.28}$$

We then require that $F(u_1)\to 0$ for $u_1\to\infty$ which imposes another condition on E and S. Thus the separation constant S and energy E are determined from the condition in Eq. (2.25), and the condition that the continued solution for $F(u_1)$ in Eq. (2.27) vanishes at infinity for which we can take a suitable large value of u_1. The energies we have obtained from this simple approach agree with the accurate values of Refs. 14 and 15.

III. MODEL WAVE FUNCTIONS

We now develop some model wave functions incorporating the general properties we have discussed, which give fairly accurate values for the energy and some spatial properties of an electron in a finite-dipole field, and an insight into the physical structure. Here onwards we will take $Z=1$.

A. Ground state wave function

For the ground state, we consider a wave function

$$\psi_0=NF(u)G(v), \quad F(u)=\frac{1}{1+au}e^{-\alpha u}, \quad G(v)=(1+bv)e^{\beta v}, \quad \alpha=R(-E/2)^{1/2}, \tag{3.1}$$

with N being the normalization constant. This wave function incorporates the asymptotic behavior in Eq. (2.10) with $m=0$. The parameters β and b are determined by using the coalescence and cusp conditions in Eqs. (2.14) and (2.15) which imply

$$-\alpha-\frac{a}{1+a}-\beta-\frac{b}{1+b}=-R, \qquad -\alpha-\frac{a}{1+a}+\beta+\frac{b}{1-b}=R. \tag{3.2}$$

These equations lead to

$$b=\left[\frac{\alpha+a/(1+a)}{1+\alpha+a/(1+a)}\right]^{1/2}, \qquad \beta=\alpha+R+\frac{a}{1+a}-\frac{b}{1-b}. \tag{3.3}$$

TABLE I. Values of the parameter a, normalization constant N, energy E, and expectation values $\langle r_b\rangle$, $\langle 1/r_b\rangle$, and $\langle r_a\rangle$, from the model wave function in Eq. (3.1) for the ground state, along with the accurate values from Ref. 15 in brackets, for some values of R.

R	a	N	$-E$	$\langle r_b\rangle$	$\langle 1/r_b\rangle$	$\langle r_a\rangle$
10.0	0.89	0.501	0.40023	1.504	0.997	10.14
			(0.40023)	(1.502)	(0.999)	(10.14)
8.0	0.87	0.488	0.37555	1.508	0.996	8.19
			(0.37555)	(1.505)	(0.998)	(8.19)
6.0	0.83	0.463	0.33507	1.521	0.990	6.28
			(0.33508)	(1.517)	(0.993)	(6.28)
5.0	0.78	0.436	0.30353	1.540	0.982	5.37
			(0.30355)	(1.533)	(0.987)	(5.36)
4.0	0.75	0.412	0.25826	1.582	0.965	4.49
			(0.25829)	(1.572)	(0.970)	(4.49)
3.0	0.69	0.367	0.19009	1.702	0.916	3.74
			(0.19015)	(1.689)	(0.924)	(3.74)
2.0	0.59	0.280	0.08808	2.200	0.754	3.43
			(0.08813)	(2.191)	(0.759)	(3.43)
1.5	0.489	0.192	0.03144	3.332	0.538	4.17
1.3	0.418	0.139	0.01397	4.684	0.400	5.39
1.1	0.317	0.0763	3.347×10^{-3}	8.755	0.230	9.32
1.0	0.250	0.0450	9.758×10^{-4}	15.18	0.141	15.7
			(1.025×10^{-3})	(16.17)	(0.129)	(16.7)
0.9	0.163	0.0177	1.204×10^{-4}	39.7	0.060	40.1

Thus, there is only one independent parameter which we take to be a. The quantity α depends on the energy E as in Eq. (3.1), which is determined iteratively by requiring that the input energy for determining α as in Eq. (3.1) is equal to the expectation value of the output energy

$$E=\frac{\langle\psi_0|H|\psi_0\rangle}{\langle\psi_0|\psi_0\rangle}. \tag{3.4}$$

Only about two or three iterations are required for obtaining an equality to four decimal places. The independent parameter a is determined variationally. It may be noted that the only nontrivial integrals are the u-integrals

$$I_n=\int_1^\infty \frac{e^{-2\alpha u}}{(1+au)^n}du. \tag{3.5}$$

With the substitution $x=(1+au)/(1+a)$ one gets

$$I_n=\frac{e^{2\alpha/a}}{a(1+a)^{n-1}}E_n(z),\quad z=\frac{2\alpha(1+a)}{a}, \tag{3.6}$$

where

$$E_n(z)=\int_1^\infty \frac{e^{-zx}}{x^n}dx \tag{3.7}$$

are the exponential integrals for which one has[22] accurate expressions. The values of the parameter a, normalization constant N, energy E, and the average values of some position variables, are given in Table I. These values obtained from the model wave function based on some local properties are generally close to the accurate values obtained from elaborate variational calculations.[15]

There are some aspects of the solutions which deserve attentions. One point is that for large values of R, the solutions tend to the hydrogenic solutions localized around the point $r_b=0$. In the present case it implies that

$$e^{-\alpha u+\beta v}\to e^{-r_b}\quad \text{for } R\to\infty \tag{3.8}$$

so that

$$\alpha\to\tfrac{1}{2}R,\quad \beta\to\tfrac{1}{2}R,\quad \text{for } R\to\infty. \tag{3.9}$$

For $R=10$, we get $\alpha=4.47$, $\beta=4.58$ which is reasonable. It may also be noted that the virial ratio

$$V_r=\frac{\langle \mathbf{r}_b\cdot\boldsymbol{\nabla}V\rangle}{\langle p^2\rangle} \tag{3.10}$$

which is the ratio of the terms on the right-hand side and left-hand side of Eq. (2.18), should be 1 for the exact energy eigenfunctions. The values of this ratio for our model wave function are 1.00, 1.00, 1.01, 1.00, 0.98 for $R=5$, 3, 2, 1.5, 1.0, respectively, which indicates the good quality of the wave function.

B. Lowest energy state with $m=1$

For the lowest energy state with $m=1$, we take a model wave function

$$\begin{aligned}&\psi_1=N(u^2-1)^{1/2}(1-v^2)^{1/2}F(u)G(v)e^{i\phi},\\ &F(u)=\frac{1}{(1+au)^2}e^{-\alpha u},\\ &G(v)=(1+bv)e^{\beta v},\\ &\alpha=R(-E/2)^{1/2},\end{aligned} \tag{3.11}$$

with N being the normalization constant. This wave function incorporates the asymptotic behavior in Eq. (2.10) with $m=1$. The parameters β and b are determined by the coalescence and cusp conditions in Eqs. (2.14) and (2.15) which imply

TABLE II. Values of the parameter a, normalization constant N, energy E, and expectation values $\langle r_b\rangle$, $\langle 1/r_b\rangle$, and $\langle r_a\rangle$, from the model wave function in Eq. (3.11) for the lowest energy $m=1$ state, and the energies from numerical calculations in brackets, for some values of R.

R	a	N	$-E$	$\langle r_b\rangle$	$\langle 1/r_b\rangle$	$\langle r_a\rangle$
10.0	0.735	0.173	0.03591 (0.03596)	5.92	0.218	12.6
9.0	0.716	0.140	0.02895 (0.02900)	6.27	0.208	12.1
8.0	0.688	0.106	0.02140 (0.02144)	6.86	0.193	11.9
7.0	0.658	0.0742	0.01358 (0.01361)	7.94	0.171	12.2
6.0	0.610	0.0435	6.300×10^{-3} (6.317×10^{-3})	10.4	0.136	13.9
5.0	0.514	0.0156	1.235×10^{-3} (1.237×10^{-3})	19.3	0.079	22.1
4.5	0.423	0.00527	1.79×10^{-4} (1.82×10^{-4})	42.3	0.040	44.7

$$-\alpha-\frac{2a}{1+a}-\beta-\frac{b}{1+b}=-\frac{1}{2}R,$$
$$-\alpha-\frac{2a}{1+a}+\beta+\frac{b}{1-b}=\frac{1}{2}R. \tag{3.12}$$

These equations lead to

$$b=\left[\frac{\alpha+2a/(1+a)}{1+\alpha+2a/(1+a)}\right]^{1/2},$$
$$\beta=\alpha+\frac{1}{2}R+\frac{2a}{1+a}-\frac{b}{1-b}. \tag{3.13}$$

The remaining parameter a is determined variationally. The quantity α depends on the energy E as in Eq. (3.11), which is determined iteratively by requiring that the input energy for determining α is equal to the expectation value of the output energy

$$E=\frac{\langle\psi_1|H|\psi_1\rangle}{\langle\psi_1|\psi_1\rangle}. \tag{3.14}$$

The values of the parameter a, normalization constant N, the energy E, and the average values of some position variables are given in Table II. The energies from the model wave function are close to the values obtained from the numerical analysis described in Sec. II E. The virial ratio in Eq. (3.10) which should be 1 for the exact energy eigenfunctions is again close to 1 for our model wave function. It takes the values 1.01, 1.01, 1.01, 1.00, 0.99 for $R=10$, 8, 6, 5, 4.5, respectively. This indicates the good quality of the wave function based on the general structural properties.

C. First excited state with $m=0$

There is a tendency for the excited states to collapse to the lowest energy state in a variational approach. This we avoid by requiring that the wave function satisfies the virial relation in Eq. (2.18) for the energy eigenstates. For the first excited state with one node in $F(u)$, i.e., $n_u=1$, $n_v=0$, $m=0$, we take a model wave function

$$\psi_{01}=NF(u)G(v),$$
$$F(u)=\frac{1}{(1+au)^2}(1-au)e^{-\alpha u},$$
$$G(v)=(1+bv)e^{\beta v},$$
$$\alpha=R(-E/2)^{1/2}, \tag{3.15}$$

with N being the normalization constant. This wave function has the required the asymptotic behavior in Eq. (2.10) with $m=0$ and has a node at $u=1/a$. The parameters β and b are determined by the coalescence and cusp conditions in Eqs. (2.14) and (2.15) which imply

$$-\alpha-\frac{2a}{1+a}-\frac{a}{1-a}-\beta-\frac{b}{1+b}=-R,$$
$$-\alpha-\frac{2a}{1+a}-\frac{a}{1-a}+\beta+\frac{b}{1-b}=R. \tag{3.16}$$

These equations lead to

$$b=\left[\frac{\alpha+a(3-a)/(1-a^2)}{1+\alpha+a(3-a)/(1-a^2)}\right]^{1/2},$$
$$\beta=\alpha+R+\frac{3a-a^2}{1-a^2}-\frac{b}{1-b}. \tag{3.17}$$

The remaining parameter a is determined by requiring that the virial relation in Eq. (2.18) is satisfied. The quantity α depends on the energy E as in Eq. (3.15), which is determined iteratively by requiring that the input energy for determining α is equal to the expectation value of the output energy

$$E=\frac{\langle\psi_{01}|H|\psi_{01}\rangle}{\langle\psi_{01}|\psi_{01}\rangle}. \tag{3.18}$$

The values of the parameter a, normalization constant N, the energy E, and the average values of some position variables are given in Table III. The energies from the model wave function are close to the values obtained from the numerical analysis described in Sec. II E.

IV. MINIMUM VALUE OF R

The minimum value of R for which bound states exist in a finite-dipole potential, known as the Fermi–Teller radius, is a very interesting quantity which has been analyzed from different approaches..[3–5,17,23] Here we present a simple description in terms of the WKB approach which leads to the correct result.

A. WKB approach

For the bound states in the limit of $E\to0$, the wave functions extend over a wide domain and vary slowly at large distances. Therefore WKB approximation would be applicable in this limit, in particular for the u-variable equation. Substituting the separable form

$$\psi(u,v,\phi)=f(u)g(v)e^{im\phi} \tag{4.1}$$

into the Schrödinger equation in Eq. (2.3), one obtains

TABLE III. Values of the parameter a, normalization constant N, energy E, and expectation values $\langle r_b\rangle$, $\langle 1/r_b\rangle$, and $\langle r_a\rangle$, from the model wave function in Eq. (3.15) for the first excited $m=0$ state with one node in $F(u)$, and the energies from numerical calculations in brackets, for some values of R.

R	a	N	$-E$	$\langle r_b\rangle$	$\langle 1/r_b\rangle$	$\langle r_a\rangle$
10.0	0.8131	0.450	0.05172 (0.05190)	6.26	0.225	14.6
9.0	0.7937	0.399	0.04646 (0.04660)	6.43	0.220	13.8
8.0	0.7697	0.348	0.04054 (0.04075)	6.65	0.213	13.1
7.0	0.7397	0.297	0.03391 (0.03416)	6.97	0.204	12.5
6.0	0.7008	0.244	0.02657 (0.02686)	7.47	0.191	12.1
5.0	0.6489	0.191	0.01868 (0.01900)	8.29	0.173	12.0
4.0	0.5769	0.136	0.01076 (0.01105)	9.87	0.146	12.7
3.0	0.4738	0.081	0.00404 (0.00422)	13.7	0.106	15.7
2.0	0.3345	0.031	0.00043 (0.00045)	30.4	0.051	31.6

$$(u^2-1)\frac{d^2f}{du^2}+2u\frac{df}{du}-\frac{m^2}{u^2-1}f+\frac{1}{2}R^2E(u^2-1)f = -Af, \quad u\geqslant 1, \tag{4.2}$$

$$(v^2-1)\frac{d^2g}{dv^2}+2v\frac{dg}{dv}-\frac{m^2}{v^2-1}g-2ZRvg + \frac{1}{2}R^2E(v^2-1)g=-Ag, \quad |v|\leqslant 1, \tag{4.3}$$

where A is the separation constant. It may noted that taking out the threshold factors of $f(u)$ and $g(v)$, as in Eq. (2.4), leads to Eqs. (2.5) and (2.6) with $S=A+|m|(|m|+1)$. We now apply the WKB approximation to Eq. (4.2).

For $E\to 0$, the wave function in the u-variable extends over a large domain, and we consider Eq. (4.2) for large values of u,

$$\frac{d^2f}{du^2}+\frac{2}{u}\frac{df}{du}-\frac{m^2}{u^4}f+\frac{1}{2}R^2Ef+\frac{A}{u^2}f=0. \tag{4.4}$$

This is similar in structure to the radial equation in spherical coordinates. As in the case of the radial equation for spherical coordinates, to make the WKB approximation more effective,[24] we introduce a variable x,

$$u=e^x \tag{4.5}$$

which leads to

$$\frac{d^2f}{dx^2}+\frac{df}{dx}+e^{2x}\left(\frac{1}{2}R^2E+\frac{A}{u^2}-\frac{m^2}{u^4}\right)f=0. \tag{4.6}$$

Using

$$f=e^{-x/2}\eta \tag{4.7}$$

one obtains

$$\frac{d^2\eta}{dx^2}-\frac{1}{4}\eta+e^{2x}\left(\frac{1}{2}R^2E+\frac{A}{u^2}-\frac{m^2}{u^4}\right)\eta=0. \tag{4.8}$$

The WKB approximation for this equation leads to the usual WKB relation for the energies,

$$\int_1^{u_0}\left[\frac{1}{2}R^2E+\frac{A-1/4}{u^2}-\frac{m^2}{u^4}\right]^{1/2}du=(n_u+1/2)\pi \tag{4.9}$$

with $n_u=0,1,\ldots$. It may be noted that one gets[24] an additional $-1/(4r^2)$ term in the WKB analysis of the radial equation in spherical coordinates also. Clearly, for $A>1/4$ the outer turning point u_0 and the integral in Eq. (4.9) tend to infinity for $E\to 0$, so that one has an infinite number of bound states for $A>1/4$. On the other hand, for $A<1/4$, the integrand is imaginary and there are no bound states. Therefore,

$$A=\tfrac{1}{4} \tag{4.10}$$

is the critical value[3] of the separation constant for the existence of the bound states. It is interesting to observe that this value is independent of the value of m, which has been noted[23] from other considerations. Substituting this value of the separation constant into Eq. (4.3), multiplying by $g(v)$ and integrating, one obtains for $E\to 0$,

$$R_{\min}=\frac{\frac{1}{4}\int g^2dv+\int(1-v^2)\left(\frac{dg}{dv}\right)^2dv+m^2\int\frac{g^2}{1-v^2}dv}{2\int vg^2dv}. \tag{4.11}$$

It allows us to determine the critical value of R for different values of m and different number of nodes in $g(v)$. For model wave functions, this relation gives an upper bound for the critical radius for a given value of m. Here we consider some model wave functions to estimate the critical radius.

B. Model estimations of $R_{\min}$

As a model wave function we consider a simple wave function for $m=0$,

$$g(v)=1+bv \tag{4.12}$$

with which Eq. (4.11) leads to

$$R=\frac{3}{16b}+\frac{9}{16}b. \tag{4.13}$$

This has a minimum value of

$$R_{\min}=0.6495 \quad \text{at} \quad b=3^{-1/2}, \tag{4.14}$$

which is fairly close to the accurate value of 0.6393. It is interesting to note that we can check the quality of the wave function in terms of the coalescence and cusp conditions in Eqs. (2.14) and (2.15) which together, for $m=0$, lead to

$$\frac{1}{g}\frac{dg}{dv}\bigg|_1+\frac{1}{g}\frac{dg}{dv}\bigg|_{-1}=2R, \quad m=0. \tag{4.15}$$

For the wave function in Eq. (4.12), this leads to

$$\frac{b}{1-b^2}=R. \tag{4.16}$$

Using this equation in Eq. (4.13) and solving for R, we get $R=0.6571$ which is fairly close to the optimum value in Eq. (4.14). This illustrates the point that the coalescence and cusp property simulates the optimum property to a significant extent.

As a more general case, we consider a wave function for a general m,

$$g(v)=(1-v^2)^{|m|/2}\ e^{\beta v} \tag{4.17}$$

which includes the threshold behavior. The integrations involved in evaluating R in Eq. (4.11) are straightforward, the general term being

$$e_n=\int_{-1}^{1} e^{2\beta v}\ v^n\ dv=\frac{1}{2^n}\left(\frac{d}{d\beta}\right)^n\frac{1}{\beta}\sinh(2\beta). \tag{4.18}$$

Minimizing R in Eq. (4.11) with respect to β leads to

$$\begin{aligned} R_{\min}&=0.6412 \quad \text{for } m=0 \text{ at } \beta=0.5868\\ &=3.801 \quad \text{for } m=1 \text{ at } \beta=1.517\\ &=10.50 \quad \text{for } m=2 \text{ at } \beta=3.07. \end{aligned} \tag{4.19}$$

These values may be compared with the accurate value[15] of 0.6393 for $m=0$, and the value of 3.79 for $m=1$ obtained by Coulson and Walmsley.[23]

With a slightly more complicated wave function for $m=0$,

$$f(v)=(1+bv)e^{\beta v}, \tag{4.20}$$

the optimum value of $R_{\min}$ from Eq. (4.11) comes out to be 0.63946 for $\beta=0.913$, $b=-0.301$, which is quite close to the accurate value[15] of 0.6393.

V. FINITE-DIPOLE POTENTIAL IN TWO DIMENSIONS

We now consider the properties of an electron in a finite-dipole potential in two dimensions. This would be relevant for an electron and a polar molecule in a junction. It would also be theoretically interesting to analyze the variation of the properties we have considered, when the dimension changes from three to two.

A. Basic equations

The elliptic coordinates in two dimensions with the foci on the z-axis, are similar to the u and v variables in Eq. (2.1) but in two dimensions which may be taken to be the xz-plane. One then gets[25]

$$\begin{aligned} \nabla^2&=\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial z^2}\\ &=\frac{4}{R^2(u^2-v^2)}\left[(u^2-1)\frac{\partial^2}{\partial u^2}+u\frac{\partial}{\partial u}+(1-v^2)\frac{\partial^2}{\partial v^2}-v\frac{\partial}{\partial v}\right],\\ u&=\frac{r_a+r_b}{R}, \quad v=\frac{r_a-r_b}{R},\\ r_a&=|\mathbf{r}-\mathbf{R}/2|, \quad r_b=|\mathbf{r}+\mathbf{R}/2|, \end{aligned} \tag{5.1}$$

and the area element

$$dA=\left(\frac{R}{2}\right)^2\frac{u^2-v^2}{[(u^2-1)(1-v^2)]^{1/2}}du\,dv. \tag{5.2}$$

These expressions can be obtained by taking derivatives and differential elements, or as part of three-dimensional elliptic cylinder coordinates.[24] The Schrödinger equation for the electron in a finite-dipole potential in Eq. (2.2) but in two dimensions, is

$$\begin{aligned} -\frac{1}{2}\left(\frac{2}{R}\right)^2\frac{1}{u^2-v^2}\Bigg[&(u^2-1)\frac{\partial^2}{\partial u^2}+u\frac{\partial}{\partial u}+(1-v^2)\frac{\partial^2}{\partial v^2}\\ &-v\frac{\partial}{\partial v}\Bigg]\psi+\frac{2Z}{R}\left(\frac{1}{u+v}-\frac{1}{u-v}\right)\psi=E\psi. \end{aligned} \tag{5.3}$$

The equation is separable, and with

$$\psi(u,v)=F(u)G(v) \tag{5.4}$$

one gets

$$(u^2-1)\frac{d^2F}{du^2}+u\frac{dF}{du}+\frac{1}{2}R^2E(u^2-1)F=-SF, \tag{5.5}$$

$$(v^2-1)\frac{d^2G}{dv^2}+v\frac{dG}{dv}-2ZRvG+\frac{1}{2}R^2E(v^2-1)G=-SG, \tag{5.6}$$

with S being the separation constant. These equations are the same as Eqs. (2.5) and (2.6) with $|m|$ replaced by $-1/2$, so that many of the properties in two dimensions can be deduced from the corresponding ones obtained from Eqs. (2.5) and (2.6), with $|m|$ replaced by $-1/2$.

B. Some general properties

We begin by considering some structural properties of the wave functions.

Following the analysis in Sec. II B, and replacing $|m|$ by $-1/2$, we obtain for the asymptotic behavior,

$$\begin{aligned} &F(u)\to u^{-1/2}e^{-\alpha u}, \quad u\to\infty,\\ &\alpha=R(-E/2)^{1/2}, \end{aligned} \tag{5.7}$$

which gives the leading behavior in the asymptotic region. The coalescence and cusp relations also can be obtained by following the analysis in Sec. II C, and replacing $|m|$ by $-1/2$. They lead to

$$\left.\frac{1}{F}\frac{dF}{du}\right|_{u=1}-\left.\frac{1}{G}\frac{dG}{dv}\right|_{v=1}=-2ZR \tag{5.8}$$

and

$$\left.\frac{1}{F}\frac{dF}{du}\right|_{u=1}+\left.\frac{1}{G}\frac{dG}{dv}\right|_{v=-1}=2ZR. \tag{5.9}$$

The virial relation in Eq. (2.18) is applicable to the two-dimensional case as well.

The procedure for obtaining the numerical solutions is the same as in Sec. II E, with $|m|$ replaced by $-1/2$ in all the equations. In our analysis, we take $Z=1$ and confine our discussion to only the ground state.

C. Model wave function for the ground state

For the ground state, we consider a model wave function

$$\psi_0 = NF(u)G(v),$$
$$F(u) = \frac{1}{(1+au)^{1/2}} e^{-\alpha u},$$
$$G(v) = (1+bv)e^{\beta v}, \tag{5.10}$$
$$\alpha = R(-E/2)^{1/2},$$

with N being the normalization constant. This wave function incorporates the asymptotic behavior in Eq. (5.7). The parameters β and b are determined by using the coalescence and cusp conditions in Eqs. (5.8) and (5.9) which imply

$$-\alpha - \frac{a/2}{1+a} - \beta - \frac{b}{1+b} = -2R,$$
$$-\alpha - \frac{a/2}{1+a} + \beta + \frac{b}{1-b} = 2R. \tag{5.11}$$

These equations lead to

$$b = \left[\frac{2\alpha + a/(1+a)}{2+2\alpha+a/(1+a)}\right]^{1/2},$$
$$\beta = \alpha + 2R + \frac{a/2}{1+a} - \frac{b}{1-b}. \tag{5.12}$$

There is only one independent parameter and we take it to be a which is determined variationally. The quantity α depends on the energy E as in Eq. (5.10), which is determined iteratively by requiring that the input energy for determining α is equal to the expectation value of the output energy

$$E = \frac{\langle \psi_0 | H | \psi_0 \rangle}{\langle \psi_0 | \psi_0 \rangle} \tag{5.13}$$

evaluated with the area element in Eq. (5.2). The values of the parameter a, energy E, average values of some position variables and the virial ratio in Eq. (3.10) are given in Table IV. The energies obtained from the model wave function based on some local properties are close to the values obtained from the numerical analysis discussed in Sec. II E with $|m|$ replaced by $-1/2$. The virial ratio which should be 1 for the exact energy eigenfunctions, is close to 1 for our model wave function. It should be noted that the binding energies in the two-dimensional case are significantly greater than the binding energies in the three-dimensional case.

D. Minimum value of *R*

For obtaining the minimum value of R for which bound states exist, we take the separable form in Eq. (5.4). Since the wave function is spread over a large domain for $E \to 0$, one can use the WKB approach to analyze the u-part of the wave function. For $E \to 0$, the equation for $F(u)$ in Eq. (5.5) for large values of u tends to

$$\frac{d^2F}{du^2} + \frac{1}{u}\frac{dF}{du} + \frac{1}{2}R^2EF + \frac{S}{u^2}F = 0. \tag{5.14}$$

Using $u = e^x$, we get

TABLE IV. Values of the parameter a, energy E, expectation values $\langle r_b \rangle$, $\langle 1/r_b \rangle$, and $\langle r_a \rangle$, and the virial ratio V_r in Eq. (3.10), for the model wave function in Eq. (5.10) in two dimensions, along with the energies from numerical calculations in brackets, for some values of R.

R	a	$-E$	$\langle r_b \rangle$	$\langle 1/r_b \rangle$	$\langle r_a \rangle$	V_r
5.0	0.70	1.7994 (1.7994)	0.498	3.95	5.03	1.01
3.0	0.83	1.6640 (1.6641)	0.497	3.99	3.05	1.00
2.0	0.84	1.4929 (1.4930)	0.498	4.00	2.09	1.00
1.5	0.78	1.3216 (1.3217)	0.504	3.99	1.63	1.00
1.0	0.68	0.9948 (0.9948)	0.538	3.85	1.23	1.01
0.7	0.56	0.6430 (0.6429)	0.631	3.47	1.08	1.01
0.5	0.44	0.3242 (0.3242)	0.852	2.76	1.14	1.02
0.3	0.238	0.04692 (0.0470)	2.10	1.24	2.24	1.04
0.2	0.089	0.00265 (0.00275)	8.10	0.342	8.17	0.97
0.15	0.026	8.3×10^{-5}	15.5	0.126	15.6	0.94

$$\frac{d^2F}{dx^2} + \left[\frac{1}{2}R^2E + \frac{S}{u^2}\right]e^{2x}F = 0, \tag{5.15}$$

and the WKB relation for the bound states leads to

$$\int \left[\frac{1}{2}R^2E + \frac{S}{u^2}\right]^{1/2} du = (n_u + 1/2)\pi, \tag{5.16}$$

with $n_u = 0,1,\ldots$. Therefore for $S > 0$, the integral tends to infinity for $E \to 0$, and one has an infinite number of bound states. To solve for the critical radius for $E \to 0$ and $S \to 0$, we multiply Eq. (5.6) by $G/(1-v^2)^{1/2}$ and integrate to obtain

$$R_{\min} = \frac{\int dv (1-v^2)^{1/2}(dG/dv)^2}{2\int dv \;\; vG^2/(1-v^2)^{1/2}}. \tag{5.17}$$

Clearly

$$R_{\min} \to 0 \tag{5.18}$$

when the slope of G tends to zero. For example, taking

$$G(v) = 1 + bv \tag{5.19}$$

will lead to $R_{\min} \to 0$ for $b \to 0$. Similarly, taking

$$G(v) = e^{\beta v} \tag{5.20}$$

will lead to $R_{\min} \to 0$ for $\beta \to 0$. Therefore one has an infinite number of bound states for an electron in a dipole potential in two dimensions, for all values of R.

VI. SUMMARY

We have analyzed the structural properties of an electron in the field of a finite-dipole with separation radius R. For the separable solutions in terms of prolate ellipsoidal coordinates, we have analyzed the asymptotic behavior when the electron is far away from the dipole, and the coalescence and cusp properties when the electron is close to the dipole charges. These simple but general properties provide a clear

insight into the structure of the wave functions. Then some simple, model wave functions are developed incorporating these properties, which give accurate values for the energies and some physical quantities, and provide a clear understanding of their physical structure. We have also analyzed the critical radius for the existence of the bound states, using the WKB approach, and obtained a simple expression for the critical radius. These considerations are extended to the dynamics in two dimensions. It is interesting to observe that in the two-dimensional case, an infinite number of bound states exist for all values of the separation radius. It may also be noted that though we have presented the results for $Z=1$, the results for other charges can be obtained from a scale transformation. In particular we have

$$E(Z,R)=Z^2E(1,ZR). \tag{6.1}$$

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