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Electric Trapping of Neutral Atoms: Stability Theory

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Abstract – The possibility to trap neutral atoms by an ac electric field using the second-order Stark effect is discussed. Criterion for the stability of ac electric trapping is theoretically investigated. The stable region is numerically determined for a configuration of six electrodes with sinusoidal and rectangular electric fields. The result shows the universal stability when [*force*]/[*frequency*]^2 is small. The effective potential depth is also calculated.

1. INTRODUCTION

The trapping of nonmagnetic and nonpolar molecules or atoms has never been reported, except for the trapping of alkaline earth atoms with a resonant light [1, 2]. If one does not use a resonant light, the largest force acting on such a particle is the second-order Stark or Zeeman effect. Since the energy shift of the particle in a stable state is always negative, the particles are attracted to a higher field. This characteristic prevents us from trapping neutral atoms in a static field. It has been realized recently that an effective potential minimum similar to the one in an rf ion trap can be generated with an ac field around a nonzero field point [3 - 6]. Although the depth of the potential produced by this method is small, it can exert a sufficiently large force on the laser-cooled atom to support against gravity. This idea was applied to the magnetic trapping of Cs atoms in the level with negative Zeeman shift [7], and also to the two-dimensional electric trapping of metastable Ne atoms [8]. In this paper, we discuss a three-dimensional ac electric trap and numerical results on the dynamics of trapped particles.

2. POTENTIAL FORM

The dipole force $\mathbf{F}$ exerted on a nonpolar neutral particle caused by the electric field $\mathbf{E}$ is

$$\mathbf{F} = (\vec{\mu} \cdot \mathrm{grad})\,\mathbf{E} = -\mathrm{grad}\,\varepsilon \quad (\varepsilon = -\frac{1}{2}\alpha|E|^2), \quad (1)$$

where $\vec{\mu}(= \alpha\mathbf{E})$ and $\alpha(> 0)$ are the dipole moment and the polarizability of the particle, respectively. In order to confine a particle statically in some volume V, the direction of the force $\mathbf{F}$ must be inward everywhere on the boundary ∂V of V:

$$\mathbf{F} \cdot d\mathbf{S} < 0. \quad (2)$$

However, because of

$$\int_{\partial V} \mathbf{F} \cdot d\mathbf{S} = \int_V \mathrm{div}\mathbf{F}\, dV, \quad (3)$$

$$\mathrm{div}\mathbf{F} = \alpha \sum_{i,j} \left(\frac{\partial^2\phi}{\partial x_i \partial x_j}\right)^2 \geq 0, \quad (4)$$

where ϕ is the scalar potential defined by $\mathbf{E} = -\mathrm{grad}\,\phi$, equation (2) is never satisfied. Thus, it is impossible to trap a particle statically by dipole force. In order to trap a particle dynamically, we impose the condition $\mathrm{div}\mathbf{F} = 0$ (as in the case of an rf ion trap); that is,

$$\sum_{i,j} \left(\frac{\partial^2\phi}{\partial x_i \partial x_j}\right)^2 = 0. \quad (5)$$

From this, we have $\frac{\partial E_j}{\partial x_i} = -\frac{\partial^2\phi}{\partial x_i \partial x_j} = 0$. If we expand electric field $\mathbf{E}$ by the coordinates around the origin, i.e., the center of the trap, the first order term should vanish. Any configuration of electrodes that has the inversion antisymmetry automatically satisfies these conditions.

Two cases are possible under these conditions:

Case 1: $\mathbf{E}(0) = 0$. In this case, the force is third order in $\mathbf{x}$, and the center of the trap is the local minimum of $|E|$. Therefore, the particle diverges in every direction (see (1)).

Case 2: $\mathbf{E}(0) \neq 0$. In this case, the force is linear in $\mathbf{x}$, and the center of the trap is a saddle point of the potential.

To proceed further, we shall first consider the system that is axially symmetric around the z-axis and antisymmetric under the inversion of the z-axis, as shown in Fig. 1. From the symmetry consideration, the scalar potential ϕ must have the form

$$\phi = d_1 z + z\{d_2 z^2 + d_3(x^2 + y^2)\} \quad (d_1 \neq 0).$$

The condition $\Delta\phi = 0$ places further restrictions:

$$\phi = d_1 z + d_2 z\{\frac{2}{3}z^2 - (x^2 + y^2)\},$$
$$\varepsilon = \frac{1}{2}\alpha|E|^2 = V_0^2\{d_4 + d_5(2z^2 - x^2 - y^2)\}. \quad (6)$$

Here, we kept only the leading term, and the higher order terms in $\mathbf{x}$ are neglected. We adopt this approximation for the rest of this paper. The potential ε has the same form as that of the rf ion trap, except that it is quadratic on the applied voltage. We can generate the same time-dependent potential as that of an rf ion trap with two pairs of electrodes, as shown in Fig. 2. In this case, the voltages of $V_1 \cos\omega t$ and $V_2 \sin\omega t$ are applied on each pair of electrodes, and the oscillation frequency of the potential is twice the frequency ω of the applied voltage. The equation of motion of this trap is described by the well-known Mathieu equation.

There are some difficulties with making electrodes like that of Fig. 2 with a size of the order of 1 mm. Let us think of a simpler electrode configuration, as shown in Fig. 3. Three pairs of electrodes are placed symmetrically on the x-, y-, and z-axes, respectively, and voltages of $\pm\xi$, $\pm\eta$, and $\pm\zeta$ are applied on each pair of electrodes. The equation of motion is, after some calculation,

$$\ddot{\mathbf{x}} = f\begin{pmatrix} Ax+bz+cy \\ By+cx+az \\ Cz+ay+bx \end{pmatrix}$$

$$\text{with}\ \begin{cases} A = (2\xi^2-\eta^2-\zeta^2)/2 \\ B = (2\eta^2-\zeta^2-\xi^2)/2 \\ C = (2\zeta^2-\xi^2-\eta^2)/2, \end{cases} \quad \begin{cases} a = -\eta\zeta \\ b = -\zeta\xi \\ c = -\xi\eta. \end{cases} \tag{7}$$

Here, we impose the condition that the time average of the force $\mathbf{F}$ at an arbitrary site be equal to zero.[1] From (7), this yields the following conditions:

$$\overline{\xi^2} = \overline{\eta^2} = \overline{\zeta^2}, \quad \overline{\eta\zeta} = \overline{\zeta\xi} = \overline{\xi\eta} = 0. \tag{8}$$

In this paper, we discuss the following two cases, which satisfy the above condition:

(1) rectangular electric field,

$$(\xi, \eta, \zeta) = \begin{cases} (V_0, 0, 0) & nT \le t < (n+\frac{1}{3})T \\ (0, V_0, 0) & (n+\frac{1}{3})T \le t < (n+\frac{2}{3})T \\ (0, 0, V_0) & (n+\frac{2}{3})T \le t < (n+1)T \end{cases}$$
$$(n = 0, 1, 2, \ldots). \tag{9}$$

(2) sinusoidal electric field,

$$\begin{cases} \xi = V_0 \cos\omega t \\ \eta = V_0 \sin\omega t \\ \zeta = V_0 \cos\gamma\omega t \end{cases} \tag{10}$$

with $\gamma > 0$, $\gamma \ne 1$.

3. EVALUATION OF THE STABILITY

In this section, we consider the stability of the solution of the equation of motion (7). We assume that the

[1] As seen from the case of an rf ion trap, this is not the necessary condition. But because of (5) (or (4)), the existence of the region where average force is inward inevitably leads to the existence of the region where the average force is outward. So, the average force should be small everywhere.

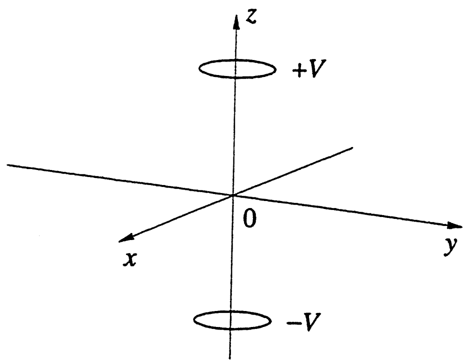

Fig. 1. Example of the electrodes, which are axially symmetric and antisymmetric under the inversion of the z-axis.

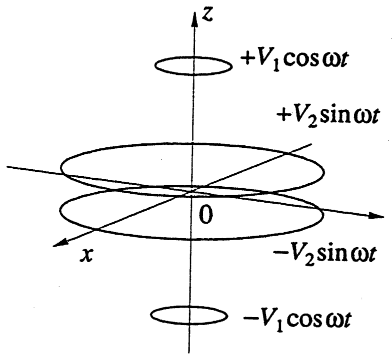

Fig. 2. Electrodes that have the same potential form as that of an rf ion trap.

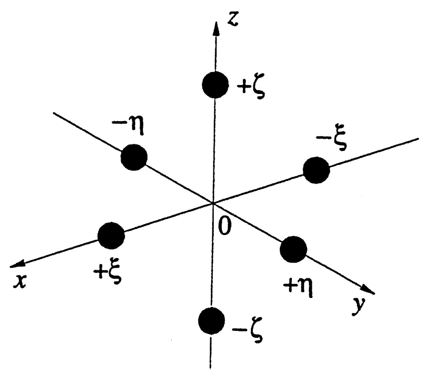

Fig. 3. Electrodes of our configuration.

coefficients of $\mathbf{x}$ in (7) are periodic in t with a period of T. Let us define the time evolution matrix $U(t)$ as

$$U(t) = \begin{pmatrix} x^{(1)}(t) & \ldots & x^{(6)}(t) \\ y^{(1)}(t) & \ldots & y^{(6)}(t) \\ z^{(1)}(t) & \ldots & z^{(6)}(t) \\ v_x^{(1)}(t) & \ldots & v_x^{(6)}(t) \\ v_y^{(1)}(t) & \ldots & v_y^{(6)}(t) \\ v_z^{(1)}(t) & \ldots & v_z^{(6)}(t) \end{pmatrix}, \tag{11}$$

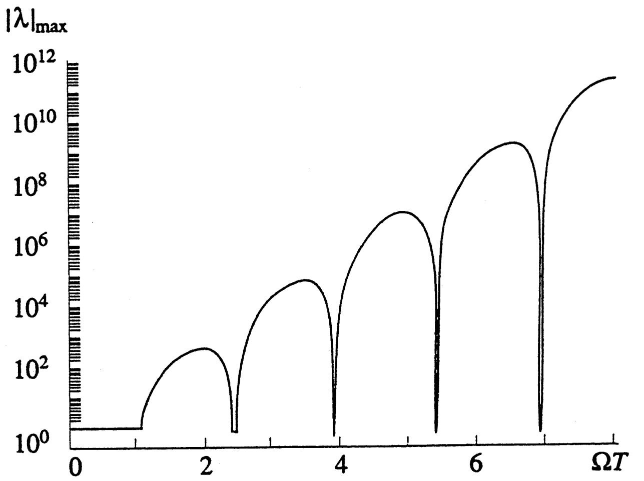

Fig. 4. Stability of the trap: rectangular electric field. Parameter $\Omega T \sim V_0/\omega$ corresponds to [*force*]$^{1/2}$/[*frequency*]. The area where $|\lambda|_{max} = 1$ is the stable region.

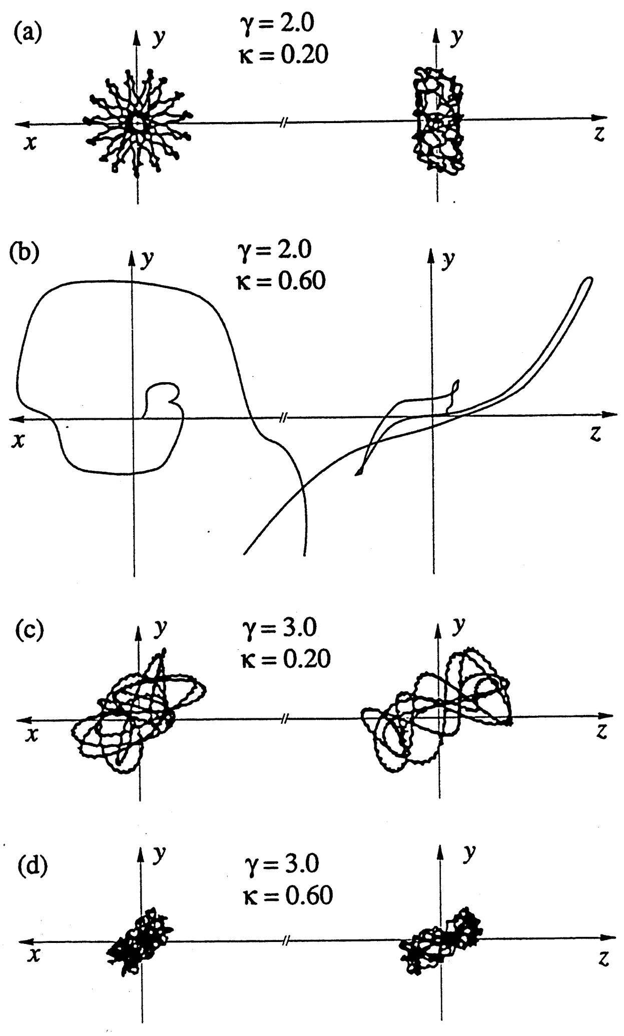

Fig. 5. Examples of the trajectory. Parameter $\kappa \equiv fV_0^2$ corresponds to [*force*]/[*frequency*]^2. (b) is unstable.

where $\mathbf{x}^{(i)}(t)$ are fundamental solutions of (7), and $\mathbf{v}^{(i)}(t) \equiv \dot{\mathbf{x}}^{(i)}(t)$. The initial condition is taken as

$$U(0) = 1. \quad (12)$$

The solution of (7) with arbitrary initial condition is given by

$$\begin{pmatrix} \mathbf{x}(t) \\ \mathbf{v}(t) \end{pmatrix} = U(t)\begin{pmatrix} \mathbf{x}(0) \\ \mathbf{v}(0) \end{pmatrix}. \quad (13)$$

Because of the periodicity of the coefficient of (7), we have

$$U(nT + t) = U(t)\{U(T)\}^n. \quad (14)$$

Let $\lambda^{(1)}, \ldots, \lambda^{(6)}$ be the eigenvalues of $U(T)$. Then, from (13) and (14), the trap is stable if

$$|\lambda^{(1)}|, \ldots, |\lambda^{(6)}| \le 1.$$

Because the left side of (7) does not contain terms proportional to v(t), $|U(t)| = 1$. Therefore, the stability condition of the trap can be written as

$$|\lambda^{(1)}|, \ldots, |\lambda^{(6)}| = 1. \quad (15)$$

Note that neither heating nor cooling exists whenever the trap is stable. When some of the eigenvalues of $U(T)$ are degenerate, the solution may not be stable even if conditions (15) are satisfied. However, we have never encountered the degenerate case in our numerical calculations, except when the electric field is zero. Therefore, we may safely conclude that the eigenvalues are nondegenerate except for rare accidental cases.

3.1. Rectangular electric field. In the case of a rectangular electric field, the equation of motion is reduced to one dimension and can be analytically solved:

$$\ddot{x} = \begin{cases} 2\Omega^2 x & (0 \le t < \frac{1}{3}T) \\ -\Omega^2 x & (\frac{1}{3}T \le t < T) \end{cases} \quad (\Omega = \sqrt{d/2}V_0), \quad (16)$$

$$U(T) = U_2 U_1, \quad (17)$$

where

$$U_1 = \begin{pmatrix} \cosh\frac{\sqrt{2}}{3}\Omega T & \frac{1}{\sqrt{2}\Omega}\sinh\frac{\sqrt{2}}{3}\Omega T \\ \sqrt{2}\Omega\sinh\frac{\sqrt{2}}{3}\Omega T & \cosh\frac{\sqrt{2}}{3}\Omega T \end{pmatrix},$$

$$U_2 = \begin{pmatrix} \cos\frac{2}{3}\Omega T & \frac{1}{\Omega}\sin\frac{2}{3}\Omega T \\ -\Omega\sin\frac{2}{3}\Omega T & \cos\frac{2}{3}\Omega T \end{pmatrix},$$

$$\lambda^2 - 2\beta\lambda + 1 = 0,$$

$$|\lambda|_{max} = \begin{cases} |\beta| + \sqrt{\beta^2 - 1} & (|\beta| > 1) \\ 1 & (|\beta| \le 1), \end{cases} \quad (18)$$

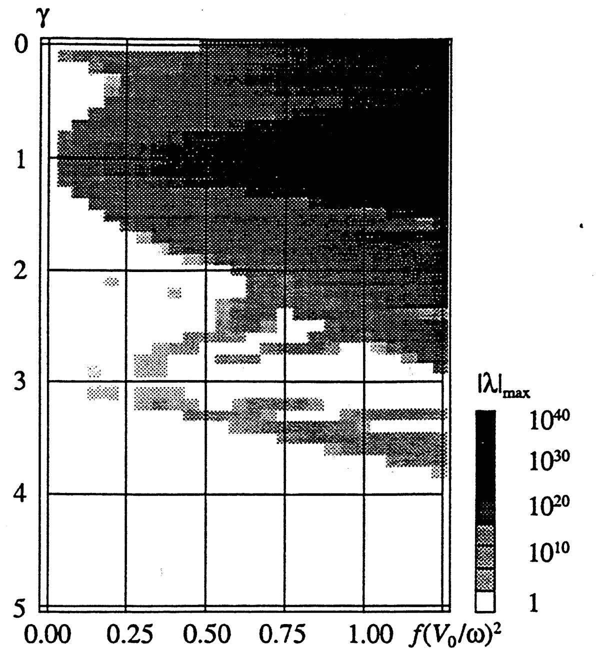

Fig. 6. Stability of the trap: sinusoidal electric field. The white part is the stable region. Logarithmic scale.

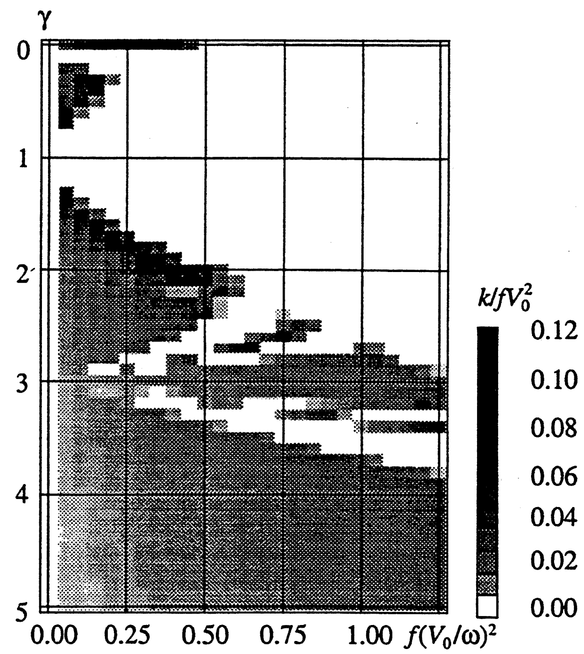

Fig. 7. Effective potential depth of the trap. The darker part has the deeper potential. Linear scale.

where

$$\beta = \cos\frac{2}{3}\Omega T\cosh\frac{\sqrt{2}}{3}\Omega T + \frac{1}{2\sqrt{2}}\sin\frac{2}{3}\Omega T\sinh\frac{\sqrt{2}}{3}\Omega T.$$

Figure 4 shows a graph of $|\lambda|_{max}$ versus ΩT. The trap is stable for small ΩT, but there also exist stable branches near $\Omega T = \frac{3}{2}\{(2n+1)\pi - \mathrm{atan}2\sqrt{2}\}$ $(n = 0, 1, \ldots)$.

4. SIMULATION

4.1. Sinusoidal electric field. For a sinusoidal electric field, the trajectory of the particle is calculated using the Runge–Kutta method. Figure 5 shows some examples of the trajectory.

To evaluate the stability, $U(T)$ and its eigenvalues $|\lambda^{(1)}|, \ldots, |\lambda^{(6)}|$ are solved for various γ and $(V_0/\omega)^2$. To obtain the result for an arbitrary γ, we may approximate γ with a rational number n/m. Then, the coefficients in (7) are periodic functions of t with a period of $T = 2\pi m/\omega$. In the present calculation, we chose $m = 10$, and (7) is integrated for $n = 0, 1, \ldots, 50$. Figure 6 shows the stability of the trap. The shade of the graph shows the magnitude of $|\lambda|_{max}$ in a log scale. The white part is the stable region where $|\lambda|_{max} = 1$. For $\gamma = 1$, in which case condition (8) is not satisfied, there is no stable region.

The estimation of the effective potential was done in the following way. We tracked the motion of the particle starting from the center of the trap with a fixed velocity $\mathbf{v}_0 = (0, 0, v_0)$ up to $t = 2T$ and estimated the maximum distance r_{max} from the center. If we approximate the trap potential with a static harmonic potential, the effective potential ε_{eff} is given by

$$\varepsilon_{eff}(\mathbf{x}) = \frac{1}{2}kx^2 \quad \text{with} \quad k \equiv (v_0/r_{max})^2. \qquad (19)$$

Figure 7 shows the graph of coefficient k of the effective potential normalized by fV_0^2 as a function of γ and $(V_0/\omega)^2$.

5. CONCLUSION

We have shown numerically that our ac electric trap of a neutral particle is stable for small $[force]/[frequency]^2 \sim f(V_0/\omega)^2$. For an atom of $\alpha \sim 10^{-38}$ Fm^2, a trap with a size of 1 mm will easily hold atoms by applying V_0 = 1 kV. The trapping force is approximately 10 times larger than the gravity force mg. The above example shows that the ac electric field is a practical tool to trap atoms and molecules which have no angular momentum. If a higher order branch of the stable region is used, the trap works as a device to separate atoms with different α/m.

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