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Efficient computational scheme for ion dynamics in RF-field of Paul trap

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We have developed an efficient computational scheme for integration of the classical Hamilton equations describing the ion dynamics confined in the radio-frequency field of the Paul trap. It has permitted a quantitative treatment of cold atom-ion resonant collisions in hybrid atom-ion traps with taking into account unremovable ion micromotion caused by the radio-frequency fields (V.S. Melezhik et. al., Phys. Rev. A100, 063406 (2019)).

The important element of the hybrid atom-ion systems is the electromagnetic Paul trap confining the charged ion. The oscillating motion of the confined ion is defined by two frequencies of the Paul trap. It is the frequency of the order of 100 kHz due to the constant electric field and the radio-frequency of about 1–2 MHz defined by the alternating electromagnetic field of the ion trap. The necessity to accurately treat the ion motion in the combined field with two time scales defined by these two very different frequencies has demanded to develop the stable computational scheme for integration of the classical Hamilton equations for the ion motion. Moreover, the scheme must be stable on rather long time-interval of the ion collision with the cold atom $\sim 10 \times 2\pi/\omega_a$ defined by the atomic trap frequency $\omega_a \sim 10\,\text{kHz}$ and in the moment of the atom-ion collision when the Hamilton equations are strongly coupled. The developed numerical method takes into account all these features of the problem and makes it possible to integrate the system of coupled quantum-semiclassical equations with the necessary accuracy and quantitatively describes the processes of atomic-ion collisions in hybrid traps, including resonance effects.

Key words and phrases: cold atoms and ions, Paul trap, radio-frequency field, classical Hamilton equations, computational scheme

1. Introduction

In the last decade, there has been great interest in ultracold hybrid atomic-ion systems, which is due to the new opportunities that arise here for quantum

simulation of various processes and effects from solid state physics to high-energy physics: electron-phonon coupling in solid state physics, critical phenomena in high-energy physics, quantum information processing etc. [1]. However, a realization of the hot proposals with cold atom and ions is impeded by the unremovable ion micromotion caused by the radio-frequency fields of the Paul traps used for confining ions in the hybrid confined atom-ion systems [1]. In the recent work [2] a quantum-semiclassical computational scheme for treating the collisional atom-ion dynamics in the confined geometry of the hybrid atom-ion traps was suggested where the ion micromotion caused by the radio-frequency fields of the ion trap was taken into account. In this work the following problem was considered: an ion confined in a time-dependent radio-frequency Paul trap with linear geometry, while the atom is constrained to move into a quasi-one-dimensional waveguide within the ion trap. In this approach the atom-ion dynamics was treated semiclassically, namely the atom dynamics is governed by the time-dependent Schrödinger equation, whereas the ion motion is described by the classical Hamilton equations of motion. Both equations were integrated simultaneously.

The quantum-semiclassical computational method [3]–[6] specifically designed for particle collisions such as the problem of ionisation of the helium ion colliding with protons [5] and antiprotons [6] has been employed and extended to the time-dependent domain, as the radio-frequency ionic confinement by the Paul trap requires. It has demanded to develop a new stable computational scheme for integration the classical Hamilton equations for the ion motion. Here, we describe the scheme and demonstrate its efficiency by using as an example of the specific Li/Yb^+ atom-ion pair, since it is the most promising atomic pair to reach the s-wave regime in Paul traps and it is currently under intense experimental investigations [7]–[9].

2. Method

A schematic view of the system under investigation is given in Figure 1. The ion is assumed to be confined in a linear Paul trap, whose electric fields read as [10]:

$$\begin{aligned} \mathbf{E}_{\mathrm{s}} &= \frac{m_i}{2|e|}\omega_i^2\,(x_i, y_i, -2z_i)\,, \\ \mathbf{E}_{\mathrm{rf}} &= \frac{m_i\Omega_{\mathrm{rf}}^2 q}{2|e|}\cos(\Omega_{\mathrm{rf}}t)\,(x_i, -y_i, 0)\,. \end{aligned} \tag{1}$$

Here, m_i is the ion mass, Ω_{rf} is the radio-frequency (rf), $\omega_i = \Omega_{\mathrm{rf}}\sqrt{a/2}$ is the secular frequency, q and a are dimensionless geometric parameters (i.e. $q_z = 0$, $q_y = -q_x \equiv q$, $-a_z/2 = a_x = a_y \equiv a$, and $a \ll q^2 < 1$). We assume that the axis of the waveguide in which is travelling the colliding atom is precisely the z-axis of the Paul trap (see Figure 1). The corresponding ion-trap interaction potential is given by

$$U(\mathbf{r}_i, t) = \frac{m_i\omega_i^2}{2}\left(z_i^2 - \frac{x_i^2 + y_i^2}{2}\right) + \frac{m_i\Omega_{\mathrm{rf}}^2}{2}q\cos(\Omega_{\mathrm{rf}}t)\left(\frac{y_i^2}{2} - \frac{x_i^2}{2}\right). \tag{2}$$

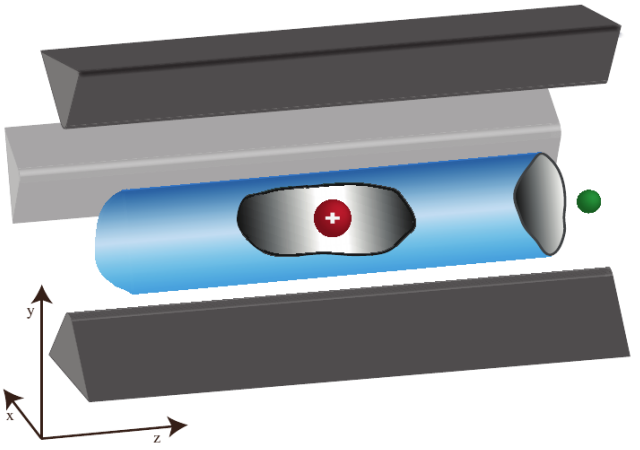

Figure 1. Pictorial illustration of the atom-ion system confined in hybrid trap. The light- and dark-grey electrodes (the big bars in the figure) of the Paul trap generate the time-dependent electric fields needed to confine the ion transversally, whereas longitudinally a static voltage is applied to ensure confinement (not shown). The atom is injected from the right to the left into a waveguide, whose centre hosts the ion. The waveguide is orientated along the longitudinal axis, z, of the linear Paul trap. In the transverse directions, x, y, the confining potential both for the atom and the ion is strong

Hence, the classical Hamiltonian describing an ion in a Paul trap is given by

$$H_i^{\text{trap}}(\mathbf{p}_i, \mathbf{r}_i, t) = \frac{\mathbf{p}_i^2}{2m_i} + U(\mathbf{r}_i, t). \tag{3}$$

When the atom is confined in the optical waveguide within the Paul trap, the ion experiences its presence via the atom-ion interaction $V_{ai}(|\mathbf{r}_a - \mathbf{r}_i(t)|)$, where $\mathbf{r}_a$ defines the atom coordinates. The full classical ion Hamiltonian is therefore given by

$$H_i(\mathbf{p}_i, \mathbf{r}_i, t; \mathbf{r}_a) = H_i^{\text{trap}}(\mathbf{p}_i, \mathbf{r}_i, t) + \langle V_{ai}(|\mathbf{r}_a - \mathbf{r}_i(t)|)\rangle, \tag{4}$$

where

$$\langle V_{ai}(|\mathbf{r}_a - \mathbf{r}_i(t)|)\rangle = \langle \Psi(\mathbf{r}_a, t; \mathbf{r}_i)|V_{ai}(|\mathbf{r}_a - \mathbf{r}_i(t)|)|\Psi(\mathbf{r}_a, t; \mathbf{r}_i)\rangle \tag{5}$$

is the quantum mechanical average of the atom-ion interaction over the atomic density instantaneous distribution. We see that the ion Hamiltonian has parametric dependence on the atom position $\mathbf{r}_a$. It leads at the moment of the atom-ion collision to the strong non-separability of the Hamilton equations

$$\begin{aligned} \frac{d}{dt}\mathbf{p}_i &= -\frac{\partial}{\partial \mathbf{r}_i} H_i(\mathbf{p}_i, \mathbf{r}_i, t; \mathbf{r}_a), \\ \frac{d}{dt}\mathbf{r}_i &= \frac{\partial}{\partial \mathbf{p}_i} H_i(\mathbf{p}_i, \mathbf{r}_i, t; \mathbf{r}_a) \end{aligned} \tag{6}$$

describing the ion dynamics and, as a consequence, to the requirement of sufficient stability of the computational scheme to this strong perturbation.

The set of classical equations (6) together with the Schrödinger equation for the atomic wave function $\Psi(\mathbf{r}_a, t, \mathbf{r}_i)$ form the complete set of dynamical equations for describing the confined atom-ion collision in hybrid traps [2]. In order to integrate simultaneously the equations we need proper initial conditions with physical significance. At the beginning of the collisional process, the atom and the ion are assumed to be far away from each other such that they do not interact ($V_{ai} = 0$). In particular, the atom is initially in the ground state of the atomic trap with the longitudinal colliding energy, that is, $E_{\mathrm{coll}} \ll 2\hbar\omega_0$, whereas the ion performs fast (with respect to atom motion) oscillations in the Paul trap with mean transversal $\bar{E}_\perp$ and longitudinal $\bar{E}_\parallel$ energies. Since the atom approaches the region of interaction with the ion very slowly ($E_{\mathrm{coll}}/\hbar \ll \omega_0 \ll \omega_i, \Omega_{\mathrm{rf}}$), the initial position of the ion does not influence the scattering process itself, which depends only on $\bar{E}_\perp$ and $\bar{E}_\parallel$. Specifically, the classical solution of the ion equations of motion (Mathieu equation) in the Paul trap (without the atom) are well approximated by $A_j \cos(\omega_i t + \phi_j)[1 + q_j \cos(\Omega_{\mathrm{rf}} t)/2]$, $\forall\, j = x, y, z$ [11].

The associated kinetic energy depends on the amplitude A_j, but not on the phase ϕ_j. Therefore, we choose, without loss of generality, the ion position at the initial time $t = 0$ in the trap centre with transversal energy, $E_\perp$, and longitudinal energy, $E_\parallel$. This can be summarised with the following set of initial conditions:

$$\begin{aligned} \mathbf{r}_i(t=0) &= (0,0,0), \\ p_{i,x}(t=0) &= \sqrt{2m_i E_\perp}, \\ p_{i,y}(t=0) &= 0, \\ p_{i,z}(t=0) &= \sqrt{2m_i E_\parallel}. \end{aligned} \tag{7}$$

These initial conditions set the mean values of the ion transversal and longitudinal energies as $\bar{E}_\perp = 1.64 E_\perp$ (calculated numerically for our trap parameters $\Omega_{\mathrm{rf}} = 2\pi \times 2\,\mathrm{MHz}$, $\omega_i = 2\pi \times 63\,\mathrm{kHz}$, $a = 0.002$ and $q = 0.08$) and $\bar{E}_\parallel = E_\parallel/2$, which is in qualitative agreement with the estimate

$$\bar{E}_\perp = \frac{E_\perp}{2}\left[1 + \left(\frac{q\Omega_{\mathrm{rf}}}{2\omega_i}\right)^2\right] \simeq 1.3 E_\perp \tag{8}$$

from the first-order solution of the Mathieu equation [11], [12].

For the integration of the Hamilton equations of motion, which involve three considerably different scales of frequencies, namely Ω_{rf}, ω_i as well as ω_0 in the quantum mechanical average $\langle \Psi(\mathbf{r}_a, t; \mathbf{r}_i) | V_{ai}(|\hat{\mathbf{r}}_a - \mathbf{r}_i(t)|) | \Psi(\mathbf{r}_a, t; \mathbf{r}_i) \rangle$, we employed the second-order Störmer–Verlet method [13].

Simultaneously to the forward in time propagation $t_n \to t_{n+1} = t_n + \Delta t$ of the atom wave-packet $\Psi_j(r_a, t_n) \to \Psi_j(r_a, t_{n+1})$ we integrate the Hamilton equations (6) with the initial conditions (7), which describe the dynamics of

the ion in the Paul trap. To this end, we have adapted the Störmer–Verlet method [13] to our problem

$$\begin{aligned}
\mathbf{p}_i^{(n+1/2)} &= \mathbf{p}_i^{(n)} - \frac{\Delta t}{2}\frac{\partial}{\partial \mathbf{r}_i} H_i(\mathbf{p}_i^{(n+1/2)}, \mathbf{r}_i^{(n)}), \\
\mathbf{r}_i^{(n+1)} &= \mathbf{r}_i^{(n)} + \frac{\Delta t}{2}\left\{ \frac{\partial}{\partial \mathbf{r}_i} H_i(\mathbf{p}_i^{(n+1/2)}, \mathbf{r}_i^{(n)}) + \frac{\partial}{\partial \mathbf{r}_i} H_i(\mathbf{p}_i^{(n+1/2)}, \mathbf{r}_i^{(n+1)}) \right\}, \quad (9) \\
\mathbf{p}_i^{(n+1)} &= \mathbf{p}_i^{(n+1/2)} - \frac{\Delta t}{2}\frac{\partial}{\partial \mathbf{r}_i} H_i(\mathbf{p}_i^{(n+1/2)}, \mathbf{r}_i^{(n+1)}).
\end{aligned}$$

Here,

$$\mathbf{p}_i^{(n)} = \mathbf{p}_i\left(t_n\right), \quad \mathbf{p}_i^{(n+1/2)} = \mathbf{p}_i\left(t_n + \frac{\Delta t}{2}\right), \quad \mathbf{p}_i^{(n+1)} = \mathbf{p}_i\left(t_n + \Delta t\right),$$

and the same definition for $\mathbf{r}_i^{(n)}$.

3. Numerical Example

The computational scheme (9) was successfully applied for numerical integration of the system of differential equations (6) with the initial conditions (7) for the Li/Yb^+ atom-ion systems confined in the hybrid traps with three absolutely different time-scales $t_{\rm rf} = 2\pi/\Omega_{\rm rf} \ll t_i = 2\pi/\omega_i \ll t_0 = 2\pi/\omega_0$ defined by the frequencies of Paul trap ($\Omega_{\rm rf} = 2\pi \times 2\,\text{MHz}$ and $\omega_i = 2\pi \times 63\,\text{kHz}$) and atomic waveguide ($\omega_0 = 2\pi \times 10\,\text{kHz}$). These three time-scales define the demand to the computational scheme. The scheme must be stable in rather long time-interval (time of atom-ion collision) $\sim 10t_0 = 10 \times 2\pi/\omega_0$ and, from the other side, it must accurately treats the fast oscillations defined by the frequency $\Omega_{\rm rf}$ of the rf-field.

In Figure 2 we present the calculated trajectory of the ion in the Paul trap (X_i variable) when there is no interaction with the atom: $V_{ia} = 0$. Here, the convergence over the step of integration on time $\Delta t \to 0$ is demonstrated as well as the stability of the computational scheme over the entire integration interval $0 \leqslant t \leqslant 10t_0$. The efficiency of the computational scheme was confirmed by the calculation of the scattering parameters in the atom-ion resonant collisions confined in hybrid traps [2] and can be applied for other resonant low-dimensional atomic and atom-ion systems.

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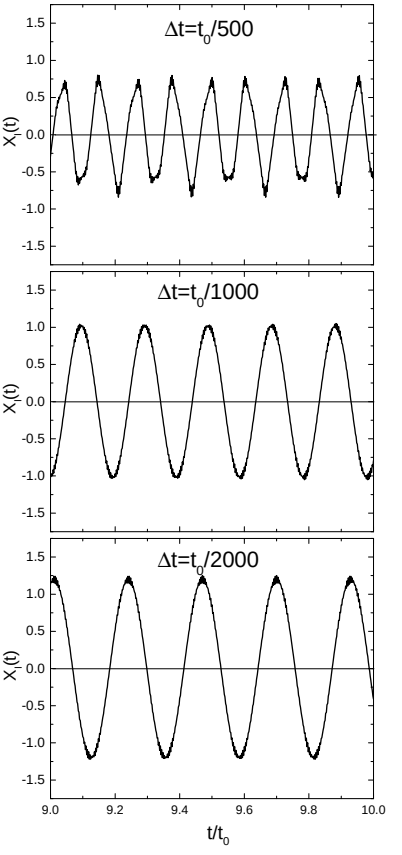

Figure 2. The calculated evolution in time of the ion trajectory ($X_i(t)$-variable), being initially at the state with $E_\perp/k_B = E_\parallel/k_B = 4.25\mu$K. The time scale is defined by the frequency $t_0 = 2\pi/\omega_0$ of the atomic waveguide-like trap ($\omega_0 = 2\pi \times 10\,$kHz)

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Эффективная вычислительная схема для описания динамики иона в радиочастотном поле ловушки Пауля

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В статье разработана эффективная вычислительная схема для интегрирования классических уравнений Гамильтона, описывающих динамику ионов пленённых радиочастотным полем ловушки Пауля. Она позволила провести количественные расчёты резонансных атомно-ионных столкновений в гибридных атомно-ионных ловушках с учётом неустранимого микродвижения ионов, вызванного радиочастотными полями (V.S. Melezhik et. al., Phys. Rev. A100, 063406 (2019)).

Важным элементом гибридных атомно-ионных систем является электромагнитная ловушка Пауля, удерживающая заряженный ион. Колебательное движение пленённого иона определяется двумя частотами ловушки Пауля. Это частота порядка 100 кГц из-за постоянного электрического поля и радиочастоты 1–2 МГц определяется переменным электромагнитным полем ионной ловушки. Необходимость точного описания движения ионов в комбинированном поле с двумя временными шкалами, задаваемыми двумя сильно различающимися частотами, потребовала разработки устойчивой вычислительной схемы для интегрирования классических уравнений (Гамильтона) движения ионов. Кроме того, требуется устойчивость схемы на достаточно большом интервале времени столкновения иона с холодным атомом $\sim 10 \times 2\pi/\omega_a$, определяемом частотой атомной ловушки $\omega_a \sim 10$ кГц, и в сам момент столкновения атома с ионом при сильной связи уравнений Гамильтона. Разработанный численный метод учитывает все отмеченные особенности задачи и позволяет с необходимой точностью интегрировать систему связанных квантово-квазиклассических уравнений и количественно описывать процессы атомно-ионных столкновений в гибридных ловушках, включая резонансные эффекты.

Ключевые слова: холодные атомы и ионы, ловушка Пауля, радиочастотное поле, классические уравнения Гамильтона, вычислительная схема