A simple inquiry on the critical electric dipole moment in one space dimension

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The magnitude of an electric dipole moment must be larger or equal to a certain critical value to support bound states. This is not a widely known fact that nevertheless is easy to understand on heuristic terms and relatively easy to calculate. This critical dipole moment, p_C, has been calculated in 2 and 3 dimensions. It has been ascertained that it does not exist in one dimension or, at least, that it is not computable. In this work, after giving simple arguments on the existence of this critical moment, we compute p_C in one dimension.

Keywords: 1D critical electric dipole; 1D quantum system.

El valor de un momento dipolar eléctrico debe ser mayor o igual a un valor crítico para que admita estados ligados. Este no muy conocido hecho puede comprenderse en forma muy simple y su valor calculado en forma relativamente simple como lo hacemos en este trabajo. Se ha calculado el momento crítico en 2 y 3 dimensiones y se ha sugerido que no existe en una dimensión o que, al menos, no se le puede calcular. Damos argumentos simples para argüir su existencia y lo calculamos exactamente en una dimensión.

Descriptores: Dipolo eléctrico crítico en una dimensión; sistemas cuánticos unidimensionales.

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1. Introduction

Electric dipoles, $\mathbf{p}(=q\mathbf{d})$, support 3D bound states only if the magnitude, $p=|\mathbf{p}|$, of the dipole moment is larger than or equal to

$$p_C = (0.6393)\, 4\pi\epsilon_0\hbar^2/q_e m_e = 5.420\times 10^{-30}\mathrm{C}\cdot\mathrm{m},$$

where q_e and m_e are, respectively, the charge and mass of the electron [1-8]. The consequences of this property can be seen in that an electron binds to certain polar molecules like H_2O (water), with $p = 6.19\times 10^{-30}$ C· m, but not to others, like H_2S (rotten egg or open sewer gas), with $p = 3.26\times 10^{-30}$ C·m [8]. This curious feature can be understood from scaling properties of the Schrödinger equation with the result that if there exists a bound state with binding energy E, then there necessarily exists another bound state with energy $\beta^2 E$, where β any real number. For details of the argument see in Ref. 5. This property also manifests itself in scattering studies where the calculated cross- sections did not completely agree with the observed ones in the case of polar molecules [2,9,11]. The explanation of such behaviour was found to be related to the fact that, for binding electrons, it is not enough for a molecule to have a non-vanishing dipole moment, p, it is also necessary for p to be greater than a certain critical value, p_C [11].

An intuitive way of understanding the mentioned features is to consider the following argument: Two point charges, one posively and the other negatively charged, of fixed magnitude and approaching each other, will produce in the limit $|\mathbf{d}|\to 0$, a point dipole of zero magnitude, $p=0$, which definitively cannot cause binding (Fig. 1). It should be also clear that a sufficiently extended physical dipole (that is, two faraway charges) should have bound states; as the system, dipole plus charge, could be regarded as a hydrogen atom perturbed by another charge. As the separation between the charges is made to decrease, the bound state would disappear as the electron gets expelled —and the dipole moment would vanish afterwards as $d\to 0$ with q fixed. Hence, there would be a minimum separation, d_{min}, which is just enough to bind the charge [5,6,9-11]. We have argued for the existence of a $p_C = qd_{\mathrm{min}}$. This is a well-known result in three dimensions [1,10,11].

But, in spite of the apparent generality of the argument given above, it has been shown that a critical electric dipole moment does not exist in two dimensions, that is, in 2D $p_C = 0$ [3,5]. It has been also suggested that the non-

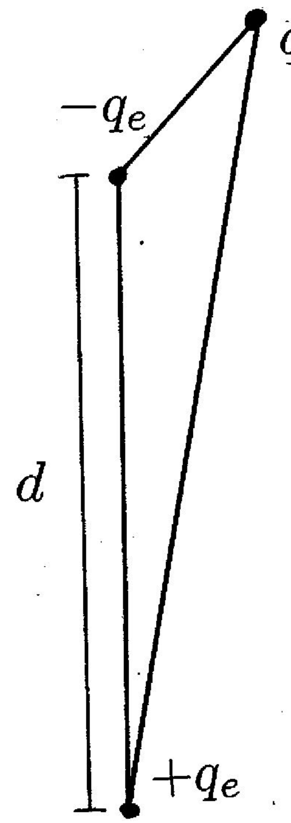

FIGURE 1. Schematic representation of a charged particle in the presence of a physical —that is, point charges at a finite separation— electric dipole. Of course, in one dimension we need to picture all the charges on a single straight line.

existence of the critical dipole also happens in one dimension. This claim is based on the mistaken belief in the existence of an infinite energy ground state in the one-dimensional hydrogen atom problem, a belief disproved a long time ago [13,14,25], for the existence of this type of state would mean that the 1D hydrogen atom Hamiltonian is not Hermitian [12,14].

In this work, our aim is to calculate the 1D critical dipole moment using rather simple quantum arguments, proving along the way that the claim of its non-existence is false. We again point out that the only objective of this paper is the calculation of the 1D p_C. It is important to notice that the value we compute is also the critical dipole moment for a 1D physical dipole with charges separated at a finite distance, as p_C is separation independent. This is explicitly proven in the Appendix. The importance of this 1D result, apart from the purely pedagogical, becomes clear when we recall the relevance attained by excitons in condensed matter and from the search for quantum computing devices using dipole-like 1D interactions, see Ref. 27 to 29.

2. First, a simple estimation

We begin estimating the 1D critical dipole moment. Think of the problem as a 1D hydrogen atom perturbed by another charge, and consider the interaction modelled by the 1D Coulomb potential,

$$V_0(x) = -\frac{\lambda}{|x|}, \tag{1}$$

where $\lambda = qk$ and q_e the charge of the nucleus. Let us pinpoint that the potential (1) is usually referred to as the one-dimensional Coulomb potential but, strictly speaking, the *correct* Coulomb potential in one dimension is $-2\pi|x|$. We use the one-dimensional potential (1) —just for the record, the problem associated with the 1D Coulomb potential (1) was first solved (both relativistically and non-relativistically) in Ref. 23 and 24. The associated energy spectrum is

$$E_n = -\, q_e^2/(8\pi\epsilon_0 a_B n^2),$$

$n=1,2,3,\ldots$, where $a_B=4\pi\epsilon_0\hbar^2/(q_e^2 m_e)$ is the Bohr radius. The ground state energy is $-q_e^2/(8\pi\epsilon_0 a_B)$ [12-16]. To estimate the distance, d, at which ionization of a one-dimensional atom occurs due to the presence of another charge, q_e, [5] and obtain a rough value for the critical dipole moment, we need to equate the repulsion energy $E_{re}=q_e^2/(4\pi\epsilon_0 d)$ with the energy of the ground state, E_1. We obtain

$$p_{crit}^{(est)} \simeq q_e\, d = 8\pi\epsilon_0/(\hbar^2 q_e m_e).$$

On comparing this result with (10), we see that this estimate is sixteen times larger than the exact value.

3. Using the Schrödinger equation to find the critical value of the dipole moment

In one dimension, the physical dipole with charges $\pm q_e$, separated at a distance d, is

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

But, given the separation independence of the 1D critical moment, it is more direct to use the well-known one-dimensional point-dipole potential [5]

$$V_{\rm dp}(x) = \frac{p}{x|x|}, \quad \text{where} \quad k \equiv q_e/(4\pi\epsilon_0), \tag{3}$$

and search for bound states using the Schrödinger equation with the potential (3), corresponding to zero energy, as must be done to find the critical electric dipole moment [2,5].

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

$$-\frac{\hbar^2}{2m}\frac{d^2\Psi}{dx^2} + q_e\frac{p}{x|x|}\Psi(x) = E\Psi(x). \tag{4}$$

Notice that for $x > 0$, the potential is repulsive, hence $\Psi(x > 0) = 0$ [3]. Thus $x = 0$ acts as an impenetrable barrier and any particle has zero probability of crossing from the left to the right- hand side and viceversa [12,17]. This feature can be traced back to the superselection rule (SR) [18,19] that is known to act in the quantum problem defined in (4). The SR prevents any relationship between the happenings on the left-with those on the right-hand side of the origin. The two sides can be described as effectively disconnected even in classical terms [4].

We should also pinpoint that for $x < 0$, our quantum problem (4) reduces, after taking into account the effect of the superselection rule, to the problem with a $-1/x^2$ potential. This problem admits states of any negative energy —see Refs. 3, 4, and 11 and the references therein. A way of getting a "normal" bound state for such a system, hence also to our problem, is through renormalization, which enables us to obtain a non-zero energy state with a normalizable wave function. This state is, however, not a standard quantum state in the sense of elementary quantum mechanics [4,11].

To proceed with the solution, let us make the change $x = -y$ in Eq. (4); we obtain

$$-\frac{d^2\Psi}{dy^2} - \frac{\alpha}{y^2}\Psi(y) = -\xi\Psi(y) \tag{5}$$

where $\alpha \equiv 2m_e p q_e/(4\pi\epsilon_0\hbar^2) > 0$ and $\xi \equiv -2mE/\hbar^2$. We write $\Psi(y)$ as the power series

$$\Psi(y) = \sum_{j=0}^{\infty} a_j y^{j+\nu}. \tag{6}$$

Substituting (6) into (5), it becomes

$$\sum_{j=0}^{\infty} a_j y^{j+\nu-2}[(j+\nu)(j+\nu-1)+\alpha]=\xi\sum_{j=0}^{\infty} a_j y^{j+\nu}, \tag{7}$$

leading to the recurrences

$$\begin{aligned}[\nu(\nu-1)+\alpha]a_0 =&0,\\ [\nu(\nu+1)+\alpha]a_1 =&0, \quad \text{and}\\ [(\nu+j+2)(\nu+j+1)+\alpha]a_{j+2} =&\xi a_j.\end{aligned} \tag{8}$$

From Eqs. (8), we conclude that all the odd coefficients vanish; furthermore we find $\nu_\pm = (1 \pm \sqrt{1-4\alpha})/2$ as possible values for the leading exponent. We have demonstrated the existence of two independent solutions, $\Psi_+(y)$ and $\Psi_-(y)$, behaving near $y = 0$ as

$$\Psi_\pm(y) \sim a_0\sqrt{y}e^{\pm\sqrt{1/4-\alpha}\ln y}. \tag{9}$$

For these solutions to be well behaved, the quantity $\sqrt{1/4-\alpha}$ has to be imaginary. Thus $\alpha \geq 1/4$ for bound states to exist, and therefore $\alpha = 1/4$ is the value we need [3,4,20]. Armed with this value, we can directly obtain the critical value of the point electric dipole moment in one dimension as

$$p_C = \frac{\pi\epsilon_0}{2}\frac{\hbar^2}{q_e m_e} = 1.052\times 10^{-30}\ \text{C}\cdot\text{m}. \tag{10}$$

We emphasize again that *a physical dipole should have the same critical value as the point dipole*. We do not need to pursue the solution further, but we consider it important to mention that the $1/x^2$ potential leds to an extremely peculiar quantum problem which requires renormalization or other advanced techniques to reveal its rather interesting properties [4,5,11,22].

Summarizing, a one-dimensional dipole does not always support bound states. For a 1D electric dipole to be able to bind charged particles, its dipole moment must be larger than or at least equal to p_C [4,5,11].

4. Conclusion

As a conclusion to the calculation of the one-dimensional critical point dipole problem, we state that the *dipole moment critical value* for allowing bound states is

$$p_C = 1.052\times 10^{-30}\ \text{C}\cdot\text{m}. \tag{11}$$

Moreover, it can be shown that the system supports at most *a single renormalized bound state* [3,4]. The existence of a critical value for the electric dipole in one dimension matches the well-established result in three dimensions. Any 1D system with an electric dipole moment smaller than p_C cannot bind charged particles. However, in two dimensions a critical electric dipole does not exist. The electric dipole potential in two dimensions supports at least one bound state no matter how small the two-dimensional moment [5]. Hence, the two dimensional case is remarkable. One may even wonder is if this property is shared by all even-dimensional electric dipoles.

We can compare the results of this electric problem with the rather different properties of the corresponding magnetic problem, also known as the Störmer problem, in which chaotic and regular motion has been found [30-33]. It is also worth noting that we would expect to find an anomaly in the one-dimensional quantum interaction of an electron with the field of an electric dipole [21]. We remind the reader that an anomaly arises whenever the classical invariance of a system is violated upon quantization, or when a quantity that vanishes according to classical physics acquires a non-zero value when quantum dynamics is used [26].

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APPENDIX

The critical dipole does not depend on the charge separation

In one dimension the Schrödinger for the problem of an *extended* dipole is

$$\frac{d^2}{dx^2}\psi(x) - \mu\left(\frac{q_e}{|x-d/2|} - \frac{q_e}{|x+d/2|}\right)\psi(x) = 4\mathcal{E}\psi(x) \tag{A.1}$$

where d is the separation between charges (Fig. 1),

$$\mu \equiv \frac{2m}{\hbar^2}\frac{q_e p}{4\pi\epsilon_0}, \tag{A.2}$$

and

$$\mathcal{E} \equiv -\frac{m_e E}{2\hbar^2} d^2. \tag{A.3}$$

Assume we have solved the Schrödinger Eq. (A.1) and obtained the ground state energy, $\mathcal{E}_1$, as a function of the dimensionless dipole moment μ:

$$\mathcal{E}_1 = \mathcal{E}^{\text{gs}}(\mu). \tag{A.4}$$

Now we decrease μ by reducing gradually the charge —we are assuming that the distance d between the charges is fixed and that the charge reduction is just a strategy for establishing the d-independence— until the energy, $\mathcal{E}_1$, vanishes and all the bound states have been squeezed out: that is, until $\mathcal{E}^{\text{gs}}(\mu_C) = 0$. This condition tells us the critical dipole moment p_C has the form

$$p_C = \left(\frac{\mu_C}{2}\right)\left(\frac{4\pi\epsilon_0\hbar^2}{q_e m}\right). \tag{A.5}$$

The critical dipole is therefore completely independent of the separation d as μ_C does not depend on d —since it is simply the μ-value at which the largest energy eigenvalue of the quantum Eq. (A.1) vanishes. Notice that this property can be also argued from the role played by d as just a scale-fixing factor for the energy [see (14)] with no relevance for the dipole moment [13]. The independence of p_C on the separation between charges has hence been proven. This argument has been borrowed from Refs. 5 and 11. See also Ref. 9.

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