The interaction of an electron with a polar molecule is shown to be the simplest realization of a quantum anomaly in a physical system. In particular, the existence of a critical dipole moment for electron capture and formation of anions, which has been confirmed experimentally and numerically, is derived as a manifestation of the anomaly associated with quantum symmetry breaking of the classical scale invariance exhibited by the point-dipole interaction. Analysis of symmetry breaking for this system is implemented within two different models: point dipole subject to an anomaly and finite dipole subject to explicit symmetry breaking. Moreover, the critical value is shown to be a "fixed point," that is, independent of the size of the finite dipole, thereby highlighting the relevance of the anomaly mechanism.

PACS numbers: 03.65.Ge, 11.10.Gh, 11.30.-j, 31.15.-p
which can be regarded as a generalized inverse square potential with an anisotropic coupling strength. As usual, in Eq. (1), the polar angle \( \theta \) is measured from the direction of the dipole moment, and we assume that the problem occurs in ordinary three-dimensional space. The coupling can be rewritten in a dimensionless form

\[
\lambda = \frac{-2mK_e}{\hbar^2} p Q = \frac{p}{p_0},
\]

with \( m \) being the reduced mass of the system and \( K_e \) the electrostatic constant. In Eq. (2) the characteristic dipole moment \( p_0 \) sets the scale for our analysis and is the relevant dimension parameter whose order of magnitude will provide an estimate for criticality (charge capture). For the particular case of an electron interacting with a polar molecule, \( Q = -e \), and \( p_0 = e a_0/2 \approx 1.271 \, D \), where \( a_0 \) is the Bohr radius and \( D \) is the debye [25]. The corresponding Hamiltonian

\[
H = -\frac{\hbar^2}{2m} \left[ \nabla^2 + \lambda \cos \theta \right],
\]

is explicitly scale and conformally invariant, as the analysis below shows.

The corresponding classical Lagrangian \( L = m v^2/2 - V(r) \) has an associated action that is invariant under the scale transformations \( t \rightarrow \tau t, r \rightarrow \rho r \) (with \( \tau > 0 \) and \( \rho > 0 \), \( \rho^2 = \tau \); this property is shared by the larger class of homogeneous potentials of degree \(-2\) [12], which also includes the two-dimensional delta-function potential. In the language of dimensional analysis, this symmetry means that the point-dipole potential has no characteristic dimensional scales and the coupling \( \lambda \) is dimensionless [29].

The symmetry analysis under time reparametrizations can be generalized to [30,31] \( t \rightarrow \tilde{t} = t - \alpha f(t), r \rightarrow \tilde{r}(\tilde{t}) = J^t r(t) \), with \( J = \left[ dt/d\tilde{t} \right] \). Invariance of the action occurs only when the following two conditions are simultaneously satisfied: (i) \( \delta = 1/2 \) and (ii) \( f(t) \) is quadratic in \( t \). This selects the \( SO(2,1) \) conformal group, just as for the inverse square potential [14], the magnetic monopole [30], and the magnetic vortex [31], with the following three generators: (i) the Hamiltonian \( H \), Eq. (3), associated with time translations \( t \rightarrow t - \alpha \) [for \( f(t) = 1 \)]; (ii) the dilation generator

\[
D = t H - \frac{1}{4} \left( r \cdot \mathbf{p} + \mathbf{p} \cdot r \right), \tag{4}
\]

associated with the scale transformation defined in the previous paragraph, with \( \tau = 1 - \alpha \) [for \( f(t) = t \)]; and (iii) the conformal generator

\[
K = H t^2 - \frac{1}{2} (\mathbf{p} \cdot r + r \cdot \mathbf{p}) t + \frac{1}{2} m r^2, \tag{5}
\]

associated with the special conformal transformation \( 1/t \rightarrow 1/t + \alpha \) [for \( f(t) = t^2 \)]. The corresponding commutators \([D,H] = -i \hbar H, [D,K] = i \hbar K \), and \([H,K] = 2i \hbar D \) show that these three operators form an \( SO(2,1) \) algebra [32].

We will now examine how scale invariance is broken at the quantum-mechanical level. This symmetry breaking manifests itself in the appearance of a critical dipole moment, whose existence and numerical value we will establish next by generalizing our treatment of the inverse square potential [15]. This can be accomplished by writing the Schrödinger equation for the point dipole in spherical coordinates, with the separation of variables \( \Psi(r,\theta,\phi) = u(r)\Theta(\theta)e^{im\phi}/r \), where the azimuthal dependence corresponds to conservation of the axial component \( L_z \) of angular momentum. Then, the corresponding equations for \( r \) and \( \theta \) are explicitly given by

\[
\frac{d^2 u(r)}{dr^2} + \left( E + \frac{\gamma}{r^2} \right) u(r) = 0, \tag{6}
\]

and

\[
\hat{A} \Theta(\theta) = \gamma \Theta(\theta), \tag{7}
\]

where

\[
\hat{A} = -\Lambda^2 + \lambda \cos \theta, \tag{8}
\]

and \( \Lambda^2 = L^2/\hbar^2 \) is the dimensionless angular momentum (squared). Equations (6) and (7) constitute a coupled system of eigenvalue equations linked by the separation constant \( \gamma \). Notice that Eq. (6) can be interpreted as defining an
where $\lambda_{\text{ISP}} \equiv \gamma$. In addition, $\gamma$ is implicitly related to the actual coupling $\lambda$ of the point-dipole potential by means of the eigenvalue equation (7); this relation can be obtained by recasting Eq. (7) into matrix form through the matrix

$$M(\gamma, \lambda) = -A(\lambda) + \gamma \mathbb{I},$$

where $\mathbb{I}$ is the identity matrix. Then, specializing to $m = 0$, and in the basis provided by normalized Legendre polynomials, $\sqrt{(2l + 1)/2} P_l(\cos \theta)$, the matrix elements of $M(\gamma, \lambda)$ become

$$M_{ll'}(\gamma, \lambda) = [l(l + 1) + \gamma] \delta_{ll'} - \lambda \left\{ \frac{l}{\sqrt{(2l - 1)(2l + 1)}} \delta_{l',l-1} + \frac{(l + 1)}{\sqrt{(2l + 1)(2l + 3)}} \delta_{l',l+1} \right\},$$

while the corresponding characteristic equation is

$$D(\gamma, \lambda) \equiv \det M(\gamma, \lambda) = \begin{vmatrix} \gamma & -\frac{\lambda}{\sqrt{3}} & 0 & \cdots & \frac{\lambda}{\sqrt{15}} & (6 + \gamma) & \cdots \\ -\frac{\lambda}{\sqrt{3}} & 2 + \gamma & -\frac{2\lambda}{\sqrt{15}} & \cdots & \cdots & \cdots & \cdots \\ 0 & -\frac{2\lambda}{\sqrt{15}} & (6 + \gamma) & \cdots & \cdots & \cdots & \cdots \\ \vdots & \vdots & \vdots & \ddots & \cdots & \cdots & \cdots \\ \vdots & \vdots & \vdots & \cdots & \ddots & \cdots & \cdots \\ \vdots & \vdots & \vdots & \cdots & \cdots & \ddots & \cdots \\ \frac{\lambda}{\sqrt{3}} & 0 & \cdots & \cdots & \cdots & \cdots & \cdots \end{vmatrix} = 0.$$ \hspace{1cm} (11)

Finally, the required critical dipole moment $\gamma^{(s)}$ is determined from the corresponding critical inverse-square coupling $\gamma^{(s)}$, i.e.,

$$D(\gamma^{(s)} , \lambda^{(s)}) = 0.$$ \hspace{1cm} (12)

It should be noticed that the existence of symmetry breaking for the dipole potential with critical moment $\lambda^{(s)}$ can be viewed as a consequence of the corresponding symmetry breaking for the inverse square potential, which occurs for $\gamma^{(s)} = 1/4$ (for $l = 0$ in three dimensions), when the ground state energy takes zero value [15]. It then follows [from Eq. (12)] that there exists a critical value of the dimensionless dipole moment equal to $\lambda^{(s)} \approx 1.279$ [33], which amounts to the familiar critical dipole moment $p^{(s)} \approx 1.625 \ D$ [19–23]. Extensive empirical and numerical studies have confirmed the existence of a critical dipole moment of a similar value for a large number of molecules [27,28]. This remarkable universal property of polar molecules can be regarded as the simplest physical example of a quantum anomaly.

The fact that the predictions arising from the quantum anomaly analyzed in the previous paragraph agree with the corresponding empirical and numerical findings requires further elaboration. In effect, a polar molecule is better modeled as a finite dipole, with an interaction potential

$$V(r) = K_e Qq \left( \frac{1}{R_+} - \frac{1}{R_-} \right) = K_e \frac{Qp \cos \theta}{r^2} + V_{sb}(r),$$ \hspace{1cm} (13)

where $R_{\pm}$ represents the distance to the charge $Q$ from the positive and negative charges of the dipole. Equation (13) displays the point-dipole potential (1), with $p = qa$ ($l = 1$), supplemented by a symmetry-breaking potential $V_{sb}(r)$, which includes higher-order multipoles (for $l > 1$ and $r > a/2$, with moments $\sim qa^l = pa^{l-1}$), as well as the contribution to the potential for $r < a/2$. In short, in this model, the SO(2,1) symmetry of potential (1) undergoes explicit symmetry breaking by the introduction of additional terms in the Hamiltonian. The corresponding Schrödinger equation with potential (13) can be derived by separation of variables in prolate spheroidal coordinates [34], thus providing a solution [21–23,35] that illustrates the effect of adding explicit symmetry-breaking terms.

A priori, it is by no means obvious that the approximate point-dipole representation captures the correct behavior and the correct numerical value of the critical dipole moment. However, as we will show next, this is indeed the case. In other words, even though the finite dipole introduces a length scale $a$ and amounts to an example of explicit symmetry breaking, the existence of a critical dipole moment as well as its numerical value are independent of $a$. In fact, this result is confirmed by the explicit solution of the problem with potential (13). In short, the simplified point-dipole model exhibits an anomaly, whose relevance lies in that it yields a robust prediction—one that survives when the finite size of the molecule is considered.

Let us now see the dimensional argument that proves the statement of the previous paragraph. The characteristic dimensional parameters for the dynamics of the finite dipole are $\hbar$, $m$, $q$, and $a$, as well as the finite charge $Q$; moreover, the interaction only involves the product $Qq$. Then, according to Buckingham’s Pi theorem of dimensional analysis [36],

3
\[ E_{gs} = -\frac{\hbar^2}{2ma^2} F(\lambda), \]  
(14)

where \( \lambda \) is the dimensionless combination of the given parameters that we previously defined in Eq. (2) and \( F(\lambda) \) is an arbitrary function of \( \lambda \). On the other hand, the critical value of the dimensionless coupling, \( \lambda^{(*)} \), occurs when the ground state energy \( E_{gs} \) takes zero value. Thus, the critical dipole moment is defined by the condition

\[ F(\lambda^{(*)}) = 0, \]  
(15)

whose solution is a dimensionless number independent of the size \( a \) of the dipole. In particular, the critical value survives in the limit \( a \to 0 \), which amounts to the ideal point dipole. This shows that the point-dipole model with anomalous symmetry breaking predicts the correct physics of the finite dipole, for which the symmetry is explicitly broken.

In conclusion, we have found theoretical and empirical evidence—further confirmed by numerical computations—of the existence of a quantum anomaly in molecular physics. Specifically, this anomaly is manifested by the formation of anions through electron capture by polar molecules with supercritical dipole moments and, to our knowledge, represents the simplest realization of quantum-mechanical symmetry breaking in a physical system.

This research was supported in part by CONICET and ANPCyT, Argentina (L.N.E., H.F., and C.A.G.C.) and by the University of San Francisco Faculty Development Fund (H.E.C.). Instructive discussions with Profs. Carlos R. Ordóñez and B. Montgomery Pettitt are gratefully acknowledged by H.E.C.

[3] An introductory discussion of the three types of symmetry breaking, with elementary examples of each kind, can be found in B. R. Holstein, hep-ph/0010033.
[18] In addition to the work of Refs. [16,17], the interpretation of dimensional transmutation as an anomaly is critically revisited in A. Cabo, J. L. Lucio, and H. Mercado, *Am. J. Phys.* **66**, 240 (1998). However, their analysis—limited to the scattering solutions—misses relevant information conveyed by the bound-state sector of the theory.
[25] The debye \( D \) is a characteristic scale for molecular dipole moments, defined to be exactly \( 1 \, D = 10^{-18} \) esu-cm.
This property implies that, quantum-mechanically and for a sufficiently strong potential, the Hamiltonian fails to be bounded from below and is not self-adjoint, despite its Hermitian character. A relevant example of the application of the technique of self-adjoint extensions can be found in Ref. [16], where it is applied to the two-dimensional delta-function potential. This point is related to Ref. [10].

Let $D_N(\gamma, \lambda)$ be the upper left truncation of the determinant $D(\gamma, \lambda)$ [Eq. (11)] associated with the first $N$ rows and columns. In particular, $D_2(\gamma, \lambda)$ already yields the value $\lambda = 3\sqrt{3}/4 \approx 1.299$. Then, iteration with the recurrence relation $D_N(\gamma, \lambda) = [N(N-1) + \gamma] D_{N-1}(\gamma, \lambda) - (N-1)^2 \lambda^2 D_{N-2}(\gamma, \lambda)/(2N-1)(2N-3)$ provides the desired critical value to any degree of precision.


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