Addendum to "Quantum theory of the stability region of an ion in a Paul trap"

Leilei Yan,[1,2] Mang Feng,[1,*] and Kelin Wang[3]

[1]*State Key Laboratory of Magnetic Resonance and Atomic and Molecular Physics, Wuhan Institute of Physics and Mathematics, Chinese Academy of Sciences, Wuhan 430071, China*

[2]*University of the Chinese Academy of Sciences, Beijing 100049, China*

[3]*Department of Modern Physics, University of Science and Technology of China, Hefei 230026, China*

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The authors call attention to a previous work [Kelin Wang, Mang Feng, and Juhao Wu, Phys. Rev. A **52**, 1419 (1995)] for quantum-mechanically studying the stability region of the Paul trap, where the calculation does not work for the case of zero dc voltage. But the ions can be confined experimentally at zero dc voltage which is understandable via the Mathieu equation. We present a quantum-mechanical study for such a case as a supplement.

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The Paul trap [1], since its invention, has become an important setup in the exploration of nonlinear physics and quantum physics. The charged particles confined in the trap can demonstrate nonlinearity, such as chaos-order transition [2,3], the Duffing oscillator [4], and configuration phase transition [5]. Moreover, we may encode qubits into the electronic states of the confined charged atoms for quantum information storage. If the charged atoms are laser-cooled down to low temperature of the order of micro-Kelvins, their vibrational modes can be employed as a data bus for quantum information processing [6–8].

The time-dependent potential is essential to the confinement of the charged particles in the Paul trap [9]. Besides the requirement from the Earnshaw theorem [10], whether the particles can be confined or not depends on the stability region of the trap, which is determined by the Mathieu equation. However, in terms of quantum mechanics, any cold particle behaves as a wave function, whose characteristic can be fully described by the Schrödinger equation. So it is of great interest to see what happens for a cold particle in a Paul trap by a purely quantum-mechanical treatment, rather than by the classical Mathieu equation.

A previous work [11] published by some of the authors focused on the quantum-mechanical understanding of the stable confinement of a single Paul-trapped ion, in which the stability region is related to the convergence of a nonlinear equation [11,12] and a larger stability region has been found than by using the Mathieu equation. However, this treatment does not work for the case of zero dc voltage of the external electric field, i.e., $U = 0$ (defined later), which is a singularity of the treatment. Nevertheless, the case of $U = 0$ does belong to the stability region solved by the Mathieu equation, and, as far as we know, the condition $U = 0$ is usually employed experimentally for stably trapping ions [13].

The present work focuses on the case of zero dc voltage by the Schrödinger equation for the condition to confine ions. Like in Ref. [11], we still relate the stability region to the convergence of the nonlinear equation deduced from the reduction of a time-dependent Schrödinger equation into a time-independent one. To avoid that singularity, we solve the nonlinear equation by an alternative method, from which we show a condition between the ac voltage and the ac frequency for stably confining the ion, and, more interestingly, this stability condition is less stringent than that determined either by the Mathieu equation or by the quantum-mechanical way in Ref. [11].

In terms of Ref. [1], the Paul-trapped ion behaves the same in both x and y directions with the secular frequency $\Omega^2_{x(y)}(t) = \frac{q}{mr_0^2}[U + V\cos(\omega t)]$, with the charge q and the mass m of the trapped ion, the radius r_0 of the trap, the dc voltage U, and the ac voltage V owning the frequency ω. The motion of the ion in the z direction is slightly different, whose secular frequency is $\Omega^2_z(t) = \frac{q}{mr_0^2}[U - V\cos(\omega t)]$. Usually, the trap axis is defined along the z direction, and x and y directions are called radial directions.

In the case of $U = 0$, we may consider three identical Schrödinger equations for the trapped particle in three dimensions if we mathematically omit the π phase difference in the micromotion between the x-y plane and the z axis. As a result, the one-dimensional motion of a Paul-trapped ion is described as

$$i\hbar\frac{\partial}{\partial t}\Psi(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi(x,t) + \frac{m}{2}\Omega^2(t)x^2\Psi(x,t), \quad (1)$$

with $\Omega^2(t) = \frac{q}{mr_0^2}V\cos(\omega t)$. Using the same transformations as in Refs. [11,12], we may have a new Schrödinger equation,

$$i\hbar\frac{\partial}{\partial s}\Phi(\xi,s) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial \xi^2}\Phi(\xi,s) + \frac{m}{2}F(t)\xi^2\Phi(\xi,s), \quad (2)$$

where we have $F(t) = \frac{1}{2}\ddot{\varphi}\varphi - \frac{1}{4}\dot{\varphi}^2 + \Omega^2(t)\varphi^2$, and

$$\Psi(x,t) = \Phi(\xi,s)e^{i\beta(t)x^2 - \frac{\hbar}{m}\int_0^t \beta(\tau)d\tau}, \quad (3)$$

with $\beta(t) = \frac{m\dot{\varphi}(t)}{4\hbar\varphi(t)}$, $\xi = \frac{1}{\sqrt{\varphi(t)}}x$, and $s = \int_0^t \varphi^{-1}(\tau)\,d\tau$. In the previous treatments [11,12], we have $F(t)$ as a constant, which reduces the solution of Eq. (2) to a simple harmonic oscillator since the constant related to the dc voltage U is nonzero. Moreover, $U = 0$ is a singularity in that treatment.

In the present treatment, to avoid the divergence due to the singularity, we solve the nonlinear equation $F(t)$ by an alternative method. We still suppose $F(t)$ to be a constant C,

*mangfeng@wipm.ac.cn

which is a very small number in comparison with ω^2, but nonzero. However, in the present case of $U = 0$, the solution strongly depends on the initial state of the trapped ion. For convenience of our description, we below replace $\cos(\omega t)$ in the potential by $\cos(\omega t + \frac{\pi}{2})$, which shifts the time-dependent potential by a $\pi/2$ phase but does not change the physical essence of the solution.

As a result, Eq. (2) is reduced to be a simple harmonic oscillator equation, whose solution can be found in the textbook and whose validity depends on the convergence of the following equation:

$$2\varphi(t)\ddot{\varphi}(t) - \dot{\varphi}^2(t) + \frac{4qV}{mr_0^2}\cos\left(\omega t + \frac{\pi}{2}\right)\varphi^2(t) = 4C. \quad (4)$$

By defining $\varphi(t) = \sum_{n=0}^{\infty}\phi_n \cos^n(\omega t + \frac{\pi}{2})$, we obtain following recurrence equation:

$$\phi_{n+2} = -\frac{T_1^{n+2} - T_2^n + 4vT_3^{n-1}}{2(n+1)(n+2)\phi_0\omega^2}, \quad (5)$$

with $\phi_0\phi_2 = \frac{1}{4}\phi_1^2 + \frac{C}{\omega^2}$, $v = \frac{qV}{mr_0^2}$, and

$$T_1^n = \sum_{l+k=n}\phi_l\phi_k[2k(k-1) - lk]\omega^2 - \phi_0\phi_n[2n(n-1)]\omega^2,$$

$$T_2^n = \sum_{l+k=n}\phi_l\phi_k(2k^2 - lk)\omega^2,$$

$$T_3^n = \sum_{l+k=n}\phi_l\phi_k.$$

Once the recurrence in Eq. (5) is convergent, we may find the solution to Eq. (2) and thereby we know that the ion is stably confined in the trap. On the contrary, the divergence of Eq. (5) means instability of the ion in the trap.

To solve Eq. (5), we must determine the first two terms ϕ_0 and ϕ_1, whose values depend on the initial wave function of the trapped ion. As an example, we consider that the ion is initially confined in the vibrational ground state of the simple harmonic oscillator [14]

$$\psi(x,0) = \left(\frac{2\sigma}{\pi}\right)^{\frac{1}{4}} e^{-\sigma x^2}. \quad (6)$$

In comparison to the solution of Eq. (2) [11,12], i.e.,

$$\Psi_n(x,t) = D_n\left(\frac{1}{\varphi(t)}\right)^{\frac{1}{4}} H_n(Ax)e^{i\beta(t)x^2 - \frac{A^2x^2}{2}} e^{-i\frac{E_n}{\hbar}\int_{t_0}^{t}\frac{d\sigma}{\varphi(\sigma)}}, \quad (7)$$

where $D_n = \sqrt{\frac{m\sqrt{C}}{\hbar\sqrt{\pi}2^n n!}}$, $A = \sqrt{\frac{m\sqrt{C}}{\hbar\varphi(t)}}$, and $E_n = (n + \frac{1}{2})\sqrt{C}\hbar$, we have $\psi(x,0) = \Psi_0(x,0)$, implying $\sigma = \frac{A^2}{2}$ and $\beta(0) = 0$. If we take $\varphi(0) = 1$, we may obtain $\phi_0 = 1$ and $\phi_1 = 0$. We find numerically that the convergence of Eq. (5) is strongly relevant to v/w^2 and C/w^2, where the convergence occurs only within the regime $0 < v/w^2 < R$, with R the critical value, and R decreases for smaller C/w^2, as shown in Table I, where the minimum value of R is 2.35 in the case of $C/w^2 \to 0$. This implies that the ion is always stably trapped if $v/w^2 \in (0,2.35)$ is satisfied. This is a condition for the stability region of a Paul-trapped ion, different from that associated with the dc and ac voltages. In comparison, the Mathieu equation gives $v/\omega^2 \in (0,0.46)$ [1] with no dc voltage, and the rough estimate by quantum treatment in Fig. 2 in Ref. [11] is $v/\omega^2 \in (0,0.8)$ for $U \to 0$. So our solved restriction is less stringent, implying a bigger stability region. This result reflects from another angle the fact that the trapped ion under the government of quantum mechanics is more stable than the classical counterpart.

We have to mention that the condition in Eq. (5) for convergence is somewhat general because $\phi_0 = 1$ and $\phi_1 = 0$ come from $\beta(0) = 0$ and $\varphi(0) = 1$, which are reasonable assumptions based on $\psi(x,0) = \Psi_n(x,0)$. This implies that if the trapped ion is initially in a higher eigenstate or even in a superposition of the eigenstates of the simple harmonic oscillator, rather than in the ground state, $\phi_0 = 1$ and $\phi_1 = 0$ remain unchanged and the treatment above still works. In other words, the initial states of the trapped ion only change the wave packet of the ion in the time evolution, but not the condition for convergence.

Considering the realistic parameter values in a single $^{40}Ca^+$ ion in a Paul trap, such as $V = 300$ V, $\omega/2\pi = 16$ MHz, and

TABLE I. Convergence of Eq. (5) under different values of C/ω^2 and v/ω^2, where $n*$ is defined as the critical number of the series expansion terms of $\varphi(t)$ at which $(\phi_{n+2}/\phi_n - 1)$ changes suddenly from negative to positive, meaning divergence. The divergence occurs at $n* \to \infty$ when $R = v/\omega^2 = 2.75$, 2.45, and 2.35 for $C/\omega^2 = 0.04$, 0.01, and approaching 0, respectively. Therefore, if $0 < v/\omega^2 < R$, we consider $\varphi(t)$ to be always convergent.

$\frac{C}{\omega^2} = 0.04$	v/ω^2	6	5	4	3.8	3.6	3.4	3.2	3.1	3.08	3.06	3.04	3.02	3	2.98	2.96
	$n*$	352	492	954	1111	1400	1821	2907	3865	4000	4441	4589	5057	5270	5946	6499
	v/ω^2	2.94	2.92	2.9	2.89	2.88	2.87	2.86	2.85	2.84	2.83	2.82	2.81	2.80	2.79	2.78
	$n*$	7196	8064	9500	9924	10773	11777	13011	14151	16016	17798	19806	22744	28037	35370	47575
$\frac{C}{\omega^2} = 0.01$	v/ω^2	6	5	4	3.8	3.6	3.4	3.2	3	2.9	2.8	2.78	2.76	2.74	2.72	2.7
	$n*$	362	475	847	1018	1236	1562	2165	3323	4120	5792	6543	6895	7540	8483	8960
	v/ω^2	2.68	2.67	2.66	2.65	2.64	2.63	2.62	2.61	2.6	2.59	2.58	2.57	2.56	2.55	2.54
	$n*$	10155	10991	11598	12742	13395	14505	15386	17174	18384	19782	20330	21020	22985	25930	29684
$\frac{C}{\omega^2} \to 0$	v/ω^2	6	5	4	3.8	3.6	3.4	3.2	3	2.9	2.8	2.78	2.76	2.7400	2.72	2.7
	$n*$	335	445	815	905	1087	1403	1883	2585	3161	3911	4322	4733	5189	5304	5806
	v/ω^2	2.68	2.66	2.64	2.62	2.6	2.58	2.56	2.54	2.52	2.5	2.48	2.46	2.44	2.42	2.4
	$n*$	6521	6643	7212	7573	8946	9331	10492	11562	12766	14995	18285	22599	24450	33610	37343

$r_0 = 1.2$ mm, we define the radial pseudopotential frequency $\omega_r = qV/(\sqrt{2}mr_0^2\omega)$ [15]. In our case, the constant C is the effective frequency of the simple harmonic oscillator potential, and thereby we may suppose $C = \omega_r^2$. The straightforward calculation results in $v/\omega^2 = 0.05$ and $C/\omega^2 = 1.3 \times 10^{-3}$, completely satisfying the conditions required above for the stability region.

Before ending the discussion, we should emphasize the following points. The results obtained can be also applied to many ions confined in the Paul trap provided they are vibrating in center-of-mass mode. In addition, it is necessary to keep the cooling lasers always on in the ion-trapping experiments, in which the laser cooling plays the role of damping in the model. Our solution in the absence of the damping term should still work when the damping is introduced into the model. Moreover, due to fabrication imperfection, the realistic trap potential is not perfectly quadratic, but also includes additional hexapole or octopole potentials. The modified potential in the trap will definitely change the stability regime we solved. Besides, the nonlinearity due to those multipolar potentials will spoil the stability region by heating the trapped ion if the ion deviates from the equilibrium position. However, this case is beyond the scope of the present paper. The detailed study in this aspect is based on the Duffing oscillator model [4,16].

In conclusion, for the Paul-trapped ion at $U = 0$, we have still considered that the stability region is related to the convergence of the nonlinear equation obtained from the solution to the time-dependent Schrödinger equation. Solving the nonlinear equation by an alternative method, we have found a restriction that is a helpful complement for the previously studied stability regions in Refs. [1,11] and also helps our further understanding of the problem of interest from a quantum-mechanical viewpoint.

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