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Control Of Screening Of A Charged Particle In Electrolytic Aqueous Paul Trap

Jae Hyun Park and Predrag S. Krsti

Physics Division, Oak Ridge National Laboratory, P.O. Box 2008, Oak Ridge, TN 37831-6372, USA

Abstract

Individual charged particles could be trapped and confined by the combined radio-frequency and DC quadrupole electric field of an aqueous Paul trap. Viscosity of water improves confinement and extends the range of the trap parameters which characterize the stability of the trap.

Electrolyte, if present in aqueous solution, may screen the charged particle and thus partially or fully suppress electrophoretic interaction with the applied field, possibly reducing it to a generally much weaker dielectrophoretic interaction with an induced dipole. Applying molecular dynamics simulation we show that the quadrupole field has a different effect at the electrolyte ions and at much heavier charged particle, effectively eliminating the screening by electrolyte ions and reinstating the electrophoretic confinement.

Keywords

Aqueous Paul trap; electrolyte screening; electrophoretic; molecular dynamics

INTRODUCTION

Standard, conventional applications of a quadrupole Paul trap [1], in 2D and 3D options, are in the fields of mass spectrometry and ion trapping, respectively. More recent applications include the reduced dimension micro/nano traps and are in the area of quantum information processing, for coherent quantum-state manipulation of trapped atomic ions, for functional studies with fluorescent proteins, for laser sideband cooling of the motion, for formation of ordered structures of trapped ions, etc. By default, the trap confinement functions are used in vacuum, and are characterized by the applied DC (U) and AC (V) electric fields of frequency Ω , building a quadrupole potential

$$\varphi(x, y, t) = [U - V \cos(\Omega t)] \frac{x^2 - y^2}{2R_0^2} \quad (1)$$

applied to a charged particle of mass M and charge Q in a 2D trap of lateral dimension R_0 . Application for controlling of motion and position of biomolecules, for example in a

nanopore for DNA sequencing [2-5], has raised interest in an aqueous Paul trap. We have previously shown by molecular dynamics simulation that nanoscale quadrupole Paul trap can confine charged particles in an aqueous environment [5]. If the trap is filled with a medium of viscosity ζ (for water $\zeta=8.9 \times 10^{-4}$ Pa·s) then the classical, Langevin equation of motion of a charged particle is of Mathieu type with damping which takes the form

$$\frac{d^2x}{d\tau^2} + b \frac{dx}{d\tau} + (a - 2q \cos 2\tau)x = g(\tau) \quad (2)$$

where $g(\tau)$ is the stochastic Gaussian fluctuating term, arising from the Brownian motion,

$$\tau = \frac{\Omega t}{2}, a = \frac{4QU}{MR_0^2\Omega^2}, q = \frac{2QV}{MR_0^2\Omega^2}, b = \frac{2\zeta}{M\Omega} \quad (3)$$

are dimensionless parameters which define the functions of the trap, Q and M are the trapped particle charge and mass, respectively, and R_0 is the characteristic dimension of the trap. In particular, with neglecting Brownian fluctuations we derive the stability regions of the solutions of Eq. (2), shown in Figure 1 for various viscosity parameters b . The trap will preserve its confinement functions even at zero parameter a (proportional to the DC bias U), the limits of stability for parameter q (proportional to the AC bias V) will strongly depend on the viscosity parameter b . Thus, the q parameter in vacuum ($b=0$) is limited to values less than approximately 0.9, while for $b=92$, it is limited to values less than 4500.

However, if the water in the trap contains electrolytes, as is often a case with trapped charged biomolecules (for example DNA and KCl electrolyte), it is expected that counter-charged ions in electrolyte may screen the trapped particle. This might have a negative effect on the trapping stability of the molecule because the molecule charge Q in parameter q decreases (see Eq. (3)) by screening.

The main goal of this work is to demonstrate, using a series of molecular dynamics simulations, that the quadrupole electrophoretic field of a 2D aqueous Paul trap removes and prevent the screening, preserving the confining functions in presence of an electrolyte. Direct inspiration for this work has come from the recent publication of Liu et al. [6], who investigated reduction of the electrostatic screening with applied electrophoretic field of a model of charged biomolecule in a cylindrical micro-pore filled with an electrolyte. They used continuum approach to the problem, by solving Poisson-Nernst-Planck equations. and showed that, due to the imbalance between electrophoretic drift and diffusion of ions, the effective Debye length in electrolyte around the molecule increases with increase of external bias (reflecting decrease of the concentration of the counter-ions around the molecule, i.e. descreening).

In the next section, using a charged buckyball as a model of a biomolecule, we apply atomistic, molecular dynamic approach in a aqueous quadrupole 2D Paul nanotrap filled with solvated KCl, and show the suppression of the screening effect. While the screening suppression shown by Liu et al. [6] might be present in the Paul trap too, a more efficient effect, emerging from difference in the stability ranges of the buckyball and electrolyte ions, cause the total descreening.

COMPUTATION AND RESULTS

The molecular dynamics simulations were performed with the modified GROMACS 4.0 [7] in canonical ensemble (NVT) at $T=300$ K. The simulation box consisted of core region and the surrounding buffer region, as shown in Figure 2. The $6 \times 6 \times 8$ nm³ core region was placed in the center of simulation box and 1.5 nm-thickness buffer regions were attached to the core region in x- and y-direction, resulting in the total simulation box of $9 \times 9 \times 8$ nm³, containing 11286 water molecules in the core region and 11001 water molecules in the buffer. A buckyball of diameter 0.8 nm and of negative charge $-12e$ uniformly distributed over 60 carbon atoms. The buckyball, 20 dissociated KCl molecules, and water molecules were initially located in the core region while buffer region is filled with water only. The periodic boundary conditions were applied along the axis of the 2D Paul trap (z-axis) to all particles in the trap, while in the x and y directions the periodic boundary conditions are applied only to water molecules. As a consequence, water molecules could freely move in and out the buffer region in x-y directions. However, once the ions or buckyball reached border of the buffer region they could not return back to the core box and their charges were reset to zero. The system temperature was regulated using Nosé-Hoover thermostat with time constant of 0.1 ps, while the simulation time-step was 1.0 fs. The cut-off scheme was introduced to describe the electrostatic interactions with the cut-off radius of 4 nm. In these simulations we used the MD potentials optimized as in Refs. [8-10].

We apply AC voltage $V=1$ V of frequency $\Omega=1$ GHz in the Paul trap of $R_0=50$ nm. Since the DC component of voltage (U in Eq. (1)) is easily screened at electrodes by the electrolyte ions, we apply only the AC field. This leads to the buckyball q-factor of 1.30 in Eq. (3), and 2.0 and 1.32 for potassium and chlorine ions (of charge $\pm e$), respectively. Due to large difference in masses, the buckyball b-factor in Eq. (3) is close to 357, while for K^+ and Cl^- it reaches values of ~ 3895 and 3992, respectively. The consequence of these large differences is shown in Fig. 3. While buckyball is well in the stable region of the solution of Eq. (2), the electrolytic ions are not stable, and might be expelled from the core region of the Fig. 2 (i.e. from the trap confinement region).

Figure 4 shows molecular visualization of the ion removal process in aqueous Paul trap. Only electrolytic ions and buckyball are shown in the figure. With here applied high frequency of the AC quadrupole field, it is enough 10 ns to fully expel the electrolytic ions from the “core” part of the simulation cell (Fig. 2). The process of descreening shows an exponential decrease with time, and 75% of ions are expelled in the first 2 ns. Negative chlorine ions are leaving the simulation volume somewhat faster, being helped by the Coulomb repulsion of the negatively charged buckyball. The molecular dynamics simulations take into account both inter-ion Coulomb interactions and Brownian motion and the MD simulation shows that the Brownian motion does not influence the stability behavior of this particular system. The control MD calculation, performed under identical conditions, but without applied quadrupole AC electrical field, shows a complete screening of the buckyball by the K^+ ions.

CONCLUSIONS

Molecular dynamics simulations were performed on a charged buckyball in a 2D Paul trap, immersed in a water solution of potassium chloride. Without loss of generality, an electrophoretic quadrupole field of high frequency in GHz range was applied to speed up MD calculations. The conditions of confinement stability were altered between buckyball and the electrolytic ions. A simple but remarkable result was obtained: A charged particle was not screened (and can be easily de-screened) by the electrolytic ions in an aqueous 2D Paul trap. This opens possibilities for efficient use of Paul trap for confinement and control of biomolecules and other charged particles in electrolytic aqueous environments.

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FIGURE 1. of stability of the 2D Paul trap in vacuum ($b=0$) and in damping environments of viscosity factor $b \neq 0$.

FIGURE 2.
Computational space for the molecular dynamics calculation.

FIGURE 3.
Stability of buckyball and electrolytic ions in the aqueous 50 nm 2D Paul trap with $V=1$ V and $\Omega=5$ GHz.

FIGURE 4.

Result of the MD simulation. Numbers of potassium and chlorine ions as functions of time in the aqueous Paul trap, residual in the confinement computational volume of the charged ($-12e$) buckyball, from initial 20 KCl molecules.