On the critical dipole moment in one-dimension

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In a recent paper Connolly and Griffiths (CG) calculated the minimum magnitude, \( p_{\text{crit}} \), an electric dipole must have for the dipolar system to support bound states. The difficulties one may encounter in calculating the critical dipole moment in one, two, and three dimensions are also explained. In the one-dimensional case there may not be a critical dipole moment since —they argued— in one dimension the Coulomb ground state has infinite binding energy.\(^\dagger\)

Contrary to what CG hint, in this work we are able to estimate \( p_{\text{crit}} \) using the spectrum of the one dimensional hydrogen atom.\(^\dagger\) Then, by using the point dipole potential in one dimension,

\[
V_{pd}(x) = p \frac{\kappa}{|x|},
\]

where \( \kappa \equiv q/(4\pi \varepsilon_0) \), we compute the exact value of the critical dipole moment. Therefore, contrary to the claims about its possible nonexistence, we exhibit that \( p_{\text{crit}} \) do indeed exists. Notice that the \( p_{\text{crit}} \) calculated for the point dipole model is also the critical dipole moment for a physical dipole with charges separated a certain distance since its value is independent of the separation.\(^\dagger\)

For the calculation, CG considered at first the 1D Coulomb potential, \( V_0(x) = -\lambda/|x| \), where \( \lambda = Q\kappa \), stating, following Loudon\(^\dagger\) that its ground state has an infinite binding energy. Consequently, they concluded that such feature may prevent the existence of a critical dipole moment in one dimension. Thus, if the ground state for the 1D hydrogen atom were finite, a value for the critical dipole moment could be estimated as we do below.

CG made plausible the existence of the infinite binding energy ground state by exhibiting the results of a numerical computation with the regularized potential

\[
V_\varepsilon(x) = \begin{cases} 
-\lambda/\varepsilon & \text{if } |x| \leq \varepsilon \\
-\lambda/|x| & \text{if } |x| \geq \varepsilon ,
\end{cases}
\]

where \( \varepsilon \) is a regularizing cut-off, showing that the absolute value of the ground state energy increases when \( \varepsilon \) becomes smaller. We question such argument because, in spite of the numerics, no state of infinite binding energy exist for the Hamiltonian\(^\dagger\)

\[
\hat{H}_0 = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V_0(x)
\]

of the one-dimensional hydrogen atom.

\(^\dagger\)
To obtain a correct solution of this problem, one would need first to determine the self-adjoint extensions ⁴ of (3). The energy spectrum is shown then to contain no state of infinite energy.⁵,⁶ But, although not using explicitly self-adjoint extensions, both Andrews⁷ and Núñez-Yépez and Salas-Brito⁸ had previously shown that the infinite binding energy ground state, predicted by Loudon, would vanish in the limit \( \varepsilon \to 0 \). Boya et al.⁹ have also concluded that such state needs to be discarded. Thus, analysing what happens to the ground state energy of the cut-off potential as \( \varepsilon \) gets smaller and smaller, gives no information about the ground state energy of the \( -1/|x| \) potential. In fact, the energy spectrum of the one-dimensional hydrogen atom, requiring the wave functions to vanish at the origin,¹⁰ is given by the Balmer formula,

\[
E_n = -q \frac{Q}{(8\pi\varepsilon_0 a_B n^2)}, \quad n = 1, 2, 3, \ldots
\]

where \( Q \) is the charge of the nucleus, \( a_B = 4\pi\varepsilon_0 \hbar^2 / (q Q m) \) is the Bohr radius, \( q \) is the electronic charge, and \( m \) is the mass of the electron, exactly as in the three dimensional case.⁵,⁶,⁹,¹¹,¹² The energy of the ground state is thus \( -q Q / (8\pi\varepsilon_0 a_B) \).

Moreover, once the infinite energy state is discarded, we may estimate the distance, \( d \), at which the ionization of a one-dimensional atom occurs due to the presence of another charge,⁴ \( Q \), and therefore we may get a rough estimate of the critical dipole moment equating the Coulomb repulsion energy \( E_{re} = q Q / (4\pi\varepsilon_0 d) \) with the energy of the ground state, \( E_1 \), we obtain

\[
p_{crit}^{(est)} = Q d = 8\pi\varepsilon_0 \frac{\hbar^2}{qm}.
\]  (4)

As can be seen on comparing with (11), this rough estimate is sixteen times larger than the exact value. But, its real importance is that it suggests that a critical value for the dipole moment in one-dimension may exist. Our next task is to compute \( p_{crit} \) exactly and, by doing so, to establish its existence beyond any doubt.

The Schrödinger equation describing an electron interacting with a point dipole is

\[
-\frac{\hbar^2}{2m} \frac{d^2 \Psi}{dx^2} + p \frac{\kappa}{x|x|} \Psi(x) = E \Psi(x).
\]  (5)

To solve (5) notice that for \( x > 0 \) the potential is repulsive and no bound states exist, hence \( \Psi(x > 0) = 0 \).¹³ There is as an impenetrable barrier at \( x = 0 \) so any bound particle has zero probability of crossing to the right side.¹⁴ The solutions must then approach zero as \( x \to 0 \) from the left. Introducing \( y = -x \) in Eq. (5), we get

\[
-\frac{d^2 \Psi}{dy^2} - \frac{\alpha}{y^2} \Psi(y) = -\xi \Psi(y)
\]  (6)
where \( \alpha \equiv \frac{2mpq}{(4\pi \epsilon_0 \hbar^2)} > 0 \) and \( \xi \equiv -2mE/\hbar^2 \). We write \( \Psi(y) \) as the power series

\[
\Psi(y) = \sum_{j=0}^{\infty} a_j y^{j+\nu}, \quad \text{(we assume } a_0 \neq 0) \tag{7}
\]
then substituting (7) into (6), it becomes

\[
\sum_{j=0}^{\infty} a_j y^{j+\nu-2}[(j+\nu)(j+\nu-1) + \alpha] = \xi \sum_{j=0}^{\infty} a_j y^{j+\nu}, \tag{8}
\]
leading to the relationships

\[
\begin{align*}
[\nu(\nu - 1) + \alpha]a_0 &= 0, \\
[\nu(\nu + 1) + \alpha]a_1 &= 0, \\
[(\nu + j + 2)(\nu + j + 1) + \alpha]a_{j+2} &= \xi a_j.
\end{align*} \tag{9}
\]
From (9) we conclude that all the odd-term coefficients vanish and we find two possible values for the leading exponent, \( \nu_{\pm} = (1 \pm \sqrt{1 - 4\alpha})/2 \). Therefore, there are two independent solutions, \( \Psi_{\pm} \), behaving near \( y = 0 \) as

\[
\Psi_{\pm}(y) \sim a_0 y^{1/2} e^{\pm \sqrt{1/4 - \alpha} \ln y}. \tag{10}
\]
These solutions are finite at the origin and square integrable only if \( \sqrt{1/4 - \alpha} \) is imaginary, thus \( \alpha \geq 1/4 \) for bound states to exist.\(^{13,15,16}\) Using this result we obtain the critical value of the point dipole in one dimension

\[
P_{\text{crit}} = \frac{\pi \epsilon_0 \hbar^2}{2qm}. \tag{11}
\]
We emphasize that a physical dipole has exactly the same critical value as the point dipole. Therefore, a one-dimensional dipole does not always support bound states; for that to happen the dipole moment must be larger or at least equal than \( P_{\text{crit}} \). We must point out that, even in such a case, there can only be one bound state.\(^{1,2,16}\)

**Conclusion:** In one-dimension there is a critical dipole moment \( P_{\text{crit}} = \pi \epsilon_0 \hbar^2/2qm = 1.052 \times 10^{-30} \text{ C} \cdot \text{m} \). Any one-dimensional system with an electric dipole moment smaller than \( P_{\text{crit}} \) cannot support bound states.

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1 Kevin Connolly and David J. Griffiths, “Critical dipoles in one, two, and three dimensions,” Am. J. Phys. 75, 524–531 (2007) and the references therein.

2 Jean-Marc Levy-Leblond, “Electron capture by polar molecules,” Phys. Rev. 153, 1–4 (1967).

3 Rodney Loudon, “One-dimensional hydrogen atom,” Am. J. Phys. 27, 649–655 (1959).

4 A very good discussion of finer points of the mathematics of operators in quantum mechanics can be found in G. Bonneau, J. Faraut, and G. Valent, “Self-adjoint extensions of operators and the teaching of quantum mechanics,” Am. J. Phys. 69, 322–331 (2001).

5 W. Fisher, H. Lescke, and P. Müller, “The functional-analytic versus the functional-integral approach to quantum Hamiltonians: The one-dimensional hydrogen atom,” J. Math. Phys. 36, 2313–2323.

6 I. Tsutsui, T. Fülöp, and Taksu Cheon, “Connection conditions and the spectral family under singular potentials,” J. Phys. A: Math. Gen. 36, 275–287 (2003).

7 M. Andrews, “Ground state of the one-dimensional hydrogen atom,” Am. J. Phys. 34, 1194–1195 (1966).

8 H. N. Núñez-Yépez and A. L. Salas-Brito, “Nonexistence of the nondegenerate ground state of the one-dimensional hydrogen atom,” Eur. J. Phys. 8, 306–309 (1987).

9 L. J. Boya, M. Kniecik, and A. Bohm, “Hydrogen atom in one dimension,” Phys. Rev. A 37, 3567-3569 (1988).

10 The self-adjoint extensions of Hamiltonian (3), given explicitly in Eqs. (2) and (3) of Ref. [5], and necessary for understanding all the features of the problem, is an object depending on 4 parameters, each corresponding to certain boundary conditions. The specific “part” of the extensions, used in Ref. here, in [3], and in other papers, is the one requiring Dirichlet boundary conditions, i.e. \( \psi(0) = 0 \).

11 H. N. Núñez-Yépez, C. A. Vargas, and A. L. Salas-Brito, “The one-dimensional hydrogen atom...
in momentum representation,” Eur. J. Phys. 8, 189–193 (1987).

12 V. Lutsenko, L. G. Mardoyan, G. S. Pogosyan, A. N. Sissakian, and V. M. Ter-Antonyan, “Non-relativistic Coulomb problem in a one-dimensional quantum mechanics,” J. Phys. A: Math. Gen. 22, 2739–2749 (1989).

13 Andrew M. Essin and David J. Griffiths, “Quantum mechanics of the $1/x^2$ potential,” Am. J. Phys. 74, 109–117 (2006).

14 P. Garbaczewski, and W. Karwowski, “Impenetrable barriers and canonical quantization,” Am. J. Phys. 72, 924–933 (2004).

15 This calculation is done for the radial part of the three dimensional point dipole in Ref. [4]. For the the one-dimensional $-a/x^2$ potential see Ref. [13].

16 For another discussion of the condition $\alpha \geq 1/4$ for the existence of bound states see K. S. Gupta and S. G. Rajeev, “Renormalization in quantum mechanics,” Phys. Rev. D 48, 5940–5945 (1993).