Quantization of the piezoelectric constant

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The well-known and celebrated first-primer classical analysis of a one-dimensional inversion-asymmetric assembly of electric point charges interconnected by mechanical springs shows that the system is piezoelectric and characterized by a parameter-dependent but constant piezoelectric coefficient d defined as the ratio between the change in system length and the change in electric field. The former system is the simplest system displaying the phenomenon of piezoelectricity. We demonstrate that a quantum-mechanical analysis of the Hamiltonian for the same system of electric point charges and mechanical springs leads to a piezoelectric constant that depends not only on the system parameters but also on the eigenstate. Hence, the piezoelectric constant, determined as the ratio between the change in the expectation value of the system length and the change in the applied electric field, is quantized. It is demonstrated analytically and numerically, which is a necessary condition, that the quantized piezoelectric constant vanishes if the system Hamiltonian is inversion symmetric.

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I. INTRODUCTION

Piezoelectricity is a well-known phenomenon in materials lacking inversion symmetry [1–4] and finds use in numerous fields [5–11] such as biology, medicine, maritime applications, nondestructive testing, instrumentation, surveillance, and nanotechnology [12–21]. The classical mathematical introduction to piezoelectricity is by virtue of a simple system of electric point charges interconnected by mechanical springs [22]. It is demonstrated that an inversion-asymmetric system may display a spontaneous polarization, i.e., a nonzero polarization in the absence of external fields, in addition to a change in the polarization proportional to the strength and sign of an external mechanical field. Similarly, the exertion of an electric field may lead to the generation of mechanical strain and stress proportional to the strength and sign of the electric field. In this classical toy-model representation, the piezoelectric constant is a system constant. Likewise, in real materials (solids), the piezoelectric constant is a third-rank tensor [23,24] reflecting the fact that the piezoelectric effect depends on the applied electric-field (electric-displacement) vector component or the applied mechanical-strain (mechanical-stress) tensor component. With the modern theory of piezoelectricity introduced about three decades ago, Resta and Vanderbilt with coworkers [25–28] applied the geometric phase (Berry phase) [29–33] to evaluate cyclic adiabatic-polarization changes to accurately determine the piezoelectric material constants [34] using atomistic methods such as the density-functional theory [35].

Recently, there has been substantial activity on nanomechanical resonators [36,37]. Piezoelectric nanomechanical resonators are instrumental for applications in highly sensitive devices where extremely high Q factors (more than 10 million) are required [36]. Piezoelectricity allows vibrational resonances of a nanomechanical resonator based on, e.g., AlN [38–41] to be transformed into electrical signals which is necessary for applications in quantum computing for measuring properties of qubits at room temperature and development of quantum processing units. The extreme precision of piezoelectric nanomechanical resonators [36,42] also renders them suitable for applications where low noise and long coherence times are required, such as mirror suspensions, quantum-cavity optomechanical devices, or nanomechanical sensors. The latter examples are all useful for nanodevices like LEDs and photonics computing [39].

The present work adds new flavor to the general theory of piezoelectricity. We demonstrate, through the construction of a quantum version of Auld's toy model, that the piezoelectric constant of a small-scale system of charges and springs is quantized in the same way as the energy and other observables are. Hence, the concept of quantum piezoelectricity and a quantized piezoelectric constant is discussed in a simple way that allows direct experimental verification from the study of individual molecules or periodic structures lacking inversion symmetry. The application of the theory to larger-scale systems to determine collective modes is a very important and interesting extension. A natural way to address the latter problem would be to use the linear combination of atomic orbitals (LCAO) method or the tight-binding (TB) method where the "atom" is a single nanoscale system. Hopping between

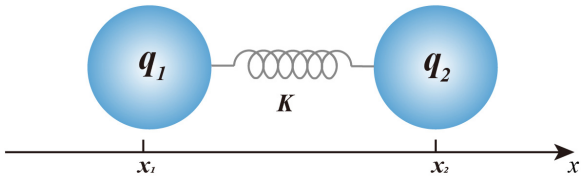

FIG. 1. The general two-particle system consisting of two point charges q_1 and q_2 with coordinates x_1 and x_2, respectively, connected by a spring with spring constant K. The system permittivity is ϵ.

"atoms" in a second-quantized formulation leads to extended (crystal) eigenstates for which crystal-like piezoelectric properties can be addressed. Using our toy system as the "atom," the crystal becomes a functionalized/artificial crystal, but it should be noted that the properties of real systems can be mimicked by appropriately fitting the spring constants and point-charge values.

A main reasoning behind this work is to avoid computationally intensive methods such as density-functional theory. Instead, our model aims to provide qualitative insight into the nature of piezoelectricity and, most importantly, to demonstrate for a simple system that the piezoelectric constant becomes quantized. Note also that the Berry-phase method is applicable to Bloch periodic systems (crystals) and therefore not suitable to address the present case of simple few-particle systems.

II. CLASSICAL PIEZOELECTRICITY

Consider the system shown in Fig. 1 consisting of two point charges q_1 and q_2 and a spring with spring constant K. The forces F_1 and F_2 on particle 1 and 2, respectively, are

$$F_1 = K(x_2 - x_1 - l_0) - \frac{q_1 q_2}{4\pi\epsilon}\frac{1}{(x_2 - x_1)^2}, \tag{1}$$

$$F_2 = -K(x_2 - x_1 - l_0) + \frac{q_1 q_2}{4\pi\epsilon}\frac{1}{(x_2 - x_1)^2}, \tag{2}$$

where ϵ is the permittivity and l_0 is the undeformed spring length. Note that the Coulomb force considered in this toy case is a one-dimensional (1D) simplification of the real three-dimensional (3D) electrostatic force between point charges. Assume $q_2 = -q_1 = q$. Then,

$$F_1 = K(x_2 - x_1 - l_0) + \frac{q^2}{4\pi\epsilon}\frac{1}{(x_2 - x_1)^2}, \tag{3}$$

$$F_2 = -K(x_2 - x_1 - l_0) - \frac{q^2}{4\pi\epsilon}\frac{1}{(x_2 - x_1)^2}, \tag{4}$$

and the system polarization is

$$P = q_1 x_1 + q_2 x_2 = q(x_2 - x_1). \tag{5}$$

In equilibrium, the forces $F_{2,eq} = -F_{1,eq}$ are both zero whereby the equilibrium coordinate difference $(x_2 - x_1)_{eq}$ can be determined. Since the equation determining $(x_2 - x_1)_{eq}$ is cubic, two possibilities can arise depending on the system parameters: (i) Three real solutions or (ii) one real solution and two complex-conjugate solutions. The physically interesting

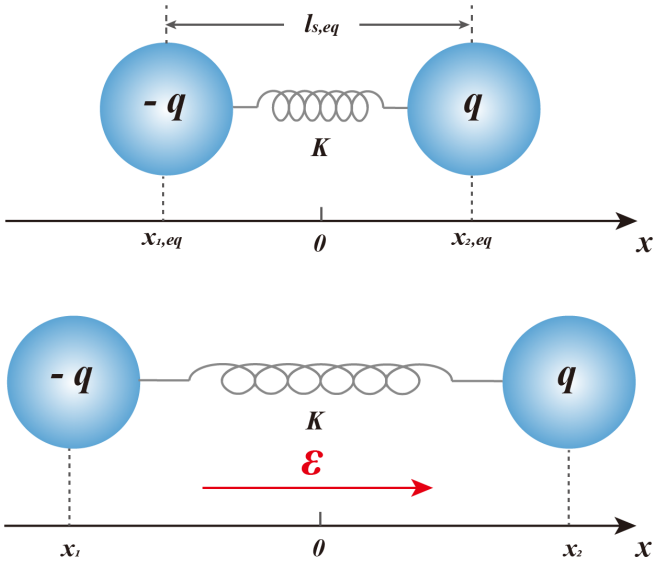

FIG. 2. The two-particle piezoelectric system consisting of two point charges q and $-q$ connected by a spring.

solutions are the real solutions. The cubic equation is

$$K(x_2 - x_1)_{eq}^3 - Kl_0(x_2 - x_1)_{eq}^2 + \frac{q^2}{4\pi\epsilon} = 0. \tag{6}$$

Applying an electric field

Consider now the inversion-asymmetric system $q_2 = -q_1 = q$ (Fig. 2). If an external electric field $\mathcal{E}$ is applied to the system, force equilibrium on the two particles are expressed as

$$F_1 - q\mathcal{E} = 0, \tag{7}$$

$$F_2 + q\mathcal{E} = 0. \tag{8}$$

If the applied electric field is small, a first-order Taylor expansion is a good approximation,

$$\begin{aligned} F_1 &= F_{1,eq} + \left.\frac{\partial F_1}{\partial x_1}\right|_{eq}\delta x_1 + \left.\frac{\partial F_1}{\partial x_2}\right|_{eq}\delta x_2, \\ \delta x_2 &= \left.\frac{\partial F_1}{\partial x_1}\right|_{eq}\delta x_1 + \left.\frac{\partial F_1}{\partial x_2}\right|_{eq}\delta x_2, \end{aligned} \tag{9}$$

$$\begin{aligned} F_2 &= F_{2,eq} + \left.\frac{\partial F_2}{\partial x_1}\right|_{eq}\delta x_1 + \left.\frac{\partial F_2}{\partial x_2}\right|_{eq}\delta x_2, \\ \delta x_2 &= \left.\frac{\partial F_2}{\partial x_1}\right|_{eq}\delta x_1 + \left.\frac{\partial F_2}{\partial x_2}\right|_{eq}\delta x_2. \end{aligned} \tag{10}$$

Equations (3)–(4) yield, for the partial derivatives,

$$\begin{aligned} \left.\frac{\partial F_1}{\partial x_1}\right|_{eq} &= -K - \frac{2q^2}{4\pi\epsilon}\frac{1}{(x_{2,eq} - x_{1,eq})^3}(-1) \\ &= -K + \frac{q^2}{2\pi\epsilon}\frac{1}{(x_{2,eq} - x_{1,eq})^3}, \end{aligned} \tag{11}$$

$$\left.\frac{\partial F_2}{\partial x_2}\right|_{eq} = -K + \frac{2q^2}{4\pi\epsilon}\frac{1}{(x_{2,eq} - x_{1,eq})^3}(1) = \left.\frac{\partial F_1}{\partial x_1}\right|_{eq}, \tag{12}$$

$$\left.\frac{\partial F_1}{\partial x_2}\right|_{eq} = K - \frac{2q^2}{4\pi\epsilon}\frac{1}{(x_{2,eq} - x_{1,eq})^3}(1) = -\left.\frac{\partial F_1}{\partial x_1}\right|_{eq}, \quad (13)$$

$$\left.\frac{\partial F_2}{\partial x_1}\right|_{eq} = K + \frac{2q^2}{4\pi\epsilon}\frac{1}{(x_{2,eq} - x_{1,eq})^3}(-1) = -\left.\frac{\partial F_1}{\partial x_1}\right|_{eq}, \quad (14)$$

and Eqs. (7)–(8) lead to the same equation

$$A\delta x_1 - A\delta x_2 = q\mathcal{E}, \quad (15)$$

where $F_{1,eq} = -F_{2,eq} = 0$ is used, and A is defined as

$$A = \left.\frac{\partial F_1}{\partial x_1}\right|_{eq} = \left.\frac{\partial F_2}{\partial x_2}\right|_{eq} = -\left.\frac{\partial F_1}{\partial x_2}\right|_{eq} = -\left.\frac{\partial F_2}{\partial x_1}\right|_{eq}. \quad (16)$$

The change in the system length $\delta\mathcal{L}$ now becomes

$$\delta\mathcal{L} = \delta(x_2 - x_1) = -\frac{q\mathcal{E}}{A}, \quad (17)$$

where Eq. (15) is used in obtaining the last equality.

Note that system stability against deformations requires

$$A = \left.\frac{\partial F_1}{\partial x_1}\right|_{eq} = \left.\frac{\partial F_2}{\partial x_2}\right|_{eq} < 0. \quad (18)$$

III. SPONTANEOUS POLARIZATION AND PIEZOELECTRICITY

In general, there is a spontaneous polarization given by

$$P_{\text{spon}} = q_1 x_{1,eq} + q_2 x_{2,eq} = q(x_2 - x_1)_{eq} = q\mathcal{L}_{eq} \neq 0, \quad (19)$$

and its value is determined by solving Eq. (6) for $\mathcal{L}_{eq} = (x_2 - x_1)_{eq}$.

The piezoelectric constant d is determined as the change in system length divided by the change in electric field,

$$d = \frac{\delta\mathcal{L}}{\delta\mathcal{E}} = -\frac{q\mathcal{E}}{A}/\mathcal{E} = -\frac{q}{A}, \quad (20)$$

which is nonzero. In obtaining the second equality, use is made of Eq. (17). Note that $d > 0$ if $q > 0$ since stability requires $A < 0$. Similarly, $d < 0$ if $q < 0$ due to the stability criterion $A < 0$.

IV. QUANTUM PIEZOELECTRICITY

The Schrödinger equation for the simple system shown in Fig. 1 is now solved so as to obtain its wave functions and energies. Attention is given to the determination of the system polarization as a function of an external electric field.

V. REDUCTION TO 1D GOVERNING EQUATIONS

Consider two charges q_1 and q_2 connected by a spring and positioned at x_1 and x_2, respectively. A 1D assumption is made for the Coulomb interaction,

$$V_{Cou}(x_1 - x_2) = \frac{q_1 q_2}{4\pi\epsilon}\frac{1}{|x_1 - x_2|}, \quad (21)$$

where ϵ is the permittivity. The elastic coupling is described by the potential term

$$V_{\text{Elas}}(x_1 - x_2) = \tfrac{1}{2}K((x_2 - x_1) - l_0)^2 = \tfrac{1}{2}K(-(x_1 - x_2) - l_0)^2, \quad (22)$$

where l_0 is the equilibrium length of the spring and K is the spring constant. Considering further that the system is exposed to an external electric field $\mathcal{E}$ directed along the positive x axis, there is a third contribution to the total potential,

$$V_{Elec}(x_1, x_2) = -q_1\mathcal{E}x_1 - q_2\mathcal{E}x_2. \quad (23)$$

The two-body Hamiltonian H now takes the form

$$\begin{aligned} H\psi = \Bigg[&-\frac{\hbar^2}{2m_1}\frac{\partial^2}{\partial x_1^2} - \frac{\hbar^2}{2m_2}\frac{\partial^2}{\partial x_2^2} + V_{Cou}(x_1 - x_2) \\ &+ V_{\text{Elas}}(x_1 - x_2) + V_{Elec}(x_1, x_2)\Bigg]\psi(x_1, x_2) \\ &= E\psi(x_1, x_2), \end{aligned} \quad (24)$$

where m_1 (m_2) is the mass of charge q_1 (q_2), ψ is the two-body wave function, and E is the energy.

It is easy to rewrite the electric field potential as

$$\begin{aligned} V_{Elec}(x_1, x_2) &= -q_1\mathcal{E}x_1 - q_2\mathcal{E}x_2 \\ &= \gamma_r(x_1 - x_2) + \gamma_c\left(\frac{m_1 x_1 + m_2 x_2}{m_1 + m_2}\right), \end{aligned} \quad (25)$$

by fixing

$$\gamma_r = -q_1\mathcal{E}\frac{m_2}{m_1 + m_2} + q_2\mathcal{E}\frac{m_1}{m_1 + m_2}, \quad (26)$$

$$\gamma_c = -(q_1 + q_2)\mathcal{E}. \quad (27)$$

From standard quantum mechanics, the Hamiltonian in x_1, x_2 can be transformed using the center-of-mass coordinate $X_G = \frac{m_1 x_1 + m_2 x_2}{m_1 + m_2}$ and the relative coordinate $X = x_1 - x_2$:

$$H = \frac{P_G^2}{2M} + \frac{P^2}{2\mu} + V_{X_G}(X_G) + V_X(X) \equiv H_{X_G} + H_X, \quad (28)$$

$$H_{X_G} = \frac{P_G^2}{2M} + V_{X_G}(X_G), \quad (29)$$

$$H_X = \frac{P^2}{2\mu} + V_X(X), \quad (30)$$

$$V_{X_G}(X_G) = \gamma_c X_G, \quad (31)$$

$$V_X(X) = \frac{q_1 q_2}{4\pi\epsilon}\frac{1}{|X|} + \frac{1}{2}K((-X) - l_0)^2 + \gamma_r X, \quad (32)$$

where

$$P_G = -i\hbar\frac{\partial}{\partial X_G}, \quad (33)$$

$$P = -i\hbar\frac{\partial}{\partial X}, \quad (34)$$

$$M = m_1 + m_2, \quad (35)$$

$$\mu = \frac{m_1 m_2}{m_1 + m_2}. \quad (36)$$

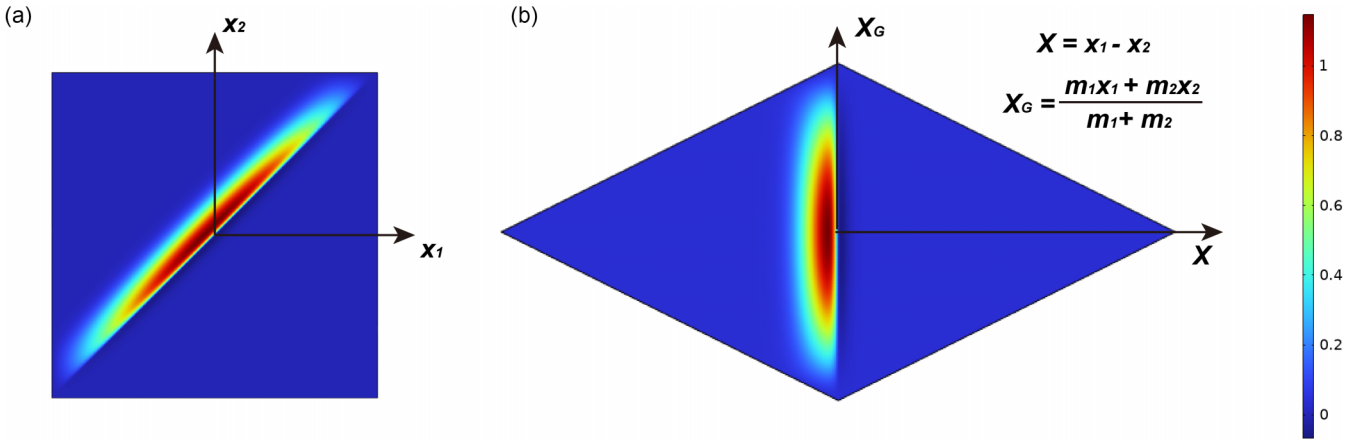

FIG. 3. A schematic drawing of the (a) square and (b) rhombus domains in x_1, x_2 and X, X_G coordinates, respectively. Also shown is the ground state (not normalized) plotted within the two domains.

The original two-dimensional (2D) Hamiltonian H problem can now be split into two $1D$ Hamiltonian problems,1D

$$H_{X_G}|\psi_{X_G}\rangle = E_{X_G}|\psi_{X_G}\rangle, \tag{37}$$

$$H_X|\psi_X\rangle = E_X|\psi_X\rangle, \tag{38}$$

$$\psi = |\psi_{X_G}\rangle \otimes |\psi_X\rangle, \tag{39}$$

$$\left(-\frac{\hbar^2}{2M}\frac{\partial^2}{\partial X_G^2} + V_{X_G}(X_G)\right)\psi_{X_G} = E_{X_G}\psi_{X_G}, \tag{40}$$

$$\left(-\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial X^2} + V_X(X)\right)\psi_X = E_X\psi_X, \tag{41}$$

where

$$\begin{aligned} H|\psi\rangle &= (H_{X_G} + H_X)(|\psi_{X_G}\rangle \otimes |\psi_X\rangle) \\ &= H_{X_G}|\psi_{X_G}\rangle \otimes |\psi_X\rangle + H_X|\psi_{X_G}\rangle \otimes |\psi_X\rangle \\ &= E_{X_G}|\psi_{X_G}\rangle \otimes |\psi_X\rangle + E_X|\psi_{X_G}\rangle \otimes |\psi_X\rangle \\ &= (E_{X_G} + E_X)|\psi_{X_G}\rangle \otimes |\psi_X\rangle = (E_{X_G} + E_X)|\psi\rangle, \end{aligned} \tag{42}$$

so that

$$E = E_{X_G} + E_X. \tag{43}$$

VI. BOUNDARY CONDITIONS

Assume an infinite barrier potential is imposed on the system such that the total wave function vanishes when $|x_1| \geqslant L$ or $|x_2| \geqslant L$. The calculational domain in $x_1 - x_2$ space corresponds to a square with side length $2L$ centered at the origin ($[-L;L] \times [-L;L]$). Transforming x_1, x_2 into center-of-mass and relative coordinates X_G, X, the square is transformed into a rhombus as shown in Fig. 3, i.e, for any function $f(x_1, x_2)$,

$$\begin{aligned} &\int_{-L}^{L} dx_1 \int_{-L}^{L} dx_2 f(x_1, x_2) \\ &= \oint_{\text{square}} dx_1\, dx_2 f(x_1, x_2) \\ &= \oint_{\text{rhombus}} dX\, dX_G f(X, X_G). \end{aligned} \tag{44}$$

In obtaining the second equality it was used that the Jacobian satisfies $|\frac{\partial(x_1,x_2)}{\partial(X,X_G)}| = 1$.

Normalization

Wave functions are normalized such that

$$\begin{aligned} &\int_{-\infty}^{\infty} dx_1 \int_{-\infty}^{\infty} dx_2\, |\psi(x_1, x_2)|^2 \\ &= \lim_{L\to\infty} \int_{-L}^{L} dx_1 \int_{-L}^{L} dx_2\, |\psi(x_1, x_2)|^2 \\ &= \lim_{L\to\infty} \oint_{\text{square}} dx_1\, dx_2\, |\psi(x_1, x_2)|^2 \\ &= \lim_{L\to\infty} \oint_{\text{rhombus}} dX_G\, dX\, |\psi(X_G, X)|^2 \\ &= \lim_{L\to\infty} \int_{-L}^{L} dX_G \int_{-2L}^{2L} dX |\psi(X_G, X)|^2 \\ &= \lim_{L\to\infty} \int_{-L}^{L} dX_G\, |\psi_{X_G}(X_G)|^2 \int_{-2L}^{2L} dX |\,\psi_X(X)|^2 = 1, \end{aligned} \tag{45}$$

which is guaranteed by fixing

$$\begin{aligned} \int_{-\infty}^{\infty} dX_G\, |\psi_{X_G}(X_G)|^2 &= 1, \\ \int_{-\infty}^{\infty} dX\, |\psi_X(X)|^2 &= 1. \end{aligned} \tag{46}$$

Note that in obtaining the fourth equality, it was used that wave functions are zero *outside* the rhombus domain and that the rhombus domain is a subset of $[-L;L]_{X_G} \times [-2L;2L]_X$.

Similarly, it follows that the expectation value for any operator that only depends on the relative coordinate $f = f(X)$ fulfills

$$\begin{aligned} \langle f(X)\rangle &= \int_{-\infty}^{\infty} dx_1 \int_{-\infty}^{\infty} dx_2\, f(X)|\psi(x_1, x_2)|^2 \\ &= \lim_{L\to\infty} \int_{-L}^{L} dX_G\, |\psi_{X_G}(X_G)|^2 \int_{-2L}^{2L} dX f(X)|\,\psi_X(X)|^2 \\ &= \int_{-2L}^{2L} dX f(X)|\,\psi_X(X)|^2, \end{aligned} \tag{47}$$

and that the expectation value for any operator that only depends on the center-of-mass coordinate $g = g(X_G)$ fulfills

$$\begin{aligned}\langle g(X_G)\rangle &= \int_{-\infty}^{\infty} dx_1 \int_{-\infty}^{\infty} dx_2\, g(X_G)|\psi(x_1,x_2)|^2 \\ &= \lim_{L\to\infty}\int_{-L}^{L} dX_G\, g(X_G)|\psi_{X_G}(X_G)|^2 \int_{-2L}^{2L} dX\, |\psi_X(X)|^2 \\ &= \int_{-L}^{L} dX_G\, g(X_G)|\,\psi_{X_G}(X_G)|^2. \end{aligned} \tag{48}$$

VII. PIEZOELECTRICITY

With the above relations it is easy to derive some important consequences for the system length in the presence of an external electric field.

A. Inversion-asymmetric systems

When $q_2 = -q_1 = q$ the system is inversion asymmetric but uncharged as a whole.

The spontaneous polarization is determined as

$$\begin{aligned}\langle P_{\text{spon}}\rangle_i &= \langle q_2x_2 + q_1x_1\rangle_{i,\mathcal{E}=0} \\ &= q\langle x_2 - x_1\rangle_{i,\mathcal{E}=0} = q\int_{-2L}^{2L} dX(-X)\,|\psi_{i,X}(X)|^2_{\mathcal{E}=0}, \end{aligned} \tag{49}$$

which is generally *nonzero* since H_X is neither even nor odd in X (and therefore the eigenstates, distinguished by a subscript i, $\psi_{i,X}|_{\mathcal{E}=0}$ are not eigenstates of parity) while $-X$ has parity -1.

The change in system length with the application of a (small) external electric field $\mathcal{E}$ is

$$\begin{aligned}\Delta\langle\mathcal{L}\rangle_i &= \langle x_2 - x_1\rangle_{i,\mathcal{E}} - \langle x_2 - x_1\rangle_{i,\mathcal{E}=0} \\ &= \langle -X\rangle_{i,\mathcal{E}} - \langle X\rangle_{i,\mathcal{E}=0} \\ &= \int_{-2L}^{2L} dX(-X)\,|\psi_{i,X}(X)|^2_{\mathcal{E}} \\ &\quad - \int_{-2L}^{2L} dX(-X)\,|\psi_{i,X}(X)|^2_{\mathcal{E}=0}. \end{aligned} \tag{50}$$

It follows from Eqs. (26), (30), and (32) that H_X and therefore the eigenstates $\psi_{i,X}$ depend on $\mathcal{E}$. Since H_X depends on $\mathcal{E}$ and is neither even nor odd in X while $-X$ has parity -1, the change in system length with the application of an electric field is generally nonzero, and the piezoelectric constant is determined by

$$d_i = \frac{\Delta\langle\mathcal{L}\rangle_i}{\mathcal{E}}. \tag{51}$$

In Fig. 4 the first four eigenstates of the two-particle piezoelectric system is plotted.

Our calculations reveal that the piezoelectric constant d_i does not depend on the eigenstate i (see Fig. 5) which is not given *a priori*. In the next section, we shall see that this result does not apply to more complicated systems such as the four-particle system.

B. Corollary on inversion-symmetric systems

It is easy to demonstrate that an inversion-symmetric system is nonpiezoelectric if the system is uncharged as a whole (which for our system implies that $q_2 = q_1 = 0$). Then the system length $\langle\mathcal{L}\rangle_i = \langle x_2 - x_1\rangle_{i,\mathcal{E}}$ is independent of the electric field $\mathcal{E}$ and the piezoelectric constant $d_i = \frac{\Delta\langle\mathcal{L}\rangle_i}{\mathcal{E}}$ is zero. Further, the spontaneous polarization must be zero, since

$$\langle P_{\text{spon}}\rangle_i = \langle q_2x_2 + q_1x_1\rangle_{i,\mathcal{E}=0} = 0. \tag{52}$$

VIII. AULD'S SYSTEM IN THE QUANTUM CASE

Consider the structure of four point charges q_1, q_2, q_3, q_4 that Auld considered [22,23] (Fig. 6). The charges q_2 and q_3 cannot move and are positioned at a fixed distance l to the left (q_2) and to the right (q_3), respectively. The charges q_1 and q_4 can both move and are positioned at distances l_a and l_b to the left and right, respectively. A spring with spring constant K and equilibrium length l_0 is connected between charges q_1 and q_2. A similar spring is connected between charges q_3 and q_4. The system Hamiltonian can be written as

$$\begin{aligned}H = &-\frac{\hbar^2}{2m_1}\frac{\partial^2}{\partial l_a^2} - \frac{\hbar^2}{2m_4}\frac{\partial^2}{\partial l_b^2} + \frac{1}{2}K(l_a - l - l_0)^2 \\ &+ \frac{1}{2}K(l_b - l - l_0)^2 + \frac{q_1q_2}{4\pi\epsilon}\frac{1}{|l_a - l|} \\ &+ \frac{q_1q_3}{4\pi\epsilon}\frac{1}{|l_a + l|} + \frac{q_1q_4}{4\pi\epsilon}\frac{1}{|l_a + l_b|} \\ &+ \frac{q_2q_3}{4\pi\epsilon}\frac{1}{|2l|} + \frac{q_2q_4}{4\pi\epsilon}\frac{1}{|l_b + l|} + \frac{q_3q_4}{4\pi\epsilon}\frac{1}{|l_b - l|}, \end{aligned} \tag{53}$$

where ϵ is the permittivity.

The spontaneous polarization operator of the system is given by

$$P_{\text{spon}} = -q_1l_a - q_2l + q_3l + q_4l_b. \tag{54}$$

A. Nonpiezoelectric system

Consider the case $q_1 = q_4 = q$ and $q_2 = q_3 = -q$ where $q \neq 0$ (Fig. 7). The total charge of the system is zero and the system is inversion symmetric. In this case, the Hamiltonian takes the form

$$\begin{aligned}H = &-\frac{\hbar^2}{2m_1}\frac{\partial^2}{\partial l_a^2} - \frac{\hbar^2}{2m_4}\frac{\partial^2}{\partial l_b^2} + \frac{1}{2}K(l_a - l - l_0)^2 \\ &+ \frac{1}{2}K(l_b - l - l_0)^2 - \frac{q^2}{4\pi\epsilon}\frac{1}{|l_a - l|} \\ &- \frac{q^2}{4\pi\epsilon}\frac{1}{|l_a + l|} + \frac{q^2}{4\pi\epsilon}\frac{1}{|l_a + l_b|} + \frac{q^2}{4\pi\epsilon}\frac{1}{|2l|} \\ &- \frac{q^2}{4\pi\epsilon}\frac{1}{|l_b + l|} - \frac{q^2}{4\pi\epsilon}\frac{1}{|l_b - l|}. \end{aligned} \tag{55}$$

Observe that the Hamiltonian is invariant subject to the operation $l_a \longleftrightarrow l_b$.

The spontaneous polarization operator is

$$P_{\text{spon}} = -ql_a + ql - ql + ql_b = q(l_b - l_a), \tag{56}$$

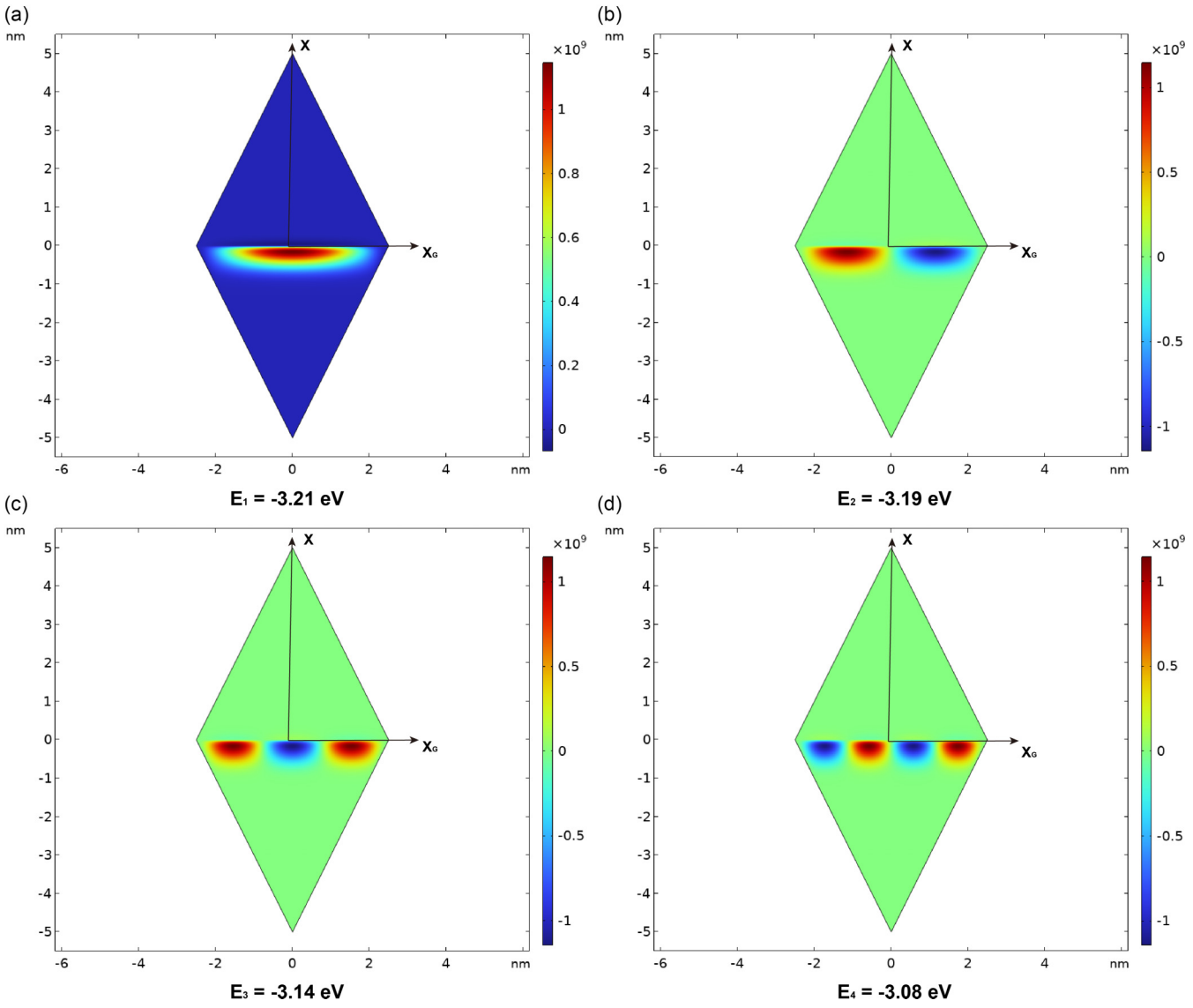

FIG. 4. The first four eigenstates plotted in X, X_G coordinates.

and it clearly changes sign under the operation $l_a \longleftrightarrow l_b$. Since the latter operation is a symmetry of the system, the spontaneous polarization must be zero.

B. Piezoelectric system

Consider now the case $q_1 = -q_4 = q$ and $q_2 = -q_3 = -q$ where $q \neq 0$ (Fig. 8). The total charge of the system is zero and the system is inversion asymmetric. In this case, the Hamiltonian takes the form

$$\begin{aligned} H = &-\frac{\hbar^2}{2m_1}\frac{\partial^2}{\partial l_a^2} - \frac{\hbar^2}{2m_4}\frac{\partial^2}{\partial l_b^2} + \frac{1}{2}K(l_a - l - l_0)^2 \\ &+ \frac{1}{2}K(l_b - l - l_0)^2 - \frac{q^2}{4\pi\epsilon}\frac{1}{|l_a - l|} \\ &+ \frac{q^2}{4\pi\epsilon}\frac{1}{|l_a + l|} - \frac{q^2}{4\pi\epsilon}\frac{1}{|l_a + l_b|} \\ &- \frac{q^2}{4\pi\epsilon}\frac{1}{|2l|} + \frac{q^2}{4\pi\epsilon}\frac{1}{|l_b + l|} - \frac{q^2}{4\pi\epsilon}\frac{1}{|l_b - l|}. \end{aligned} \tag{57}$$

The spontaneous polarization operator is

$$P_{\text{spon}} = -ql_a + ql + ql - ql_b = q(2l - l_a - l_b). \tag{58}$$

Note that the Hamiltonian and the spontaneous polarization are both unchanged under the operation $l_a \longleftrightarrow l_b$ so this symmetry does not force P_{spon} to be zero. In fact, the spontaneous polarization in general depends on the eigenstate

$$\langle P_{\text{spon}}\rangle_i = \int_{-L}^{L} dl_a \int_{-L}^{L} dl_b\, q(2l - l_a - l_b)\, |\psi_i(l_a, l_b)|^2. \tag{59}$$

IX. APPLICATION OF AN ELECTRIC FIELD

If an electric field $\mathcal{E}$ is applied to the system, the Hamiltonian changes by $H_{\mathcal{E}}$, where

$$H_{\mathcal{E}} = q_1\mathcal{E}l_a + q_2\mathcal{E}l - q_3\mathcal{E}l - q_4\mathcal{E}l_b. \tag{60}$$

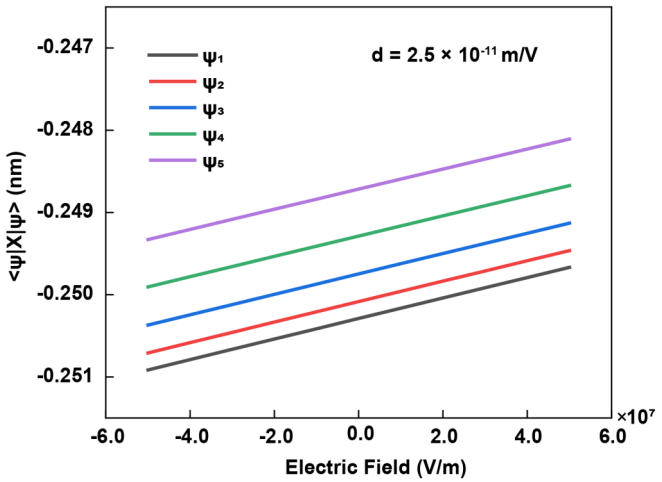

FIG. 5. A plot of the change in system length as a function of the electric field for the two-particle piezoelectric system. Note that the piezoelectric coefficient d_i does not depend on the eigenstate which is not given *a priori*.

A. Nonpiezoelectric system

For the nonpiezoelectric system,

$$H_{\mathcal{E}} = q\mathcal{E}l_a - q\mathcal{E}l + q\mathcal{E}l - q\mathcal{E}l_b = -q\mathcal{E}(l_b - l_a). \tag{61}$$

The unperturbed Hamiltonian H of the nonpiezoelectric system (i.e., the Hamiltonian in the absence of $H_{\mathcal{E}}$) is symmetric upon interchanging l_a and l_b. Therefore, all eigenstates of H are also eigenstates of the operator T that interchanges l_a and l_b [with eigenvalues $+1$ (symmetric states) and -1 (antisymmetric states)], i.e., T and H commute. All energy eigenstates of H can then be assigned as symmetric or antisymmetric upon interchanging l_a and l_b. Since $H_{\mathcal{E}}$ is odd upon interchanging l_a and l_b, it follows from first-order perturbation theory that all energies corresponding to nondegenerate eigenstates ψ^i_{ND} of the nonpiezoelectric system do not change to first order in the electric field, i.e.,

$$\langle\psi^i_{ND}|H_{\mathcal{E}}|\psi^i_{ND}\rangle = 0. \tag{62}$$

To demonstrate that piezoelectric constants indeed are zero for the present nonpiezoelectric system is difficult in the general case. First of all, the operator $\mathcal{L} = l_a + l_b$ has eigenvalue $+1$ while $H_{\mathcal{E}}$ has eigenvalue -1 upon interchanging l_a and l_b. The change in length due to the application of an electric field is given by

$$\begin{aligned}\Delta\langle\mathcal{L}\rangle_i &= \langle\psi_{i,\mathcal{E}}|\mathcal{L}|\psi_{i,\mathcal{E}}\rangle - \langle\psi_{i,\mathcal{E}=0}|\mathcal{L}|\psi_{i,\mathcal{E}=0}\rangle \\ &= \langle\psi_{i,\mathcal{E}} - \psi_{i,\mathcal{E}=0}|l_a + l_b|\psi_{i,\mathcal{E}=0}\rangle \\ &\quad + \langle\psi_{i,\mathcal{E}=0}|l_a + l_b|\psi_{i,\mathcal{E}} - \psi_{i,\mathcal{E}=0}\rangle + O(\mathcal{E}^2).\end{aligned} \tag{63}$$

For nondegenerate states, the first-order correction to the eigenstates from $H_{\mathcal{E}}$ is

$$|\psi_{i,\mathcal{E}}\rangle = |\psi_{i,\mathcal{E}=0}\rangle + \sum_{k\neq i}\frac{\langle\psi_{k,\mathcal{E}=0}|H_{\mathcal{E}}|\psi_{i,\mathcal{E}=0}\rangle}{E_{i,\mathcal{E}=0} - E_{k,\mathcal{E}=0}}|\psi_{k,\mathcal{E}=0}\rangle, \tag{64}$$

where $E_{i,\mathcal{E}=0}$ is the unperturbed energy of eigenstate $|\psi_{i,\mathcal{E}=0}\rangle$. Thus, the following applies for nondegenerate states:

$$\begin{aligned}|\psi_{i,\mathcal{E}=0}\rangle &= \text{symmetric function}, \\ |\psi_{i,\mathcal{E}}\rangle &= |\psi_{i,\mathcal{E}=0}\rangle + \text{an antisymmetric function of } O(\mathcal{E}),\end{aligned} \tag{65}$$

or

$$\begin{aligned}|\psi_{i,\mathcal{E}=0}\rangle &= \text{antisymmetric function}, \\ |\psi_{i,\mathcal{E}}\rangle &= |\psi_{i,\mathcal{E}=0}\rangle + \text{a symmetric function of } O(\mathcal{E}),\end{aligned} \tag{66}$$

where "symmetric function" ("antisymmetric function") means that the function is unchanged (changes sign) when l_a and l_b are interchanged. Since $l_a + l_b$ is symmetric upon interchanging l_a and l_b, it follows from Eq. (63) that

$$\Delta\langle\mathcal{L}\rangle_i = 0 + \text{an even function of } \mathcal{E}\ \ \forall\, i. \tag{67}$$

Hence, for nondegenerate states of a nonpiezoelectric system, the system length does not change sign when the electric field changes sign, and the piezoelectric constants vanish identically. Numerical results verify that this conclusion also holds for degenerate states.

B. Piezoelectric system

For the piezoelectric system,

$$H_{\mathcal{E}} = q\mathcal{E}l_a - q\mathcal{E}l - q\mathcal{E}l + q\mathcal{E}l_b = q\mathcal{E}(l_b + l_a - 2l). \tag{68}$$

It follows from Eq. (58) that the electric-field-induced change in polarization is proportional to the change in system length for the piezoelectric system

$$\Delta P = -q(\Delta l_a + \Delta l_b) = -q\Delta\mathcal{L}, \tag{69}$$

thus

$$\Delta\langle P\rangle_i = -q\Delta\langle\mathcal{L}\rangle_i, \tag{70}$$

where

$$\begin{aligned}\Delta\langle\mathcal{L}\rangle_i &= \langle\psi_{i,\mathcal{E}}|\mathcal{L}|\psi_{i,\mathcal{E}}\rangle - \langle\psi_{i,\mathcal{E}=0}|\mathcal{L}|\psi_{i,\mathcal{E}=0}\rangle \\ &= \langle\psi_{i,\mathcal{E}} - \psi_{i,\mathcal{E}=0}|\mathcal{L}|\psi_{i,\mathcal{E}=0}\rangle + \langle\psi_{i,\mathcal{E}=0}|\mathcal{L}|\psi_{i,\mathcal{E}} \\ &\quad - \psi_{i,\mathcal{E}=0}\rangle + O(\mathcal{E}^2).\end{aligned} \tag{71}$$

Note that it follows from both nondegenerate and degenerate perturbation theory that $|\psi_{i,\mathcal{E}} - \psi_{i,\mathcal{E}=0}\rangle$ is $O(\mathcal{E})$ and of the same symmetry as $|\psi_{i,\mathcal{E}=0}\rangle$. Thus, since $\mathcal{L}$ is unchanged with respect to interchanging l_a and l_b, $\Delta\langle\mathcal{L}\rangle_i$ is generally nonzero.

In analogy with the quantum-mechanical definition of the piezoelectric constants for two point charges connected by a spring, the quantized piezoelectric constants for the Auld system of four point charges and two springs are

$$d_i = \frac{\Delta\langle\mathcal{L}\rangle_i}{\Delta\mathcal{E}}. \tag{72}$$

Since $\Delta\langle\mathcal{L}\rangle_i$ is generally nonzero, the piezoelectric constants d_i are nonzero as well. Sometimes, it is convenient to calculate the piezoelectric constants in terms of the ratio between the change in strain and the change in electric field,

$$\tilde{d}_i = \frac{\Delta\langle\mathcal{L}\rangle_i/\langle\mathcal{L}\rangle_i}{\Delta\mathcal{E}}. \tag{73}$$

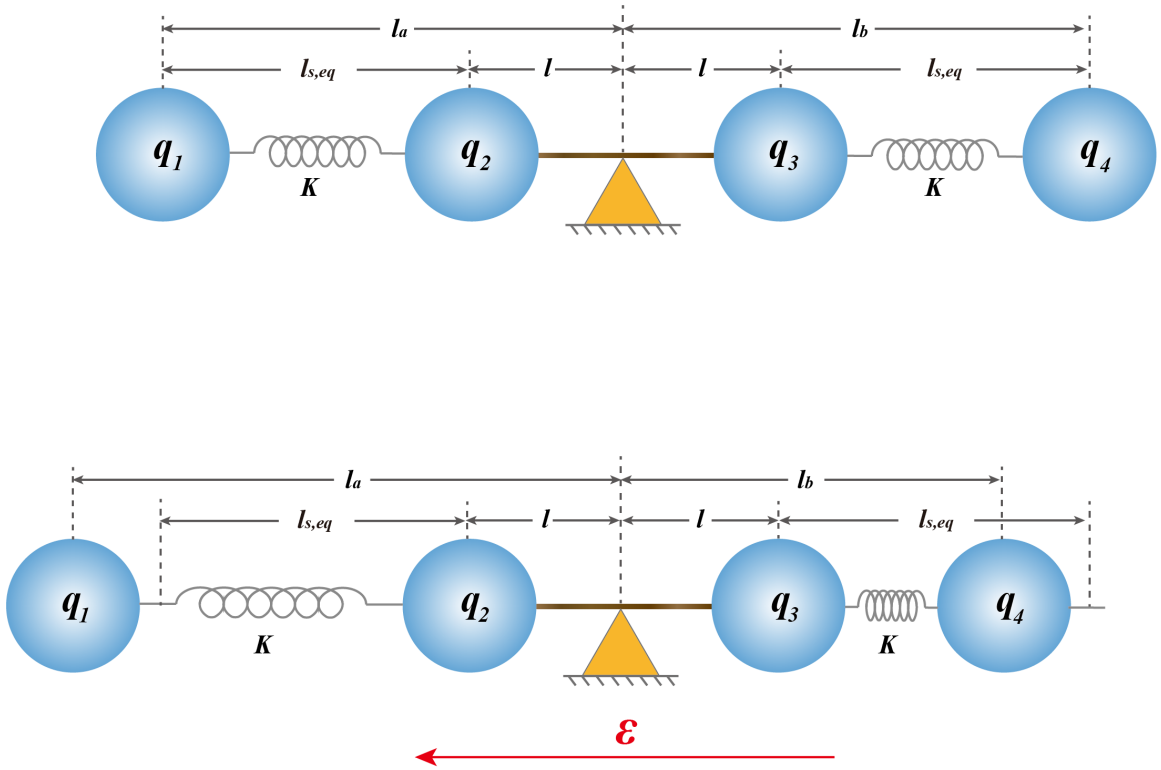

FIG. 6. Auld's system of four point charges and two springs. The illustration shows the response of a piezoelectric system to an applied electric field. The spring deformations shown in the figure correspond to either the nonpiezoelectric case where $q_2 = -q_1; q_3 = q_2; q_4 = q_1$, or the piezoelectric case where $q_2 = -q_1; q_3 = -q_2; q_4 = -q_1$.

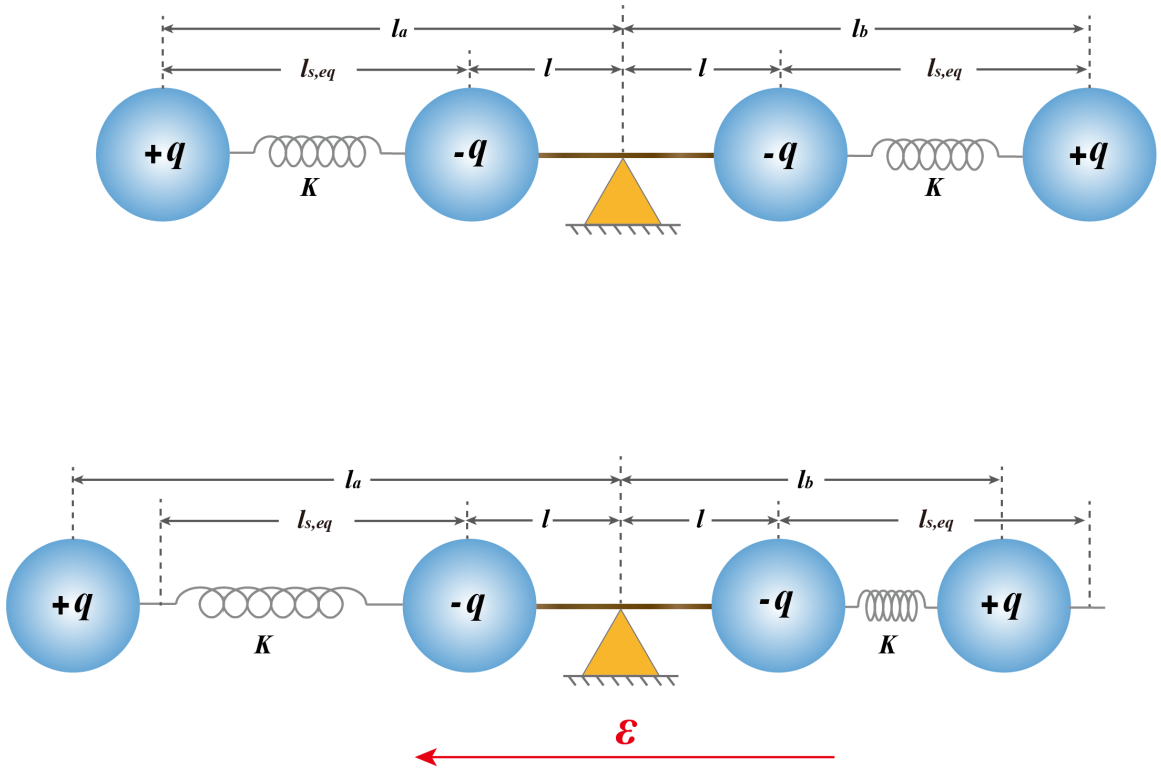

FIG. 7. Auld's system of four point charges and two springs (non-piezoelectric system). The charges counted from left to right take the values $q_1 = +q$, $q_2 = -q$, $q_3 = -q$, and $q_4 = +q$. The system length $l_a + l_b$ is unchanged subject to the application of a small electric field.

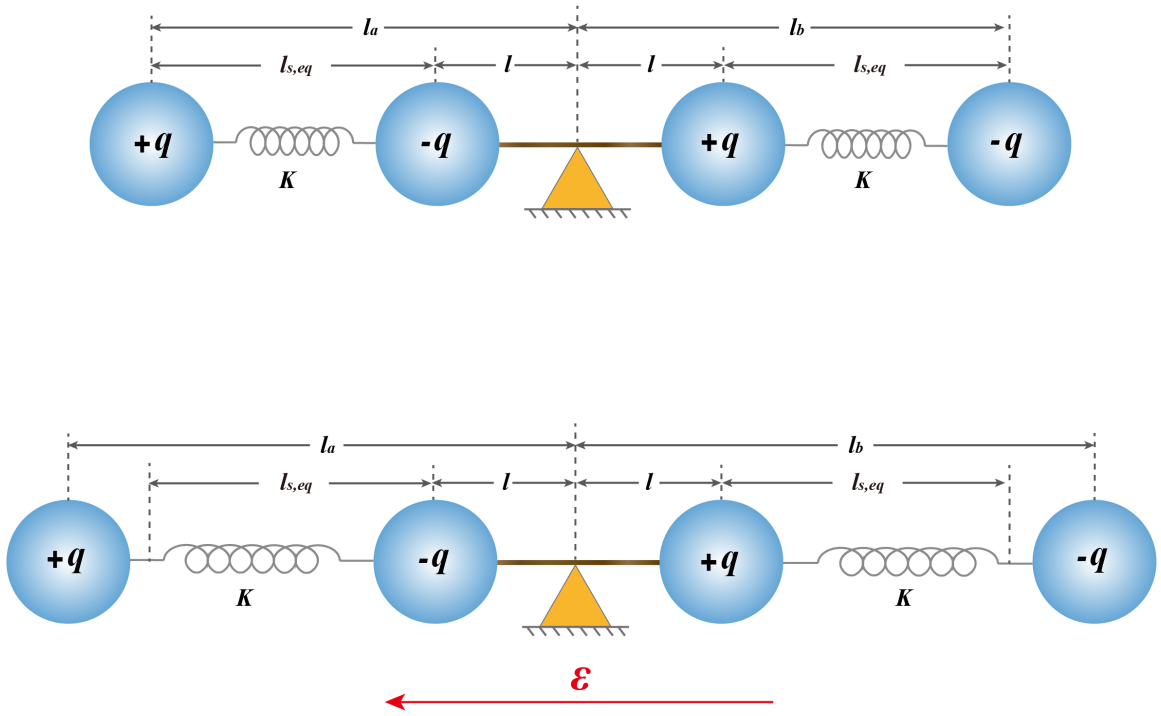

FIG. 8. Auld's piezoelectric system of four point charges and two springs (piezoelectric system). Charges from left to right take the values $q_1 = +q$, $q_2 = -q$, $q_3 = q$, and $q_4 = -q$. The system length $l_a + l_b$ changes subject to the application of a small electric field.

X. TEMPERATURE DEPENDENCE OF THE PIEZOELECTRIC CONSTANT

We will now briefly discuss how the temperature dependence of the piezoelectric constant for a simple system weakly coupled to its environment can be found using the general approach of statistical physics [43]. For any operator X of a quantum system, the temperature dependence of the average of X is given by

$$\langle X\rangle = \mathrm{Tr}(\rho X) = \sum_i \langle i|\rho X|i\rangle, \tag{74}$$

where the summation is over all eigenstates $|i\rangle$ and ρ is the statistical weight

$$\rho = \frac{\exp(-\beta H)}{Z(\beta)}. \tag{75}$$

In Eq. (75), H is the system Hamiltonian operator, $\beta = 1/(k_B T)$, k_B is Boltzmann's constant, T is the temperature, and $Z(\beta)$ is the partition function defined by

$$Z(\beta) = \mathrm{Tr}(\exp(-\beta H)). \tag{76}$$

The temperature dependence of the piezoelectric constant $d_i(T)$ can now be determined by calculating the change in the average system length due to a change in the electric field,

$$d_i(T) = \frac{\Delta \mathrm{Tr}(\rho \mathcal{L})}{\Delta \mathcal{E}}, \tag{77}$$

where $\mathcal{L}$ is the system-length operator.

XI. NUMERICAL RESULTS FOR AULD'S PIEZOELECTRIC QUANTUM SYSTEM

A. Eigenstates and energies when $\mathcal{E} = 0$

In Fig. 9, the first several wave functions of the Hamiltonian in Eq. (57) are shown. The parameters used in the calculation are listed in Table I. Similar to the nonpiezoelectric system, the unperturbed Hamiltonian H of the piezoelectric system (i.e., the Hamiltonian in the absence of $H_{\mathcal{E}}$) is symmetric upon interchanging l_a and l_b. Therefore, all eigenstates of H are also eigenstates of the operator T that interchanges l_a and l_b (with eigenvalues ± 1), i.e., T and H commute. Hence, all energy eigenstates of H can be assigned as symmetric or antisymmetric upon interchanging l_a and l_b. Observe that the ground state $S1$ with energy -124.78 eV is nondegenerate and symmetric upon interchanging l_a and l_b while the second

TABLE I. Parameters for the piezoelectric system associated with the Hamiltonian in Eq. (57).

Parameters	Value	Description
L	1.0×10^{-8} [m]	Computational domain length
l	5.0×10^{-10} [m]	Position of the fixed charge (q_2, q_3)
l_0	1.0×10^{-9} [m]	Position of the moving charge (q_1, q_4)
ϵ_0	8.85×10^{-12}[F/m]	Vacuum dielectric constant
k_C	9×10^9 [N m^2/C^2]	Coulomb constant
k	5 [N/m]	Elastic coefficient of spring
E_0	1.0×10^{-7} [V/m]	Electric field intensity
q	1.6×10^{-19} [C]	Unit charge
m_1	9.1×10^{-31} [kg]	Mass of charge q_1
m_4	9.1×10^{-31} [kg]	Mass of charge q_4

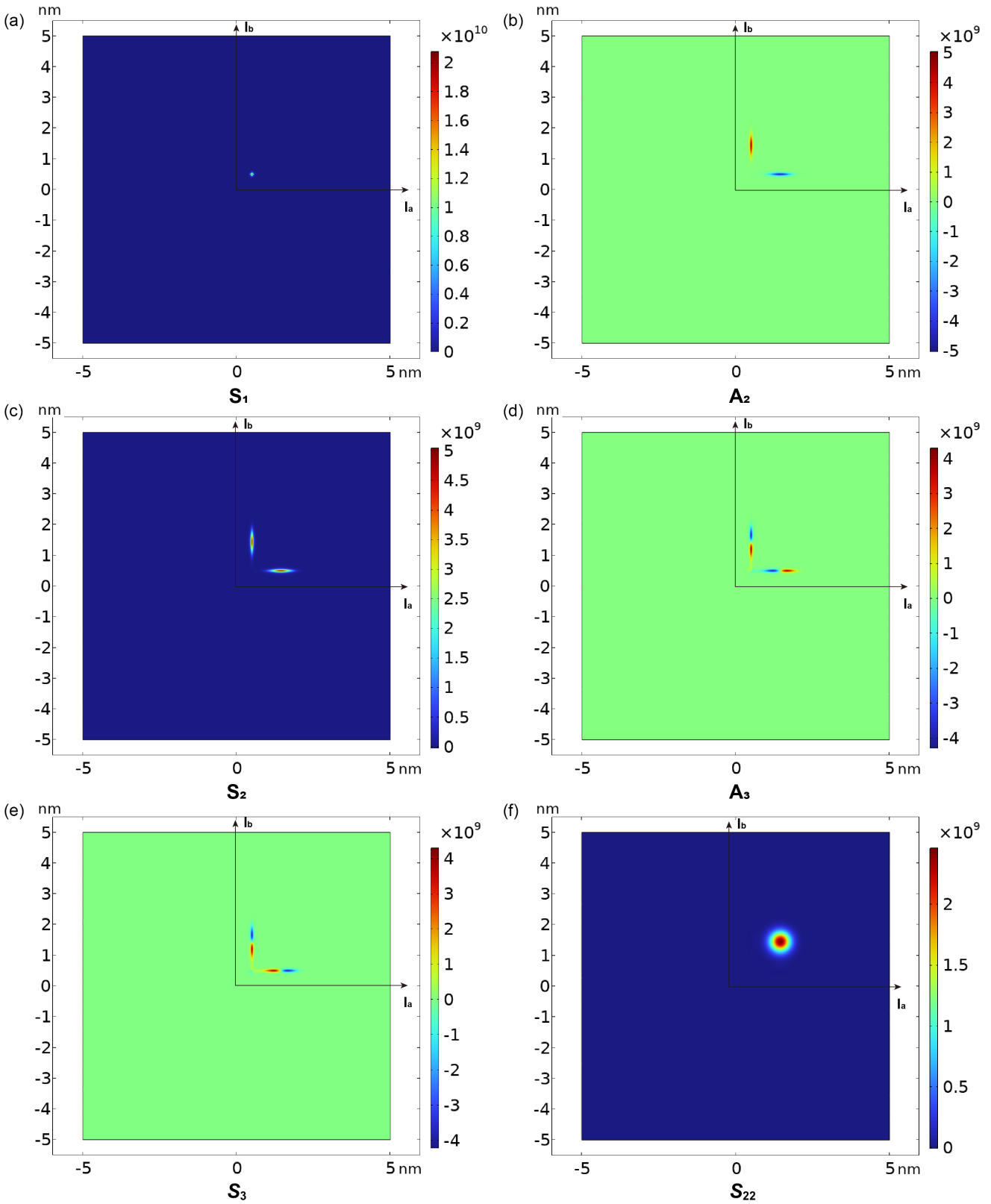

FIG. 9. The first five wave functions $S1, A2, S2, A3, S3$ and a higher excited state (the second nondegenerate state) $S22$ for Auld's piezoelectric system shown in Fig. 8. $S1$ is the ground state and the first nondegenerate symmetric state (energy -124.78 eV; top left panel). $A2$ and $S2$ are antisymmetric and symmetric degenerate states, respectively, with the (same) second-lowest energy (energy -63.14 eV; top right and middle left panels). $A3$ and $S3$ are antisymmetric and symmetric degenerate states with the (same) third-lowest energy (energy -61.72 eV; middle right and lower left panels). $S22$ is a higher-excited symmetric state and the second nondegenerate state (energy -1.46 eV; lower right panel).

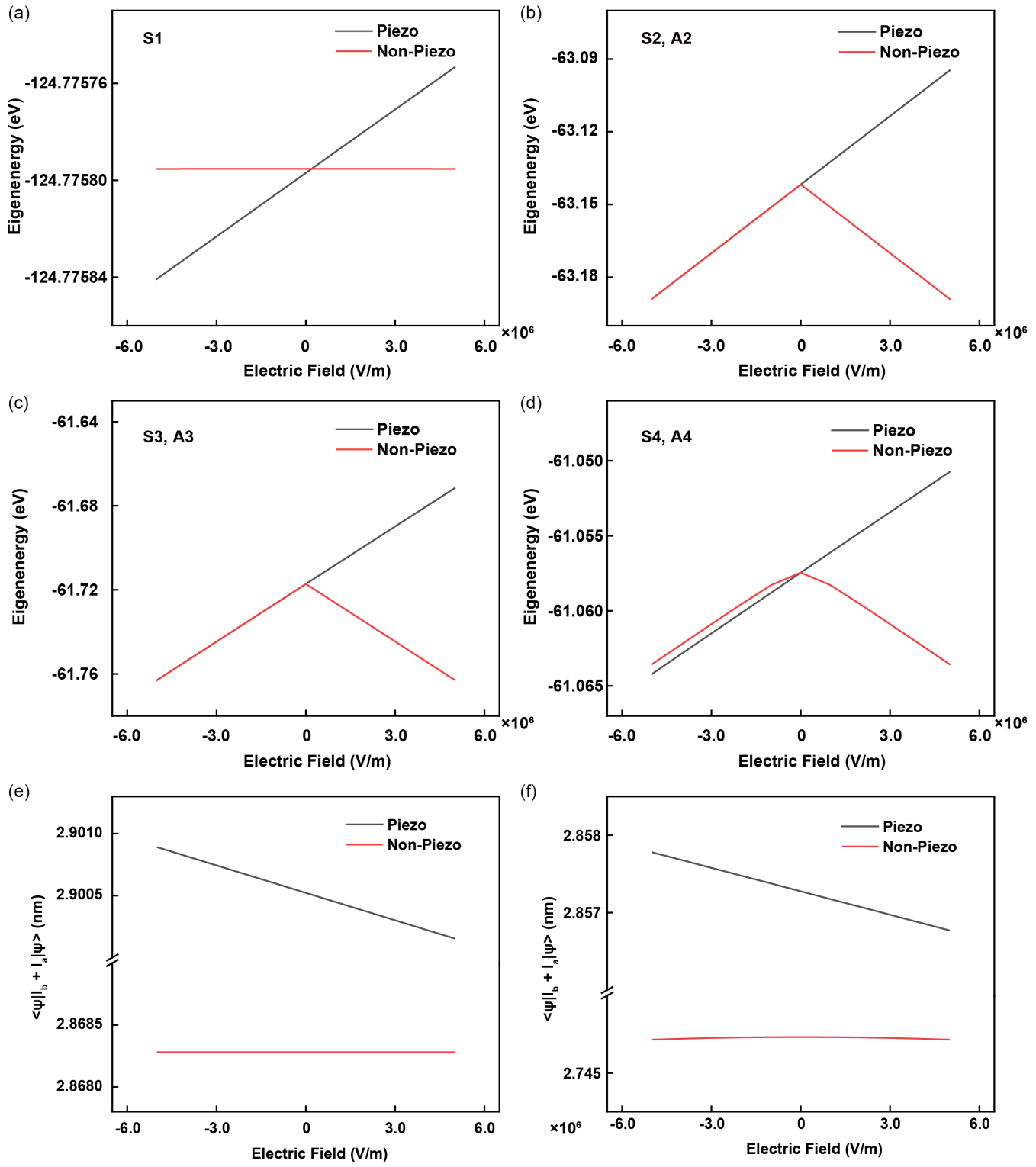

FIG. 10. Energy changes as a function of electric field for the piezoelectric and the nonpiezoelectric systems shown in Figs. 7 and 8. Energies for states $S1$, $S2$, $S3$, are $S4$ are shown in the top left, top right, middle left, and middle right panels. The energy change of $S1$ due to an applied electric field is vanishingly small to computational accuracy for both the piezoelectric and the nonpiezoelectric systems. Note that the states $S2$ and $A2$ share the same energy dependence on the electric field. The same applies to the states $S3$ and $A3$, and a similar result holds for states $S4$ and $A4$, etc. The two lower panels correspond to the second nondegenerate state (lower left) and the third nondegenerate state (lower right).

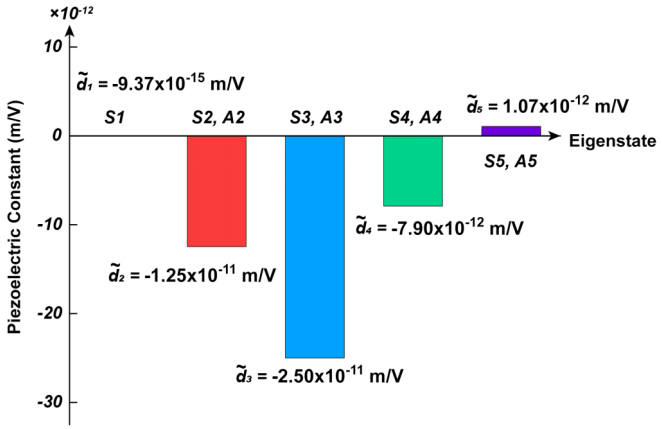

FIG. 11. Piezoelectric constants $\tilde{d}_i = \frac{\Delta\langle\mathcal{L}\rangle_i/\langle\mathcal{L}\rangle_i}{\Delta\mathcal{E}}$ computed for different eigenstates of Auld's piezoelectric system shown in Fig. 8.

($A2$) and third ($S2$) states are degenerate (energy -63.14 eV) and antisymmetric and symmetric upon interchanging l_a and l_b, respectively. Similarly, the fourth ($A3$) and fifth ($S3$) states are degenerate (-61.72 eV) antisymmetric and symmetric states upon interchanging l_a and l_b, respectively. The sixth state shown in the plot is the first-higher excited nondegenerate symmetric state $S22$ with energy -1.46 eV.

B. Energy changes due to an external electric field

In Fig. 10 changes in the first several eigenstate energies with the application of an external electric field are listed. Note that since the ground-state expectation values of the operators l_a and l_b both are equal to l (corresponding to completely compressed springs) the electric-field perturbation of the piezoelectric system [Eq. (68)] does not affect the ground-state energy since $H_{\mathcal{E}} \propto l_b + l_a - 2l$. Hence the ground-state energy is independent of the electric field to first order in the electric field. In contrast, all other state eigenstates depend on the electric field including the higher-excited nondegenerate states. Observe also that the energies of the nonpiezoelectric system (Fig. 7) are even functions of the applied electric field which is in accordance with symmetry as discussed above.

C. Piezoelectric constants

The piezoelectric constants associated with the different eigenstates of the piezoelectric system (Fig. 8) depend on the specific eigenstate for any fixed parameter set (Fig. 11). This quantum-mechanical result is fundamentally different compared to the classical piezoelectricity result for which the piezoelectric constant is a constant. Observe that the ground state is characterized by a very small piezoelectric constant $\tilde{d}_1 = \frac{\Delta\langle\mathcal{L}\rangle_1/\langle\mathcal{L}\rangle_1}{\Delta\mathcal{E}} = -9.37 \times 10^{-15}$ m/V due to its sharp localization at $l_a = l_b = l$ using first-order perturbation theory. The first six exited states ($S2, A2, S3, A3, S4, A4$) show substantially stronger piezoelectricity than the ground state (a factor of 100–1000 higher) since the former states are much less localized in $l_a - l_b$ space as inspection of Fig. 9 reveals. Note that the order of magnitude for the largest $\tilde{d}_i$ constants are similar to those of known piezoelectric semiconductors (GaAs, ZnO). Our results also confirm that for the nonpiezoelectric system (Fig. 7) the piezoelectric constant is zero for all states to computational accuracy as it must be from symmetry.

XII. CONCLUSIONS

The piezoelectric d constant of a simple one-dimensional classical inversion-asymmetric assembly of electric point charges and mechanical springs is known to be a constant but dependent on the electric charge values and the mechanical spring constants. In the present work, it is demonstrated that if the Schrödinger Hamiltonian of the same system of electric charges and mechanical springs is solved subject to open boundary conditions with respect to the moving charges, the piezoelectric constant, defined as the ratio between the expectation value of the system length and the applied electric field, becomes quantized and eigenstate dependent. It is shown that the piezoelectric constant vanishes if the system Hamiltonian is inversion-symmetric. Numerical results for eigenstates and eigenstate-dependent piezoelectric constants are discussed for two piezoelectric assemblies of point charges and mechanical springs.

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