Critical dipoles in one, two, and three dimensions

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(Received 1 November 2006; accepted 26 January 2007)

The Schrödinger equation for a point charge in the field of a stationary electric dipole admits bound states only when the dipole moment exceeds a certain critical value. It is not hard to see why this might be the case, but it is surprisingly difficult to calculate the critical dipole moment. The analogous problem should be simpler in one and two dimensions, but a general theorem forbids critical moments in one dimension, and explicit calculation shows that there is no critical moment in two dimensions. © *2007 American Association of Physics Teachers.*
[DOI: 10.1119/1.2710485]

I. INTRODUCTION

It is a remarkable fact, discovered by Fermi and Teller in the 1940s and rediscovered in the 1960s,[1] that a stationary electric dipole supports bound states if but *only* if the dipole moment exceeds a critical value:

$$p_{\text{crit}} = 0.6393\frac{4\pi\epsilon_0\hbar^2}{qm}, \tag{1}$$

where m and q are the mass and charge of the orbiting particle. For the electron,[2]

$$p_{\text{crit}} = 5.420 \times 10^{-30}\ \text{Cm}. \tag{2}$$

Even more surprising, the critical dipole moment has the same value for a physical dipole (see Fig. 1)

$$V(\mathbf{r}) = \frac{1}{4\pi\epsilon_0}\left(\frac{Q}{r_+} - \frac{Q}{r_-}\right) \tag{3}$$

as it does for the point dipole

$$V(r,\theta) = \frac{1}{4\pi\epsilon_0}\frac{p\cos\theta}{r^2} \tag{4}$$

(where $\mathbf{p}=Q\mathbf{d}$).

The purpose of this paper is to explore and explain the occurrence of a critical moment in this system. In Sec. II we recapitulate the standard arguments and offer some potentially illuminating ways of thinking about the problem. It is natural to wonder whether similar considerations apply to the one- and two-dimensional analogs, which we consider in Secs. III and IV, respectively.

II. CRITICAL MOMENT IN THREE DIMENSIONS

We start with the physical dipole: $\pm Q$ separated by a distance d. If d is large, q will form a hydrogenic system at the $+Q$ end,[3] with $-Q$ too distant to be relevant. In this limit there are obviously bound states, with the lowest energy given by the Bohr formula

$$E_1 = -\frac{mq^2Q^2}{2(4\pi\epsilon_0)^2\hbar^2}. \tag{5}$$

As we reduce the separation distance (keeping the charges constant), the approaching $-Q$ charge repels the electron, and it is plausible that at some point it will ionize the "atom" completely—closer than this separation, no bound state is possible. We can estimate the separation at which this ionization will occur. The Coulomb repulsion energy is approximately $qQ/(4\pi\epsilon_0 d)$. When this equals E_1 (in magnitude), the total energy is zero and the electron is no longer bound:

$$\frac{1}{4\pi\epsilon_0}\frac{qQ}{d} = \frac{mq^2Q^2}{2(4\pi\epsilon_0)^2\hbar^2}, \tag{6}$$

which implies

$$p = Qd = 2\left(\frac{4\pi\epsilon_0\hbar^2}{qm}\right). \tag{7}$$

This crude estimate is off by a factor of slightly more than 3 [see Eq. (1)], but it does account for the existence of a critical dipole moment.[4]

Now let us show that if there *is* a critical dipole moment, it is independent of the separation d (all that matters is the product $p=Qd$), and hence has the same value for the point dipole as for the physical dipole.[5] Schrödinger's equation for a charge q in the dipole potential, Eq. (3), is

$$-\frac{\hbar^2}{2m}\nabla^2\psi + \frac{qQ}{4\pi\epsilon_0}\left(\frac{1}{r_+} - \frac{1}{r_-}\right)\psi = E\psi. \tag{8}$$

We are interested in bound states, which is to say solutions with $E<0$. The critical moment occurs when the ground state energy goes to zero. Assume that d is fixed, and all lengths are measured in units of d: $\tilde{\mathbf{r}} \equiv \mathbf{r}/d$, $\tilde{r}_\pm \equiv r_\pm/d$, $\tilde{\nabla}^2 = d^2\nabla^2$. Then Eq. (8) assumes the dimensionless form

$$\tilde{\nabla}^2\psi - \lambda\left(\frac{1}{\tilde{r}_+} - \frac{1}{\tilde{r}_-}\right)\psi = 4\varepsilon\psi, \tag{9}$$

where

$$\lambda \equiv \frac{2m}{\hbar^2}\frac{qp}{4\pi\epsilon_0} \tag{10}$$

and

$$\varepsilon \equiv -\frac{mE}{2\hbar^2}d^2. \tag{11}$$

Suppose we have solved Eq. (9) and obtained the formula for the ground state energy[6] (in the dimensionless form ε) as a function of the dipole moment (in the dimensionless form λ): $\varepsilon_g(\lambda)$. Now we decrease λ (by reducing Q, because we are holding d fixed) until ε_g reaches zero, and the last bound state is squeezed out: $\varepsilon_g(\lambda_{\text{crit}})=0$. This condition tells us the critical dipole moment:

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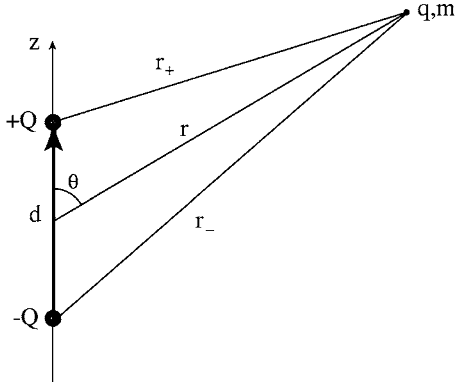

Fig. 1. Point charge q in the field of a stationary dipole.

$$p_{\text{crit}} = \left(\frac{\lambda_{\text{crit}}}{2}\right)\frac{4\pi\epsilon_0\hbar^2}{qm}. \tag{12}$$

Note that λ_{crit} does not depend on d; it is the value of λ for which the largest ε in Eq. (9) reaches zero. So p_{crit}, too, is independent of d.

This being the case, we might as well use the simplest model, the *point* dipole, to calculate p_{crit}. Schrödinger's equation[7]

$$-\frac{\hbar^2}{2m}\nabla^2\psi + \frac{qp}{4\pi\epsilon_0}\frac{\cos\theta}{r^2}\psi = E\psi \tag{13}$$

is separable in spherical coordinates. Let

$$\psi(r,\theta,\phi) = \frac{1}{r}u(r)\Theta(\theta)\Phi(\phi), \tag{14}$$

and recall that

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}. \tag{15}$$

Then Eq. (13) becomes

$$-\frac{r}{u}\frac{d}{dr}\left[r^2\frac{d}{dr}\left(\frac{u}{r}\right)\right] - \frac{1}{\Theta\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right) - \frac{1}{\Phi\sin^2\theta}\frac{d^2\Phi}{d\phi^2} + \lambda\cos\theta = -\kappa^2r^2, \tag{16}$$

where

$$\kappa \equiv \sqrt{-2mE}/\hbar\ . \tag{17}$$

Multiplying through by $\sin^2\theta$ isolates the ϕ dependence:

$$\frac{d^2\Phi}{d\phi^2} = -m_\ell^2\Phi, \tag{18}$$

where m_ℓ is the usual azimuthal separation constant. Evidently

$$\Phi(\phi) = e^{im_\ell\phi}, \tag{19}$$

and the periodicity in ϕ means that m_ℓ must be an integer. What remains is

$$\frac{r}{u}\frac{d}{dr}\left[r^2\frac{d}{dr}\left(\frac{u}{r}\right)\right] - \kappa^2r^2 = -\frac{1}{\Theta\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right) + \frac{m_\ell^2}{\sin^2\theta} + \lambda\cos\theta. \tag{20}$$

The left side of Eq. (20) is a function of r alone and the right side is a function of θ alone, so each side must be a constant—call it γ:

$$-\frac{d^2u}{dr^2} + \frac{\gamma}{r^2}u = -\kappa^2u; \tag{21}$$

$$-\frac{d^2\Theta}{d\theta^2} - \cot\theta\frac{d\Theta}{d\theta} + \left(\lambda\cos\theta + \frac{m_\ell^2}{\sin^2\theta}\right)\Theta = \gamma\Theta. \tag{22}$$

Equation (21) is the one-dimensional Schrödinger equation for the notorious $1/r^2$ potential.[8] The force is attractive as long as $\gamma<0$, but it does not support (normalizable) bound states unless $\gamma\leq-\frac{1}{4}$. One way to see this[9] is to look for solutions by the method of Frobenius: Let

$$u(r) = r^\nu\sum_{n=0}^{\infty}a_nr^n, \tag{23}$$

with $a_0\neq0$. Equation (21) becomes

$$\sum_{n=0}^{\infty}[(n+\nu)(n+\nu-1)-\gamma]a_nr^{n+\nu-2} = \kappa^2\sum_{n=0}^{\infty}a_nr^{n+\nu}, \tag{24}$$

from which it follows that

$$[\nu(\nu-1)-\gamma]a_0 = 0, \tag{25a}$$

$$[\nu(\nu+1)-\gamma]a_1 = 0, \tag{25b}$$

$$[(n+\nu+2)(n+\nu+1)-\gamma]a_{n+2} = \kappa^2a_n \quad (n=0,1,2,\ldots). \tag{25c}$$

Equation (25a) yields $\nu_\pm=(1\pm\sqrt{1+4\gamma})/2$, and Eq. (25b) gives $a_1=0$.

There are two solutions, one for ν_+ and one for ν_-. Near the origin they go like

$$u_\pm(r) \sim a_0r^{\pm\nu} = a_0r^{1/2}e^{\pm\sqrt{\gamma+(1/4)}\ \ln r}. \tag{26}$$

As $r\to0$, $\ln r\to-\infty$, so u_+ diverges unless $\gamma\leq-\frac{1}{4}$, in which case the square root is imaginary:

$$u_\pm(r) \sim a_0r^{1/2}e^{\pm ig\ \ln r}, \tag{27}$$

where $ig\equiv\sqrt{\gamma+\left(\frac{1}{4}\right)}$; both solutions go to zero at the origin. The general solution is a linear combination of u_+ and u_-, but only one combination is normalizable:[10]

$$u(r) = A\sqrt{r}K_{ig}(\kappa r), \tag{28}$$

where K_{ig} is the modified Bessel function of order ig. *Conclusion:* For a normalizable solution the separation constant must satisfy $\gamma\leq-\frac{1}{4}$. Presumably[11] the larger $|\gamma|$ becomes, the tighter is the binding, but the critical value, above which no bound states can exist, is $\gamma=-\frac{1}{4}$.

Turning now to Eq. (22), we are interested in the ground state,[12] so $m_\ell=0$:

$$-\frac{d^2\Theta}{d\theta^2}-\cot\theta\frac{d\Theta}{d\theta}+\lambda\cos\theta\Theta=\gamma\Theta. \tag{29}$$

We expand $\Theta(\theta)$ in (normalized) Legendre polynomials[13]

$$\Theta(\theta)=\sum_{\ell=0}^{\infty}d_\ell\sqrt{\frac{2\ell+1}{2}}P_\ell(\cos\theta), \tag{30}$$

which satisfy the differential equation

$$-\frac{d^2}{d\theta^2}P_\ell(\cos\theta)-\cot\theta\frac{d}{d\theta}P_\ell(\cos\theta)$$
$$=\ell(\ell+1)P_\ell(\cos\theta), \tag{31}$$

and write Eq. (29) as

$$\sum_{\ell=0}^{\infty}[\ell(\ell+1)+\lambda\cos\theta-\gamma]d_\ell\sqrt{\frac{2\ell+1}{2}}P_\ell(\cos\theta)=0. \tag{32}$$

But[14]

$$\cos\theta P_\ell(\cos\theta)=\frac{1}{2\ell+1}[(\ell+1)P_{\ell+1}(\cos\theta)$$
$$+\ell P_{\ell-1}(\cos\theta)], \tag{33}$$

so

$$\sum_{\ell=0}^{\infty}\left\{[\ell(\ell+1)-\gamma]d_\ell+\lambda\left[\frac{\ell}{\sqrt{(2\ell-1)(2\ell+1)}}d_{\ell-1}+\frac{\ell+1}{\sqrt{(2\ell+1)(2\ell+3)}}d_{\ell+1}\right]\right\}P_\ell(\cos\theta)=0. \tag{34}$$

We substitute the critical value $\gamma=-\frac{1}{4}$ and use orthogonality of the Legendre polynomials to show that

$$\left[\ell(\ell+1)+\frac{1}{4}\right]d_\ell+\lambda\left[\frac{\ell}{\sqrt{(2\ell-1)(2\ell+1)}}d_{\ell-1}+\frac{\ell+1}{\sqrt{(2\ell+1)(2\ell+3)}}d_{\ell+1}\right]=0, \tag{35}$$

for $\ell=0,1,2,\ldots$. In matrix form,

$$\begin{pmatrix}1/4 & \lambda/\sqrt{3} & 0 & 0 & \cdots\\ \lambda/\sqrt{3} & 9/4 & 2\lambda/\sqrt{15} & 0 & \cdots\\ 0 & 2\lambda/\sqrt{15} & 25/4 & 3\lambda/\sqrt{35} & \cdots\\ 0 & 0 & 3\lambda/\sqrt{35} & 49/4 & \cdots\\ \vdots & \vdots & \vdots & \vdots & \ddots\end{pmatrix}\begin{pmatrix}d_0\\ d_1\\ d_2\\ d_3\\ \vdots\end{pmatrix}$$
$$=\mathbf{0}. \tag{36}$$

Evidently the determinant of this matrix is zero. By truncating at the 2×2, 3×3, 4×4, … level, we obtain a sequence of approximations for λ:

$$\lambda_2=\frac{3}{4}\sqrt{3}=1.299\,04, \tag{37a}$$

$$\lambda_3=\frac{15}{4}\sqrt{\frac{5}{43}}=1.278\,74, \tag{37b}$$

$$\lambda_4=\frac{1}{4}\sqrt{\frac{5}{3}(1483-2\sqrt{(2)(23)(11\,701)})}=1.278\,63, \tag{37c}$$

etc. The sequence converges very rapidly—from λ_7 on the first 16 digits are stable at

$$\lambda=1.278\,629\,754\,399\,962\,5, \tag{38}$$

and the critical dipole moment, Eq. (12), is

$$p_{\text{crit}}=(0.639\,314\,877\,199\,981\,3)\frac{4\pi\epsilon_0\hbar^2}{qm}, \tag{39}$$

confirming Eq. (1).

That's for the point dipole, of course, but we know from the general theorem that the critical moment is independent of the separation of the charges, so it applies as well to the physical dipole. Still, it would be nice to check this independently. Equation (8) separates in prolate spheroidal coordinates,[15]

$$\xi\equiv\frac{r_+ + r_-}{d},\quad \mu\equiv\frac{r_+ - r_-}{d},\quad \phi, \tag{40}$$

where ϕ is the usual azimuthal angle. Note that $\xi\geq1$, $|\mu|\leq1$, and $r_\pm=(\xi\pm\mu)d/2$. The potential energy is

$$\frac{qQ}{4\pi\epsilon_0}\left(\frac{1}{r_+}-\frac{1}{r_-}\right)=-\frac{qp}{4\pi\epsilon_0}\frac{4}{d^2}\left(\frac{\mu}{\xi^2-\mu^2}\right), \tag{41}$$

and Eq. (8) takes the form

$$\nabla^2\psi+\frac{4\lambda}{d^2}\left(\frac{\mu}{\xi^2-\mu^2}\right)=\frac{4\varepsilon}{d^2}\psi. \tag{42}$$

The Laplacian in prolate spheroidal coordinates is[15]

$$\frac{4}{d^2(\xi^2-\mu^2)}\left\{\frac{\partial}{\partial\xi}\left[(\xi^2-1)\frac{\partial}{\partial\xi}\right]+\frac{\partial}{\partial\mu}\left[(1-\mu^2)\frac{\partial}{\partial\mu}\right]+\frac{\xi^2-\mu^2}{(\xi^2-1)(1-\mu^2)}\frac{\partial^2}{\partial\phi^2}\right\}. \tag{43}$$

For a separable solution

$$\psi(\xi,\mu,\phi)=X(\xi)M(\mu)\Phi(\phi), \tag{44}$$

and

$$\frac{1}{X}\frac{d}{d\xi}\left[(\xi^2-1)\frac{dX}{d\xi}\right]+\frac{1}{M}\frac{d}{d\mu}\left[(1-\mu^2)\frac{dM}{d\mu}\right]+\frac{\xi^2-\mu^2}{(\xi^2-1)(1-\mu^2)}\frac{1}{\Phi}\frac{d^2\Phi}{d\phi^2}+\lambda\mu=\varepsilon(\xi^2-\mu^2). \tag{45}$$

The ϕ dependence is the same as before:

$$\frac{d^2\Phi}{d\phi^2}=-m_\ell^2\Phi, \tag{46}$$

so $\Phi(\phi)=e^{im_\ell\phi}$ for integer m_ℓ. Putting this into Eq. (45) and noting that

$$\frac{\xi^2-\mu^2}{(\xi^2-1)(1-\mu^2)}=\frac{1}{\xi^2-1}+\frac{1}{1-\mu^2}, \tag{47}$$

we obtain the (ordinary) differential equations for $X(\xi)$ and $M(\mu)$:

$$\frac{d}{d\xi}\left[(\xi^2-1)\frac{dX}{d\xi}\right]=\left(\frac{m_\ell^2}{\xi^2-1}+\varepsilon\xi^2+\gamma\right)X, \tag{48}$$

$$\frac{d}{d\mu}\left[(1-\mu^2)\frac{dM}{d\mu}\right]=\left(\frac{m_\ell^2}{1-\mu^2}-\varepsilon\mu^2-\lambda\mu-\gamma\right)M, \tag{49}$$

where γ is the separation constant.

We are interested in the ground state (so $m_\ell=0$) at the critical point $\varepsilon=0$ (where E crosses from negative to positive, and the bound state disappears):

$$\frac{d}{d\xi}\left[(\xi^2-1)\frac{dX}{d\xi}\right]=\gamma X, \tag{50}$$

$$-\frac{d}{d\mu}\left[(1-\mu^2)\frac{dM}{d\mu}\right]-\lambda\mu M=\gamma M. \tag{51}$$

Equation (50) has the general solution

$$X(\xi)=AP_{(1/2)(-1+\sqrt{1+4\gamma})}(\xi)+BQ_{(1/2)(-1+\sqrt{1+4\gamma})}(\xi), \tag{52}$$

where P and Q are Legendre functions. $Q_\nu(\xi)$ diverges at $\xi=1$ (that is, on the line joining $-Q$ and $+Q$), and $P_\nu(\xi)$ diverges as $\xi\to\infty$ unless $-1\le\nu\le 0$.[16] It turns out[17] that ν must be $-\frac{1}{2}$, and hence

$$\gamma=-\tfrac{1}{4}. \tag{53}$$

The change of variables

$$\mu\equiv-\cos v \tag{54}$$

transforms Eq. (51) into a form we have encountered before (compare Eq. (29)):

$$-\frac{d^2M}{dv^2}-\cot v\frac{dM}{dv}+\lambda\cos vM=\gamma M. \tag{55}$$

We have already shown that for $\gamma=-\frac{1}{4}$ this delivers $\lambda=1.2786$ and the critical dipole moment Eq. (39).

Alternatively, one can solve Eq. (42) by the variational method, using a trial wave function of the form

$$\psi(\xi,\mu)=\sum_{n=0}^{\infty}C_n\phi_n(\xi,\mu), \tag{56}$$

with $\phi_n(\xi,\mu)\equiv\xi^{-p}\mu^n$, where p and $\{C_n\}$ are adjustable parameters.[18] The matrix elements of the Hamiltonian are[19]

$$H_{mn}=\int\phi_m H\phi_n\,d\tau \tag{57a}$$

$$=\frac{2\pi\hbar^2 d}{(4p^2-1)}\times\begin{cases}\dfrac{p^2(m+n-1)+mn(2p+1)}{[(m+n)^2-1]}, & (m+n)\text{ even},\\ -\dfrac{(2p+1)\lambda}{2(m+n+2)}, & (m+n)\text{ odd}.\end{cases} \tag{57b}$$

The ξ integrals converge for $p>\frac{1}{2}$. We are interested in the crossover point where the energy goes to zero; here the wave function becomes very delocalized, which is to say that p is as small as possible: $p\to\frac{1}{2}$. Because $H\psi=0$ (for the ground state), the determinant of the Hamiltonian matrix vanishes. Dropping the constants in front,

$$\begin{vmatrix}1 & 4\lambda/3 & 1/3 & 4\lambda/5 & \cdots\\ 4\lambda/3 & 3 & 4\lambda/5 & 9/5 & \cdots\\ 1/3 & 4\lambda/5 & 7/3 & 4\lambda/7 & \cdots\\ 4\lambda/5 & 9/5 & 4\lambda/7 & 11/5 & \cdots\\ \vdots & \vdots & \vdots & \vdots & \ddots\end{vmatrix}=0. \tag{58}$$

The solution for λ [which, remember, is twice the coefficient in Eq. (1)] converges very rapidly with the number of terms: At the 2×2 level we recover 1.229 04 [the same as Eq. (37a)]; 3×3 yields 1.278 74, and 30×30 (no problem for Mathematica) gives 1.278 629 754 399 962 5 (unchanged beyond 7×7), identical to what we got using the point dipole [Eq. (38)]. Once again, we obtain the critical dipole moment in Eq. (39).[20]

III. ONE DIMENSION

Calculating the critical dipole moment in three dimensions turned out to be surprisingly difficult, and one wonders whether the analogous problem might be simpler in one dimension, where the Coulomb potential takes the form[21]

$$V(x)=\frac{1}{4\pi\epsilon_0}\frac{Q}{|x|}. \tag{59}$$

The physical dipole is

$$V(x)=\frac{1}{4\pi\epsilon_0}\left(\frac{Q}{|x-d/2|}-\frac{Q}{|x+d/2|}\right), \tag{60}$$

and the point dipole would be

$$V(x)=\pm\frac{1}{4\pi\epsilon_0}\frac{p}{x^2}, \tag{61}$$

with the plus sign for $x>0$ and minus sign for $x<0$.

We begin, as before, with the large d limit, expecting to find a one-dimensional "hydrogen atom" at one end and a distant $-Q$ at the other. Unfortunately, the ground state of one-dimensional hydrogen [charge q in the Coulomb potential Eq. (59)] has infinite binding energy.[22] One way to see this is to regularize the potential (removing the singularity at $x=0$),

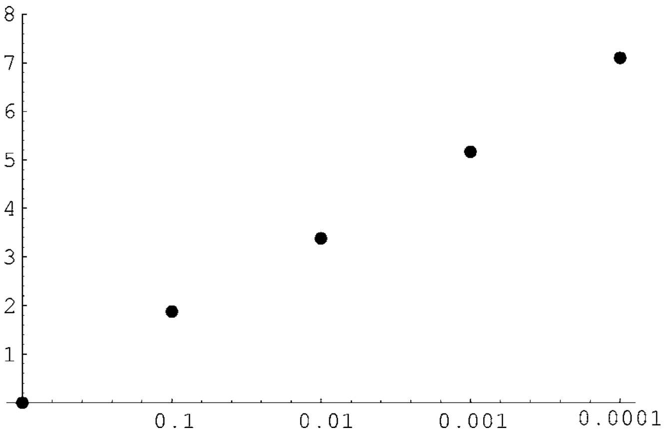

Fig. 2. Ground state energy for the regularized potential Eq. (62). The horizontal axis is ϵ, in units of $a \equiv 2\pi\epsilon_0\hbar^2/mqQ$, and the vertical axis is $a\kappa$, where $\kappa \equiv \sqrt{-2mE}/\hbar$. The graph suggests that E goes to $-\infty$ like $\ln \epsilon$, as $\epsilon \to 0$.

$$V(x) = \frac{1}{4\pi\epsilon_0}\begin{cases} 1/\epsilon, & |x| \leq \epsilon, \\ 1/|x|, & |x| \geq \epsilon, \end{cases} \tag{62}$$

solve numerically for the ground state energy,[23] and plot it as a function of the cutoff ϵ. Figure 2 indicates that the magnitude of the energy increases without limit as $\epsilon \to 0$. No matter how close we bring the $-Q$ end, it cannot ionize the atom, because $(1/4\pi\epsilon_0)Q/d = \infty$ would require $d=0$. This is hardly a proof, but it does suggest that there may not be a critical dipole moment in one dimension.

We can avoid the pathologies of the one-dimensional Coulomb potential by examining other models,[24] such as the delta-function dipole [Fig. 3(a)]:

$$U(x) = \alpha[\delta(x+d/2) - \delta(x-d/2)], \tag{63}$$

and the square-well dipole [Fig. 3(b)]:

$$U(x) = \begin{cases} V_0, & (d-a) < 2x < (d+a), \\ -V_0, & -(d+a) < 2x < -(d-a), \\ 0, & \text{otherwise}. \end{cases} \tag{64}$$

Their ground states can be obtained by solving the Schrödinger equation, but the results are disappointing (if we were hoping to find a critical separation distance): These potentials admit at least one bound state for all d, regardless of the values of α, V_0, and $a < d$. Is there perhaps a general theorem lurking here? There is. If a one-dimensional potential $U(x)$, not identically zero, vanishes outside some finite region, and if

$$\int_{-\infty}^{\infty} U(x)\, dx \leq 0, \tag{65}$$

then $U(x)$ supports at least one bound state.[25] *Conclusion:* There is no critical dipole moment in one dimension.[26]

IV. TWO DIMENSIONS

What about the two-dimensional analog? Is there a critical moment in this case, and if so, what is its value? The point-charge potential is

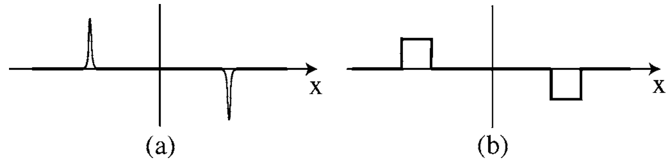

Fig. 3. (a) The delta-function dipole [Eq. (63)]. (b) The square-well dipole [Eq. (64)].

$$V(r,\theta) = \frac{1}{4\pi\epsilon_0}\frac{Q}{r}. \tag{66}$$

As always, we begin with the large d limit—a two-dimensional hydrogen atom at one end and a distant $-Q$ at the other. The ground state energy for two-dimensional hydrogen is four times its value in three dimensions,[27] and hence our crude estimate for the critical dipole moment is one fourth as great [see Eq. (7)]:

$$p_{\text{crit}} \approx \frac{1}{2}\left(\frac{4\pi\epsilon_0\hbar^2}{qm}\right). \tag{67}$$

As before, the critical dipole moment (if there is one) is independent of d, so we look first at the point dipole limit:

$$V(r,\theta) = \frac{1}{4\pi\epsilon_0}\frac{p\cos\theta}{r^2}. \tag{68}$$

Schrödinger's equation,

$$-\frac{\hbar^2}{2m}\nabla^2\psi + \frac{qp}{4\pi\epsilon_0}\frac{\cos\theta}{r^2}\psi = E\psi, \tag{69}$$

is separable in polar coordinates, where the Laplacian is

$$\nabla^2 = \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2}{\partial\theta^2}. \tag{70}$$

We seek solutions of the form

$$\psi(r,\theta) = \frac{u(r)}{\sqrt{r}}\Theta(\theta), \tag{71}$$

for which Eq. (69) reduces to

$$\left[\frac{r^2}{u}\frac{d^2u}{dr^2} - \kappa^2 r^2\right] = -\left[\frac{1}{\Theta}\frac{d^2\Theta}{d\theta^2} + \frac{1}{4} - \lambda\cos\theta\right]. \tag{72}$$

The left side is a function of r alone, and the right side is a function of θ alone, so each must be a constant—call it γ:

$$-\frac{d^2u}{dr^2} + \frac{\gamma}{r^2}u = -\kappa^2 u, \tag{73}$$

$$\frac{d^2\Theta}{d\theta^2} + \left(\gamma + \frac{1}{4} - \lambda\cos\theta\right)\Theta = 0. \tag{74}$$

Equation (73) is identical to Eq. (21); we know that the critical value of γ is $-\frac{1}{4}$. We substitute this value into Eq. (74) and obtain

$$\frac{d^2\Theta}{d\theta^2} - \lambda\cos\theta\Theta = 0. \tag{75}$$

We want a solution[28] that is periodic in θ (with period 2π) and even (for the ground state); $\Theta(\theta)$ can therefore be expressed as a Fourier cosine series:

$$\Theta(\theta) = \sum_{n=0}^{\infty} b_n \cos(n\theta). \tag{76}$$

Putting this into Eq. (75), using the identity $\cos x \cos y = (\frac{1}{2}) \times [\cos(x+y) + \cos(x-y)]$, and exploiting the orthogonality of the cosine functions, we find

$$\frac{\lambda}{2} b_1 = 0, \tag{77a}$$

$$b_1 + \frac{\lambda}{2}(2b_0 + b_2) = 0, \tag{77b}$$

$$n^2 b_n + \frac{\lambda}{2}(b_{n-1} + b_{n+1}) = 0 \quad (n = 2,3,4, \ldots), \tag{77c}$$

or, in matrix form,

$$\begin{pmatrix} 0 & \lambda/2 & 0 & 0 & \cdots \\ \lambda & 1 & \lambda/2 & 0 & \cdots \\ 0 & \lambda/2 & 4 & \lambda/2 & \cdots \\ 0 & 0 & \lambda/2 & 9 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} b_0 \\ b_1 \\ b_2 \\ b_3 \\ \vdots \end{pmatrix} = \mathbf{0}. \tag{78}$$

For a nontrivial solution the determinant of this matrix must vanish. Evaluating by minors, first along the top row, and then down the first column, we obtain

$$-\frac{\lambda^2}{2} \begin{vmatrix} 4 & \lambda/2 & 0 & 0 & \cdots \\ \lambda/2 & 9 & \lambda/2 & 0 & \cdots \\ 0 & \lambda/2 & 16 & \lambda/2 & \cdots \\ 0 & 0 & \lambda/2 & 25 & \cdots \\ \cdots & \cdots & \cdots & \cdots & \ddots \end{vmatrix} = 0. \tag{79}$$

Either $\lambda = 0$ or else the remaining determinant is zero. Would $\lambda = 0$ be acceptable? Absolutely: In this case Eq. (75) has the periodic solution $\Theta = \text{const}$, and

$$\psi(r,\theta) = A K_0(\kappa r). \tag{80}$$

Unfortunately, this means that the critical dipole moment is zero—which is to say that there is no critical dipole moment. The two-dimensional dipole (like the one-dimensional) *always* has a bound state.

Just to be sure, let's examine what happens to the ground state of the physical dipole, as the separation decreases (with Q held fixed). In this case Schrödinger's equation separates most simply in elliptic coordinates (u,v); these are closely related to the prolate spheroidal coordinates in Eq. (40), with[29]

$$\xi = \cosh u, \quad \mu = -\cos v. \tag{81}$$

The potential energy [Eq. (41)] is

$$\frac{qQ}{4\pi\epsilon_0}\left(\frac{1}{r_+} - \frac{1}{r_-}\right) = \frac{qp}{4\pi\epsilon_0} \frac{4}{d^2} \frac{\cos v}{\cosh^2 u - \cos^2 v}, \tag{82}$$

and the Laplacian[30] is

$$\nabla^2 = \frac{4}{d^2(\cosh^2 u - \cos^2 v)}\left(\frac{\partial^2}{\partial u^2} + \frac{\partial^2}{\partial v^2}\right), \tag{83}$$

so Schrödinger's equation takes the form

$$\frac{\partial^2 \psi}{\partial u^2} + \frac{\partial^2 \psi}{\partial v^2} - \lambda \cos v \, \psi = \varepsilon(\cosh^2 u - \cos^2 v)\psi. \tag{84}$$

Letting

$$\psi(u,v) = U(u)V(v), \tag{85}$$

we obtain the (ordinary) differential equations for U and V:

$$\frac{d^2 U}{du^2} - (\varepsilon \cosh^2 u + \gamma)U = 0, \tag{86a}$$

$$\frac{d^2 V}{dv^2} + (-\lambda \cos v + \varepsilon \cos^2 v + \gamma)V = 0, \tag{86b}$$

where γ is the separation constant. We are interested in the critical point $\varepsilon = 0$ (where E crosses from negative to positive):

$$\frac{d^2 U}{du^2} = \gamma U, \tag{87a}$$

$$-\frac{d^2 V}{dv^2} + \lambda \cos v \, V = \gamma V. \tag{87b}$$

Equation (87a) has the general solution

$$U(u) = A e^{\sqrt{\gamma} u} + B e^{-\sqrt{\gamma} u}. \tag{88}$$

For the ground state we want γ real, and as small as possible;[31] the limiting case is $\gamma = 0$ for which Eq. (87b) reduces to

$$\frac{d^2 V}{dv^2} - \lambda \cos v \; V = 0. \tag{89}$$

Thus we recover Eq. (75), which we already know yields a critical moment of zero.

Alternatively, we can use the variational method, with a trial wave function of the Pascual form Eq. (56). The Laplacian is[32]

$$\frac{4}{d^2(\xi^2 - \mu^2)}\left[\sqrt{\xi^2 - 1}\frac{\partial}{\partial \xi}\left(\sqrt{\xi^2 - 1}\frac{\partial}{\partial \xi}\right) + \sqrt{1 - \mu^2}\frac{\partial}{\partial \mu}\left(\sqrt{1 - \mu^2}\frac{\partial}{\partial \mu}\right)\right], \tag{90}$$

and the area element is

$$d\tau = \frac{d^2}{4} \frac{(\xi^2 - \mu^2)}{\sqrt{(\xi^2 - 1)(1 - \mu^2)}} d\xi d\mu. \tag{91}$$

The matrix elements of the Hamiltonian are

$$H_{mn} = -\frac{\hbar^2}{2m}\frac{\pi\sqrt{\pi}}{2}\frac{\Gamma(p)}{\Gamma[p+(1/2)]}\frac{(m+n)!}{2^{m+n}} \times \begin{cases} \dfrac{1}{[((m+n)/2)\,!\,]^2}\left[\dfrac{p^3}{2p+1} - \dfrac{mn}{m+n-1}\right], & (m+n)\text{ even.} \\ \dfrac{(\lambda/2)(m+n+1)}{[((m+n+1)/2)\,!\,]^2}, & (m+n)\text{ odd.} \end{cases} \tag{92}$$

In this case the limiting value of p is zero. Putting that in (and dropping the constants out front), we are left with the condition

$$\begin{vmatrix} 0 & \lambda/2 & 0 & 3\lambda/8 & \cdots \\ \lambda/2 & -1/2 & 3\lambda/8 & -3/8 & \cdots \\ 0 & 3\lambda/8 & -1/2 & 5\lambda/16 & \cdots \\ 3\lambda/8 & -3/8 & 5\lambda/16 & -9/16 & \cdots \\ \cdots & \cdots & \cdots & \cdots & \ddots \end{vmatrix} = 0, \tag{93}$$

to which an obvious solution is $\lambda=0$. Again, there is no dipole moment so small that bound states do not exist.

V. CONCLUSION

When we began this study we expected to find critical dipole moments in one and two dimensions, matching the well-established result in three dimensions. We were surprised to find that they do not exist: The electric dipole potential supports at least one bound state no matter how small the moment. All the more remarkable, then, is the three-dimensional case.[33]

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[1]The critical dipole moment was published (without explanation) by E. Fermi and E. Teller, "The capture of negative mesotrons in matter," Phys. Rev. **72**, 399–408 (1947). A derivation was given by A. S. Wightman, "Moderation of negative mesons in Hydrogen I: Moderation from high energies to capture by an H_2 molecule," *ibid.* **77**, 521–528 (1949). It was rediscovered independently by several authors more or less simultaneously, using the physical dipole model: J. E. Turner and K. Fox, "Minimum dipole moment required to bind an electron to a finite dipole," Phys. Lett. **23**, 547–549 (1966); M. H. Mittleman and V. P. Myerscough, "Minimum moment required to bind a charged particle to an extended dipole," *ibid.* **23**, 545–546 (1966). At about the same time it was obtained by several authors using a point dipole model: J.-M. Lévy-Leblond, "Electron capture by polar molecules," Phys. Rev. **153**, 1–4 (1967); W. B. Brown and R. E. Roberts, "On the critical binding of an electron by an electric dipole," J. Chem. Phys. **46**, 2006–2007 (1967). For a delightful account of the history see J. E. Turner, "Minimum dipole moment required to bind an electron—molecular theorists rediscover phenomenon mentioned in Fermi-Teller paper 20 years earlier," Am. J. Phys. **45**, 758–766 (1977). Recently, the critical dipole moment has been interpreted as an example of an anomaly—the quantum mechanical breaking of a classical symmetry (in this case scale invariance): H. E. Camblong *et al.*, "Quantum anomaly in molecular physics," Phys. Rev. Lett. **87**, 220402-1–4 (2001); S. A. Coon and B. R. Holstein, "Anomalies in quantum mechanics: The $1/r^2$ potential," Am. J. Phys. **70**, 513–519 (2002).

[2]Thus, for example, an electron should bind to the water molecule ($p=6.19\times10^{-30}$ Cm), but not to H_2S ($p=3.26\times10^{-30}$ Cm). Data from *CRC Handbook of Chemistry and Physics*, 86th ed., edited by David R. Lide (CRC Press, Boca Raton, FL, 2005). Of course, these are more complicated structures, and in particular the rotation of the molecule turns out to make a significant contribution to the binding; nevertheless, the essential prediction appears to be confirmed in the laboratory: see K. D. Jordan and F. Wang, "Theory of dipole-bound atoms," Annu. Rev. Phys. Chem. **54**, 367–396 (2003) for a comprehensive review.

[3]We're thinking of the orbiting particle as an electron, so we take q to be negative.

[4]If we take $q=-Q$ to be the electron charge, Eq. (7) yields a separation of $2a_0$, where a_0 is the Bohr radius. In other words, the critical point occurs when $-Q$ is quite close to the hydrogen atom at the $+Q$ end, so pretending that the electron is right at $+Q$ [as we did in Eq. (6)] is a poor approximation. We can do a little better using first-order perturbation theory, but it is still far from exact, because this "perturbation" is by no means small.

[5]This argument is due originally to Lévy-Leblond and Brown/Roberts (Ref. 1). A particularly elegant proof is given by Camblong *et al.* (Ref. 1).

[6]It is an awkward fact—not really relevant to the present argument—that for any $\varepsilon>0$ the energy E goes to minus infinity as $d\to0$.

[7]Don't try applying the virial theorem $2\langle T\rangle=\langle\mathbf{r}\cdot\nabla U\rangle$ to this system: It yields $\langle T\rangle=-\langle U\rangle$, and hence $\langle H\rangle=E=0$. The problem is that $\langle T\rangle$ and $\langle U\rangle$ are both infinite, in this case (though $\langle H\rangle$ is finite).

[8]See Coon and Holstein (Ref. 1); A. M. Essin and D. J. Griffiths, "Quantum mechanics of the $1/x^2$ potential," Am. J. Phys. **74**, 109–117 (2006); H. E. Camblong *et al.*, "Renormalization of the inverse square potential," Phys. Rev. Lett. **85**, 1590–1593 (2000) and references therein.

[9]A more elegant method is to factor the Hamiltonian and show that its expectation value is positive for $\gamma>-\frac{1}{4}$. See K. S. Gupta and S. G. Rajeev, "Renormalization in quantum mechanics," Phys. Rev. D **48**, 5940–5945 (1993).

[10]The other solution, $\sqrt{r}I_{ig}(\kappa r)$, diverges at large r. The normalization factor A, such that $\int_0^\infty |u|^2\,dr=1$, is $\kappa\sqrt{2\sinh(\pi g)/\pi g}$. See I. S. Gradshteyn and I. M. Ryzhik, *Table of Integrals, Series, and Products* (Academic, San Diego, 1980), Eqs. (6.576.4) and (8.332.3). Incidentally, $\langle(1/r^2)\rangle \propto \int_0^\infty (1/r)|K_{ig}(\kappa r)|^2\,dr$ is infinite, as anticipated in Ref. 7.

[11]This is not quite as obvious as it looks, because the raw $1/r^2$ potential has bound states for every negative energy, as long as $\gamma\leq-\frac{1}{4}$. The pure $1/r^2$ potential is pathological in this sense. It can be tamed in various ways (see Ref. 8); the simplest method is to introduce a (spherically symmetric) repulsive core. Brown and Roberts (Ref. 1) and O. H. Crawford, "Bound states of a charged particle in a dipole field," Proc. R. Soc. London **91**, 279–284 (1967), show that such a regularization of the potential does not affect the existence or value of the critical dipole moment.

[12]Any angular momentum about the symmetry axis can only increase the energy. Crawford (Ref. 11) does the calculation for general m_ℓ, obtaining critical dipole moments for the excited states.

[13]This method was used by Lévy-Leblond and Brown and Roberts (Ref. 1). In principle, any complete set of functions on the interval $\theta=0$ to $\theta=\pi$ would do—for example, $\{\sin(nx)\}$ or $\{\cos(nx)\}$—but Legendre polynomials have the virtue that they are eigenfunctions of L^2 [Eq. (31)], which makes the calculation much simpler.

[14]See, for instance, Ref. 10, Eq. (8.914.1).

[15]M. Abromowitz and I. A. Stegun, *Handbook of Mathematical Functions* (Dover, New York, 1965), Sec. 21. This separation is carried out by Turner and Fox, Lévy-Leblond, Mittleman and Myerscough (Ref. 1), and others.

[16]J. Spanier and K. B. Oldham, *An Atlas of Functions* (Hemisphere, New York, 1987), Chap. 59.

[17]Mittleman and Myerscough (Ref. 1) prove this by solving Eq. (48) with the ε term included, in the asymptotic regime (very large ξ), and joining this solution to $P_\nu(\xi)$ by matching the logarithmic derivatives in the overlap region. It seems that we should be able to do it without recourse to ε, which disappears from the answer, but we have not found a convincing way to do so.

[18] Turner and Fox (Ref. 1) and (in greater detail) J. E. Turner, V. E. Anderson, and K. Fox, "Ground-state energy eigenvalues and eigenfunctions for an electron in an electric-dipole field," Phys. Rev. **174**, 81–89 (1968), used a double sum $\psi(\xi,\mu)=e^{-(\alpha/2)\xi^t}\Sigma_{m,n}C_{mn}\xi^m\mu^n$, with variational parameters α, t, and $\{C_{mn}\}$. P. Pascual, A. Rivacoba, and P. M. Echenique, "Minimum dipole moment required to bind an electron in a polarizable medium," Phys. Rev. B **58**, 9584–9586 (1998) introduced the much simpler form used here.

[19] The volume element in prolate spheroidal coordinates is $d\tau=(\pi/4)d^3(\xi^2-\mu^2)d\xi d\mu$, ξ integrals run from 1 to ∞, and μ integrals from -1 to 1.

[20] The matrix in Eq. (58) is identical to the one obtained much more laboriously by Turner and Fox (Ref. 18)—which is comforting but also surprising, because their starting wave function was quite different. It is surprising, too, that the variational method converges so rapidly to the correct answer, because we have no reason to suppose that the actual ground state wave function is of either the Pascual or the Turner/Fox form. Evidently the method is peculiarly robust in the neighborhood of the crossover point $E=0$. Presumably the matrices in Eqs. (36) and (58) are similar, but we have not found the similarity transformation that relates them.

[21] It is largely a matter of taste what form we choose for the potential of a point charge in an imaginary one-dimensional universe. A referee suggests that we might take the one-dimensional analog to a point charge to be an infinite plane, with $V(x)=-\sigma x/2\epsilon_0$ for $x>0$ and $V(x)=+\sigma x/2\epsilon_0$ for $x<0$. In that case the one-dimensional "dipole" would be a parallel-plate capacitor, with $V(x)=-\sigma d/2\epsilon_0$ for $x>d/2$, $V(x)=-\sigma x/\epsilon_0$ for $-d/2<x<d/2$, and $V(x)=\sigma d/2\epsilon_0$ for $x<-d/2$), which (obviously) has no bound states for any d. But this is really a three-dimensional configuration that happens to have no y or z dependence. In any case, for the purposes of this paper a one-dimensional dipole could be any potential well with a matching hill, but V must go to zero as $|x|\to\infty$.

[22] There is some controversy about the legitimacy of this state. See C. V. Siclen, "The one-dimensional Hydrogen atom," Am. J. Phys. **56**, 9–10 (1988).

[23] This is easy, using the "shooting" method. See N. J. Giordano, *Computational Physics* (Prentice Hall, Upper Saddle River, NJ, 1997), Sec. 10.2 or D. J. Griffiths, *Introduction to Quantum Mechanics*, 2nd ed., (Prentice Hall, Upper Saddle River, NJ, 2005), Problem 2.54.

[24] In these models $U(x)$ is the potential energy, corresponding to qV in the electrostatic versions.

[25] A beautifully simple proof using the variational principle is given by K. R. Brownstein, "Criterion for existence of a bound state in one dimension," Am. J. Phys. **68**, 160–161 (2000). The theorem may not apply to the Coulomb potential [Eq. (59)], because the integral in Eq. (65) is not strictly convergent, and $U(x)$ does not vanish outside a finite region. This case, therefore, remains problematic.

[26] Of course, one could ask about asymmetric systems, in which the repulsive end is slightly larger than the attractive end, or introduce a third (positive) bump at the center, so the integral in Eq. (65) is greater than zero. In this case there is necessarily a critical separation distance, but it's not a dipole any more.

[27] B. Zaslow and M. E. Zandler, "Two-dimensional analog to the Hydrogen atom," Am. J. Phys. **35**, 1118–1119 (1967). Two-dimensional hydrogen with a logarithmic potential (arguably a more appropriate analog) has been studied by F. J. Asturias and S. R. Arágon, "The hydrogenic atom and the periodic table of the elements in two spatial dimensions," *ibid.* **53**, 893–899 (1985); it leads to a point dipole potential of the form $p\cos\theta/r$, but the critical dipole moment—if there is one—would depend on the separation of the charges, and we have not explored this case.

[28] The general solution is a linear combination of Mathieu functions, but it is only periodic for certain special values of λ. What follows is one way of determining those "allowed" values.

[29] The ordinate in Fig. 1 is now the x axis, and $x=(d/2)\cosh u\cos v$, $y=(d/2)\sinh u\sin v$.

[30] Mary L. Boas, *Mathematical Methods in the Physical Sciences*, 2nd ed., (Wiley, New York, 1983), pp. 431–434.

[31] Normalization requires $A=0$, of course. As always, the wave function is maximally delocalized as the energy approaches zero.

[32] This is not just Eq. (43) without the ϕ term—rather, it is the Laplacian for elliptic cylinder coordinates (ξ,μ,z) without the z term.

[33] One might ask whether there is a critical moment for the binding of a point charge to a magnetic dipole. Even in the classical case—the orbits of an electron in the magnetic field of the earth, for example—this problem is enormously more difficult, with chaotic as well as periodic regimes. Whole books have been written on "Størmer's problem," as it is called. As far as we know, no bound states for the quantum analog have been found. See J. R. Reitz and F. J. Mayer, "New electromagnetic bound states," J. Math. Phys. **41**, 4572–4581 (2000).

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