Design of a Biased Stark Trap of Molecules Moving Adiabatically in an Electric Field

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Abstract

It is shown that Maxwell's equations in a vacuum do not allow for a local maximum in the value of the electric field E^2, but do allow for a local minimum. Such a field minimum creates a trap of neutral particles that exhibit a Stark effect. Specific criteria are given for the design of such a trap and results of numerical calculations of sample trap potentials are presented.

I. INTRODUCTION

A suitable arrangement of biased conductors [1] leads to an electrostatic field of zero magnitude at a central location that grows to tens of kV/cm away from the center. Such a field has allowed polar molecules to be confined in far deeper potential wells than may be realized with magnetic traps [2] [3]. The neutral particles we consider do not move in a potential proportional to the electrostatic potential V, but instead, the motion is dictated by the spatial dependence of the shift quantum energy due to the local magnitude of the electric field. For this reason, the electrostatic trapping we consider does not contradict the fact that a charged particle cannot be held in stable equilibrium by electrostatic forces alone (as first pointed out by Earnshaw [4].) In the limit of adiabatic motion, the effective potential is dependent only on the particle quantum state and the local magnitude of the electric field $E = |\vec{E}|$. Although Maxwell's equations do not allow a local minimum in V, no such constraint forbids a local minimum in E. The purpose of this work is to show that it is possible to build an electrostatic trap that has a non-zero bias field at the center. Our device may serve the same purpose as the Ioffe [5]-Pritchard [6] magnetostatic trap; namely the suppression of nonadiabatic motion that occurs in regions where the field (and hence the energy splitting between quantum states) goes to zero or the gradient of the trap potential diverges. We speculate that this problem of nonadiabatic motion will be especially severe for those cases in which the Stark energy U of the molecules grows quadratically rather than linearly with electric field

Throughout this work we consider a hypothetical particle traveling in the quadratic Stark potential

$$U = \alpha E^2, \tag{1}$$

where $\vec{E}$ is the spatially dependent electric field and α is a constant. In the next section we show that Maxwell's equations allow for a local minimum in E^2, but do not allow for a local maximum. In section III we show requirements on the potential V for a local minimum in E^2 to exist and provide a practical illustration of such a biased Stark trap. The formal theorem we prove concerning biased Stark traps is stated in section IV.

II. SIMPLE PROOF THAT THERE CAN BE NO SPATIAL LOCAL MAXIMUM IN E^2

It is straightforward to show that the Laplacian of E^2 is nonnegative. We start from

$$\nabla^2 E^2 = 2\left(\partial_i E_j\right)\left(\partial_i E_j\right) + 2\left[\vec{E}\cdot\nabla^2\vec{E}\right]$$

Because $\vec{E}$ is harmonic, the term in square brackets is zero, leading to

$$\nabla^2 E^2 = 2\sum_i \left|\vec{\nabla} E_i\right|^2 \geq 0. \tag{2}$$

The fact that the Laplacian of E^2 is everywhere nonnegative proves that there cannot exist a local quadratic maximum in $E^2(x, y, z)$. In the following section we eliminate the possibility of local maxima in E^2 to any order in $\vec{r}$.

III. DESIGN OF A BIASED STARK TRAP

In what follows we investigate the specific constraints on an electric field that allow for a local minimum in U at a point at which $E^2 \neq 0$. Specifically, we find the spherical-harmonic expansion coefficients A_{lm} of the electrostatic potential that lead to a biased Stark trap.

A. Expansion of the Stark potential u in terms of spherical harmonics

Letting $u = U/\alpha E_o^2$ where E_o is the magnitude of the electric field at the center of the trap, the quadratic Stark potential becomes $u = \vec{E} \cdot \vec{E}/E_o^2$ which can be written as half of the Laplacian of V^2 by applying the condition $\nabla^2 V = 0$:

$$u = \frac{1}{2} \nabla^2 V^2 / E_o^2. \tag{3}$$

We now expand the potential about the location of the local minimum:

$$V = E_o a \sum_{\ell, m} A_{\ell m} \left(\frac{r}{a} \right)^{\ell} C^{\ell}_{m}(\theta, \phi). \tag{4}$$

Here $\overline{Y}_{\ell m}(\theta, \phi)$ are related to the normalized spherical harmonics by

$$\overline{Y}_{\ell m}(\theta, \phi) = \left(\frac{4\pi}{2\ell + 1} \right)^{1/2} Y_{\ell m}(\theta, \phi) \tag{5}$$

and a is a parameter with units of distance. Squaring this expanded form of the potential and taking the Laplacian leads to

$$u = \sum_{\ell_1, m_1, \ell_2, m_2, L} A_{\ell_1 m_1} A_{\ell_2 m_2} D^{L, \ell_1, \ell_2}_{m_1, m_2} \overline{Y}_{L, m_1 + m_2}(\theta, \phi) \left(\frac{r}{a} \right)^{\ell_1 + \ell_2 - 2}, \tag{6}$$

where $D^{L, \ell_1, \ell_2}_{m_1, m_2}$ is related to the spherical harmonic triple integral [7] and is given in terms of 3-j symbols by

$$D^{L,\ell_1,\ell_2}_{m_1,m_2} = (-1)^{m_1+m_2}(2L+1)\left[\frac{(\ell_1+\ell_2)(\ell_1+\ell_2+1)-L(L+1)}{2}\right]$$
$$\times \begin{pmatrix} \ell_1 & \ell_2 & L \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \ell_1 & \ell_2 & L \\ m_1 & m_2 & -(m_1+m_2) \end{pmatrix}, \tag{7}$$

where the factor in square brackets represents the action of the Laplacian. Note that $D^{L,\ell_1,\ell_2}_{m_1,m_2} = 0$ unless $L+\ell_1+\ell_2$ is even (because of parity), $|m_i| \leq \ell_i$, and $|\ell_1-\ell_2| \leq L \leq l_1+l_2-1$.

B. Constraints on the expansion coefficients $A_{\ell m}$ of the biased trap potential

Now we assume that the coordinate system has been fixed so that $\vec{E}_o = E_o\hat{z}$ at the origin. This choice requires

$$A_{1\pm 1} = 0 \text{ and } A_{10} = -1. \tag{8}$$

Separating those terms in the expansion of u that contain the A_{10} moment from those that do not leads to

$$u = 1 - 2\sum_{\ell>1,m} A_{\ell,m} D^{\ell-1,1,\ell}_{0,m} \overline{Y}_{\ell-1,m}(\theta,\phi)\left(\frac{r}{a}\right)^{\ell-1}$$
$$+ \sum_{\ell_1>1,\ell_2>1,m_1,m_2} \sum_{L=|\ell_1-\ell_2|}^{\ell_1+\ell_2-1} A_{\ell_1 m_1} A_{\ell_2 m_2} D^{L,\ell_1,\ell_2}_{m_1,m_2} \overline{Y}_{L,m_1+m_2}(\theta,\phi)\left(\frac{r}{a}\right)^{\ell_1+\ell_2-2}. \tag{9}$$

Let us first consider the second term in this expression, i.e., the term resulting from the expansion of $A_{10}A_{\ell,m}Y_{10}Y_{\ell,m}$. No element of this summation has a Y_{00} coefficient. This is of crucial importance. Without a Y_{00} contribution, the lowest order term cannot be positive definite. Thus if the lowest order contribution results only from a cross term with A_{10}, one cannot have a local minimum at $r=0$. At first this might make one conclude that a trap is impossible. However, the $A_{\ell\pm\ell}$ coefficients do not contribute to this sum. Thus we might be able to manage a minimum of order $r^{2\ell_n-2}$ provided

$$A_{lm} \begin{cases} = 0 \text{ for } 1 < \ell < \ell_n \\ \neq 0 \text{ for } \ell = \ell_n \text{ and } m = \pm\ell_n \\ = 0 \text{ for } \ell_n \leq \ell < 2\ell_n - 1 \text{ and } m \neq \pm\ell \end{cases}. \tag{10}$$

With these conditions and taking advantage of the fact that $A_{\ell,m}$ must equal $(-1)^m A^*_{\ell,-m}$ for V to be real, the trap potential becomes

$$
\begin{aligned}
u = 1 + &\left[-2\sum_m A_{2\ell_n-1,m} D^{2\ell_n-2,1,2\ell_n-1}_{0,m} \overline{Y}_{2\ell_n-2,m}(\theta,\phi)\right. \\
&\left.+ 2\sum_{L=0}^{l_n-1}(-1)^{\ell_n}|A_{\ell_n,\ell_n}|^2 D^{2L,\ell_n,\ell_n}_{\ell_n,-\ell_n}\overline{Y}_{2L,0}(\theta,\phi)\right]\left(\frac{r}{a}\right)^{2l_n-2} \\
&+O(r^{2\ell_n-1}). \qquad (11)
\end{aligned}
$$

Note $Y_{2\ell_n-2,m\neq 0}$ cannot be positive definite in ϕ. Thus a non-zero coefficient $A_{2\ell_n-1,m}$ with $m \neq 0$ will only serve to lower the trap depth in certain azimuthal directions. For this reason, we now assume $A_{2\ell_n-1,m} = 0$ for $m \neq 0$. These assumptions allow us to simplify Eq. (11) to

$$
\begin{aligned}
u = 1 + &\left[\gamma P_{2\ell_n-2}(\cos\theta) + |\beta|^2 \sin^{2\ell_n-2}\theta\right]\left(\frac{r}{a}\right)^{2\ell_n-2} \\
&+O(r^{2\ell_n-1}). \qquad (12)
\end{aligned}
$$

Here the non-zero expansion coefficients of the electrostatic potential are given by

$$
A_{10} = -1, \qquad (13a)
$$

$$
A_{2\ell_n-1,0} = \frac{\gamma}{(2-4\ell_n)}, \qquad (13b)
$$

$$
\begin{aligned}
A_{\ell_n,\ell_n} &= (-1)^{\ell_n} A^*_{\ell_n,-\ell_n} \\
&= \frac{\beta}{2\ell_n\sqrt{P_{2\ell_n}(0)}}. \qquad (13c)
\end{aligned}
$$

Equation (12) is our final expression for the biased electrostatic trap potential. It is valid provided the relationships of Eqs. (13a)-(13c) hold and $A_{\ell,m} = 0$ for all other coefficients with $\ell < 2\ell_n$ (coefficients of order $2\ell_n$ and greater do not contribute to order $r^{2\ell_n-2}$.) Note that although the coefficient of the $P_{2\ell_n-2}(\cos\theta)$ term is arbitrary in both sign and magnitude, the sign of the $\sin^{2\ell_n-2}\theta$ term is necessarily positive. Because $\ell_n \geq 2$, $P_{2\ell_n-2}(\cos\theta)$ has zeros in the range of $0 < \theta < \pi$, so there must be some direction for which the potential is a local minimum. Thus an extremum cannot be a local maximum, but is instead either a local minimum or a saddle point. A local minimum is created if and only if

$$\gamma > 0 \tag{14}$$

and

$$|\beta|^2 > \frac{-\gamma \, P_{2\ell_n - 2}(\cos\theta_{\rm min})}{\sin^{2\ell_n - 2}\theta_{\rm min}}. \tag{15}$$

Here $\theta_{\rm min}$ is the angle for which $P_{2\ell_n-2}(\cos\theta)/\sin^{2\ell_n-2}\theta$ is a minimum. Because we are only interested in potentials that exhibit a local minimum, γ is positive and we can redefine our scaling parameter a so that

$$\gamma = 1. \tag{16}$$

C. Design of a quadratic ($\ell_n = 2$) trap

For the case that $\ell_n = 2$, we can create an isotropic trap provided $\beta = (3/2)^{1/2}$. For this case, Eq. (12) reduces to

$$u = 1 + \left(\frac{r}{a}\right)^2 + O\left(\left(\frac{r}{a}\right)^4\right), \tag{17}$$

where

$$A_{1,0} = -1, \; A_{1,\pm 1} = 0, \tag{18a}$$

$$A_{2,2} = A_{2-2} = \frac{1}{2}, \tag{18b}$$

$$A_{2,0} = A_{2,\pm 1} = 0, \tag{18c}$$

$$A_{3,0} = -\frac{1}{6}, \tag{18d}$$

$$A_{3,\pm 1} = A_{3,\pm 2} = A_{3 \pm 3} = 0, \tag{18e}$$

$$A_{4,\pm 2} = \frac{1}{4\sqrt{15}}, \tag{18f}$$

$$A_{4,0} = A_{4,\pm 1} = A_{4,\pm 3} = 0. \tag{18g}$$

Here unspecified expansion coefficients do not affect the expansion of the Stark potential to order r^3. The constraints of Eqs. (18f) and (18g) have been added to zero out the r^3 contribution to u.

Construction of a laboratory device requires us to devise an electrode configuration that creates an electric potential meeting the constraints of Eqs. (18a)-(18g). We examine the properties of three different configurations using a combination of custom C code and the software packages SIMION (Idaho National Engineering and Environmental Laboratory) and Mathematica (Wolfrom Research). The first configuration considered, the *six-wire* trap, consists of six semi-infinite wires along the Cartesian axes. The electrodes on the positive and negative x-axes are held at a voltage of $+V$, the electrodes on the positive and negative y-axes are held at $-V$, and the electrodes on the positive and negative z-axes are held at $-V$ and $+V$, respectively. (Fig. 1.A). Symmetry arguments show that this configuration satisfies Eqs. (18a), (18c), and (18e). The other requirements are not met quantitatively, however, numerical simulations show that a trap is formed, although it suffers from significant anisotropy. The ratio between the escape potential and the potential in the center of the well for this trap is approximately 1.1.

A more isotropic trap is created if the electrode surfaces are taken to be equipotential surfaces of the ideal potential, truncated at some radius. To do this, the constants a and E_o are taken to be 1, and all $A_{\ell m}$ moments with $\ell > 4$ are taken to be zero. The electrodes are then all points within a sphere of radius 2.5 centered at the origin with $V \geq 1.5$ or $V \leq -1.5$. Electrodes created in this way are shown in Fig. 1.B1. This trap, which we call *the tennis ball trap* bears a striking resemblence to the magnetic baseball trap proposed by Bergman and et al [8] and demonstrated by Monroe et al [9]. As can be seen in Fig. 1.B2, the tennis-ball trap creates a highly creates isotropic near the origin, as predicted. The ratio of escape potential to potential at the center of the trap for this case is approximately 1.6. This configuration creates a potential that very nearly matches the ideal potential. If precise quantification of the trap potential is required, these electrodes could be created using surface machining techniques. However, the shape of the electrodes suggests a simpler design.

The third *chain-link* trap is constructed from two electrodes, each created from a long rod bent through a half torus to create a U-shape. The two electrodes are interlocked as shown in Fig. 1.C1. The negative electrode lies in the y-z plane, opening down whereas the positive electrode lies in the x-z plane, opening up. When parameters are optimized empirically, the resultant trap is fairly isotropic, as can be seen in Fig. 1.C2 and Fig. 2. In addition, the maximum electric field present in the entire configuration is substantially lower than that found in the six-wire or tennis-ball traps because of the absence of sharp edges. The parameters we determine for a roughly spherical trap are as follows: Taking the diameter of the electrode rods as d, the radius of curvature of the centerline of the half torus bend is $2d$. The center of curvature of each torus is offset $d/3$ from the origin along the z-axis toward the other half-torus. With this geometry, the field E_o in the center of the trap is $0.60\,\Delta V/d$ were ΔV is the difference of the potentials on the electrodes. The minimum potential as a function of distance from the origin for such a trap is shown in Fig. 3. The ratio between the escape E^2 potential and the center potential E_o^2 is 2.5 and the ratio between the maximum electric field in the system to E_o is 4.6. Because of its simple construction compared to the tennis-ball trap, its relative isotropy compared to the six-wire trap, and its low maximum field, this is presumably the trap most suitable for our research goals.

IV. SUMMARY

In this paper we have shown that it is both possible and practical to construct an electrostatic trap of low-field seeking particles (i.e., particles with a Stark energy that increases with increasing field strength.) We have also proven the following theorem that eliminates the possibility of creating a trap of high-field seeking particles:

Theorem: *Let $V(\vec{r})$ be a real scalar function and U be a potential function given by $U = (\vec{\nabla}V)\cdot(\vec{\nabla}V)$. Also assume a region of space for which $\nabla^2 V = 0$. If an interior point of this region contains an extremum with $\vec{\nabla}U = 0$ but $U \neq 0$, then the extremum is not a local maximum, but is instead either a local minimum or a saddle point.*

This theorem has been proven for extrema of any order. Moreover, we can always find a potential U that has a local minimum of any even order at a point where $U \neq 0$. The following corollary provides an extension to Earnshaw's theorem to neutral particles moving adiabatically in an electric field:

Corollary: *A high-field seeking particle (i.e., a particle for which the Stark energy decreases with increasing field strength) moving adiabatically in an electrostatic field cannot be held in stable equilibrium by that field alone.*

V. ACKNOWLEDGEMENTS

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FIGURES

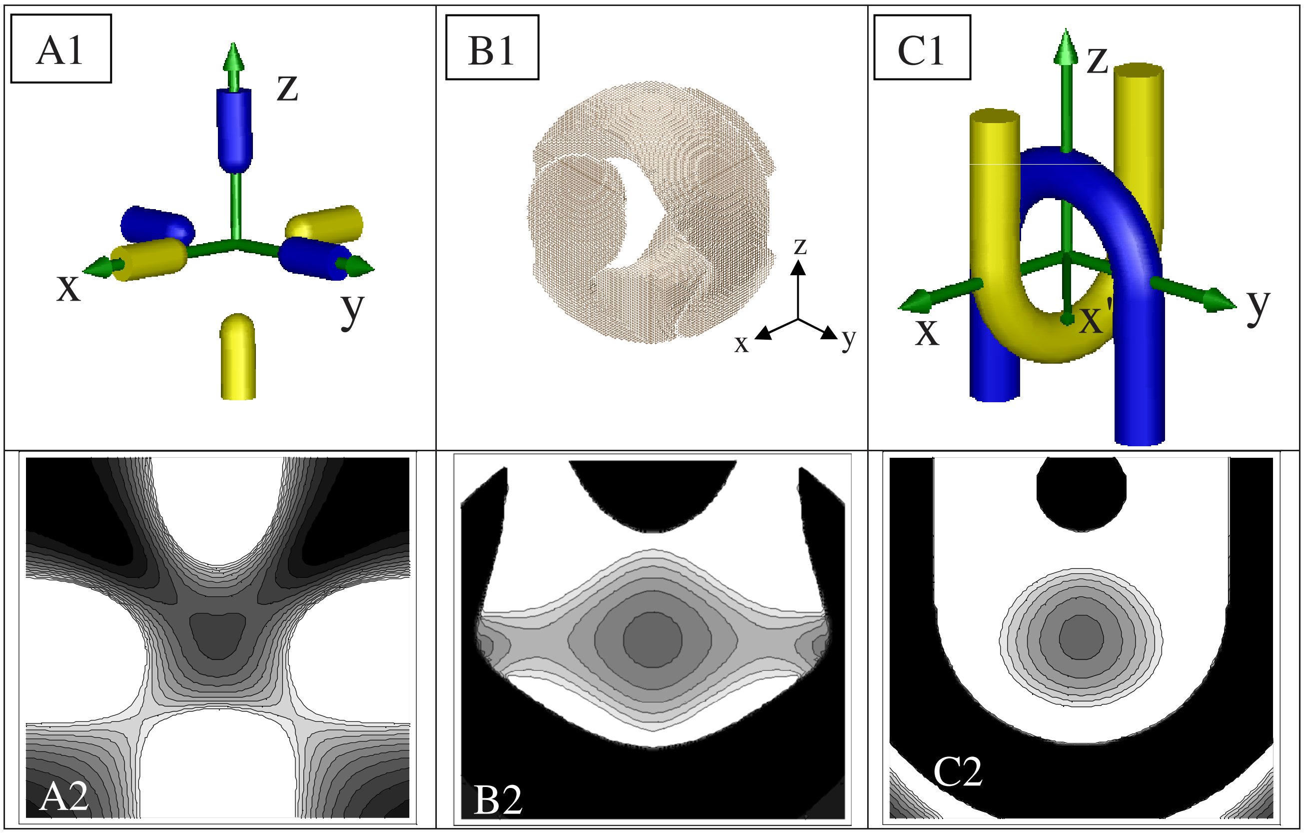

FIG. 1. Trap geometry (1) and E^2 Stark potential in the x-z plane (2) for the six-wire trap (A), tennis ball trap (B) and chain-link trap (C). The contour scale is linear with black regions indicating $E^2 = 0$ and white regions indicating values of $E^2 > 3.6E_o^2$.

Figure 1

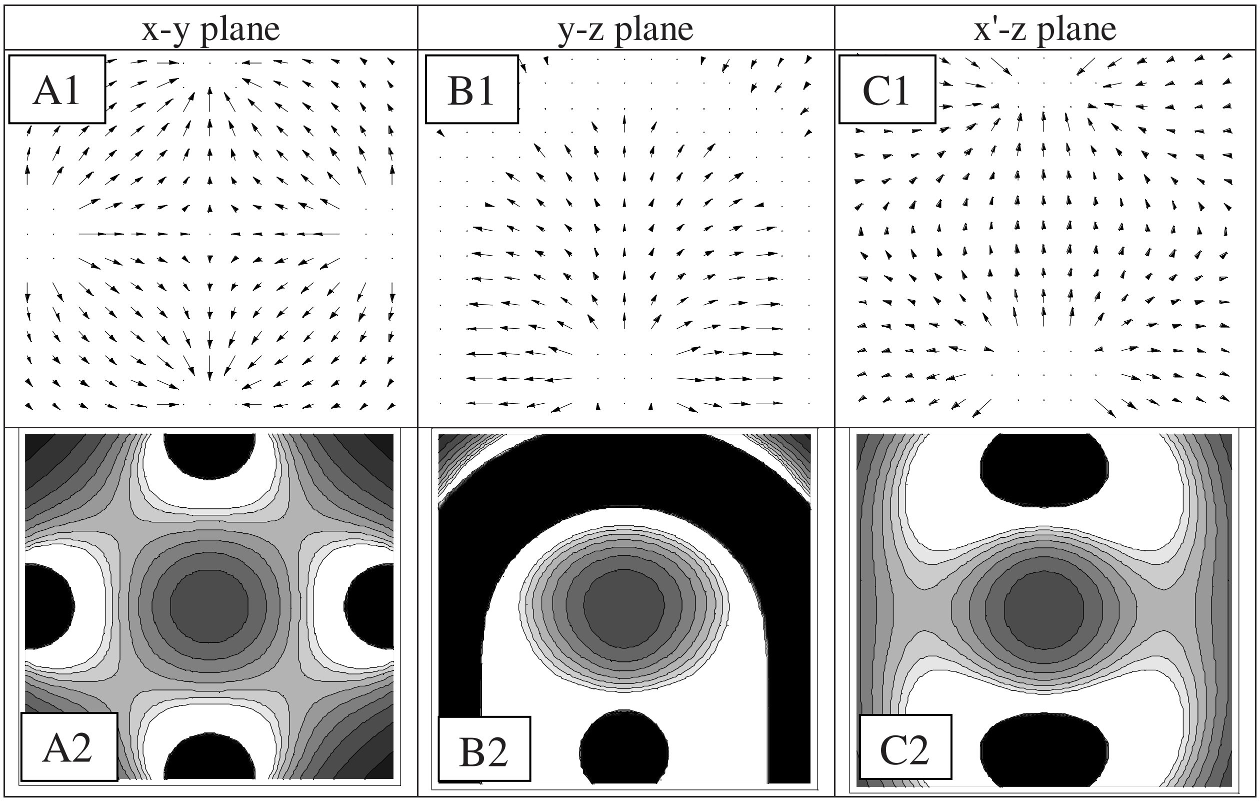

FIG. 2. Chain-link trap electrostatic field (1) and E^2 Stark potential (2) in the x-y (A), y-z (B) and x'-z (C) planes. Here x' denotes an axis parallel to the vector $\widehat{x} + \widehat{y}$. Vectors indicate magnitude and direction of the field at the origin of the vector. The vector scale varies between the electrostatic field plots. The contour plot scaling is the same as used in Fig. 1.

Figure 2

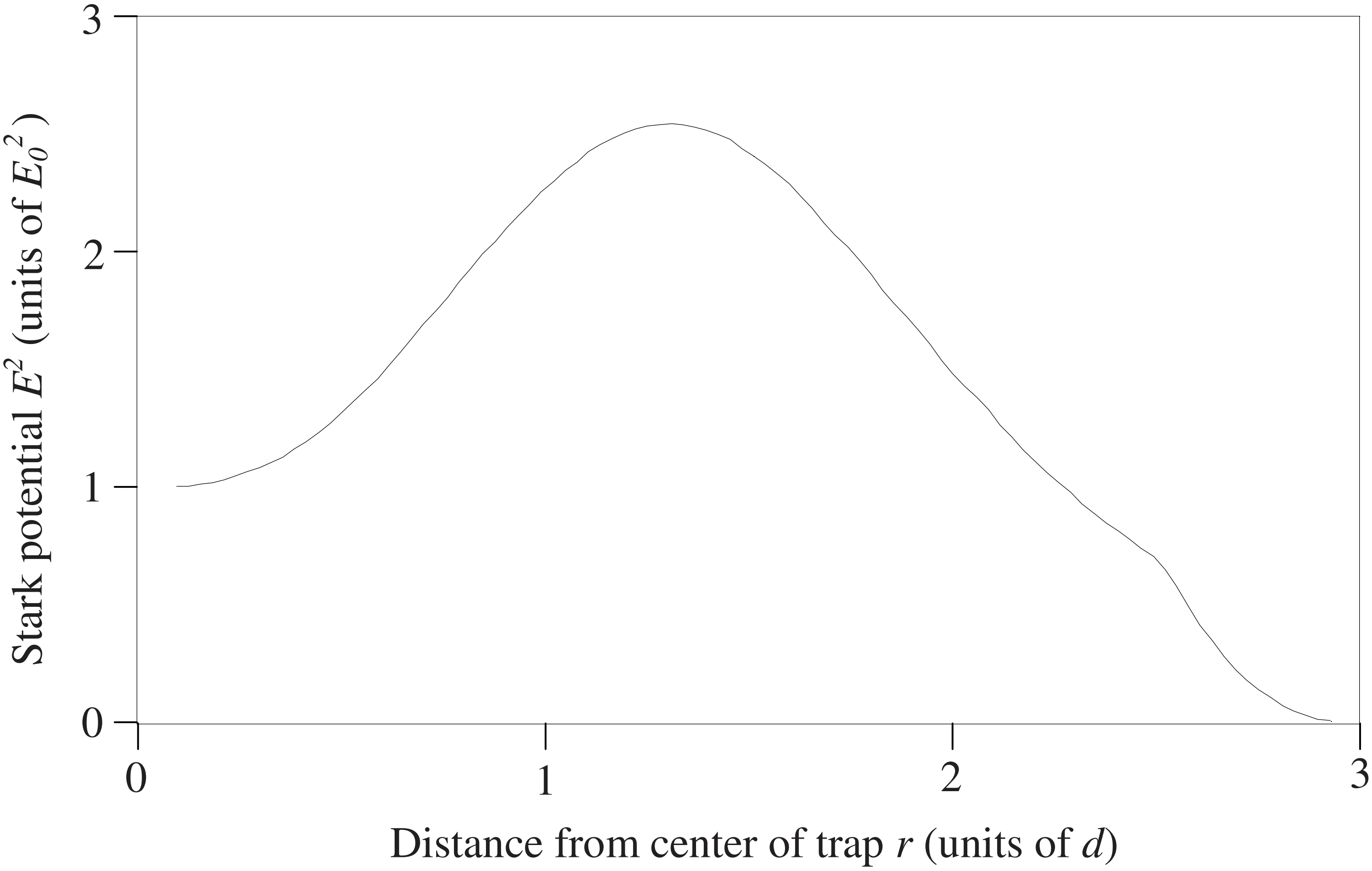

FIG. 3. Minimum value of E^2/E_o^2 on a spherical surface a distance r from the center of the chain-link trap. Here r is in units of the diameter d of the electrode rods.