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Energy Eigenstates of a Quantum Gate System

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We report exact solutions of the Poyatos–Cirac–Zoller quantum gate system with two trapped ions [*Phys. Rev. Lett.* **81**, 1322 (1998)]. It is the superposition of entangled states among the pure states of two harmonic oscillators and describes a mixed mode involving the center-of-mass and relative motions with commensurable frequencies. Theoretical analysis of the exact solutions shows that for a given trapping frequency the relative motion cannot be laser-cooled.

Quantum computation has attracted much interest because of its use in the development of polynomial-time algorithms for computational problems [1–3]. A promising quantum register is based on a collection of ions stored in a Paul trap. Two attractive schemes for performing quantum logic gates have been proposed by Cirac, Poyatos, and Zoller [4, 5], which are associated with cold or "hot" ions, respectively. The basics of the scheme with cold ions has been demonstrated experimentally by Monroe, King, and coworkers [6–8]. However, the exact solution of the Schrödinger equation for the considered system has not been derived because of difficulties in handling a system with both harmonic and Coulomb potentials. In the "hot" ion scheme, Poyatos *et al.* [5] employed only semiclassical solutions around the classical equilibrium "orbit" (a constant) [9, 10]. Feng, Duan, and coworkers [11, 12] have also given the solutions in terms of infinite series. The ions, of course, themselves exactly "solve" the Schrödinger equation and therefore are in the corresponding motional state. In particular, they were initialized to a ground state for a quantum register in previous experiments [8, 13]. To determine

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the analytically exact ground state, it is important to seek strict energy eigenstates of the system.

In this paper, we report results for solving the harmonic–Coulomb system in detail. We find that under some relationships between the frequencies of the motional mode and the quantum numbers of the relative motion, there are exact eigenstates for a set of energy eigenvalues. The exact solution is a product between wave functions of the center-of-mass (COM) and of the relative motions which have commensurable frequencies. It describes a superposition of entangled states among the pure states of two harmonic oscillators. As a "quantum data bus" these entangled mixed states will be useful.

The Poyatos–Cirac–Zoller quantum gate system is a pair of two-level ions confined in a linear trap [5]. In the presence of the static potential the Hamiltonian dominating the system is [5, 14, 15]

$$H = \frac{1}{2m}(p_1^2 + p_2^2) + \frac{1}{2} m\nu^2 (x_1^2 + x_2^2) + \frac{e^2}{4\pi\varepsilon_0 (x_2 - x_1)} \tag{1}$$

where we have assumed that the two ions possess the same mass m and are moving in the x direction with coordinates $x_2 > x_1$ and oscillation frequency ν. Setting the COM and the relative coordinates as

$$x_c = (x_1 + x_2)/2, \qquad p_c = m_c \dot{x}_c \qquad \text{for} \quad m_c = 2m \tag{2a}$$

$$r = x_2 - x_1, \qquad p_r = m_r \dot{r} \qquad \text{for} \quad m_r = m/2 \tag{2b}$$

and inserting Eqs. (2) into Eq. (1) yields the Hamiltonian with separate form $H = H_c(x_c, p_c) + H_r(r, p_r)$ whose corresponding wave function is

$$\psi = \psi_c(x_c)\psi_r(r) \qquad \text{for} \quad E = E_c + E_r \tag{3}$$

Thus we easily obtain the Schrödinger equations describing the COM and the relative motions,

$$H_c\psi_c = -\frac{\hbar^2}{2m_c}\frac{d^2\psi_c}{dx_c^2} + \frac{1}{2} m_c \nu^2 x_c^2 \psi_c = E_c\psi_c \tag{4a}$$

$$H_r\psi_r = -\frac{\hbar^2}{2m_r}\frac{d^2\psi_r}{dr^2} + \frac{1}{2} m_r \nu^2 r^2 \psi_r + \frac{e^2}{4\pi\varepsilon_0 r}\psi_r = E_r\psi_r \tag{4b}$$

The first of Eqs. (4) denotes a single harmonic oscillator with well-known solution and level. We determine the solution of Eq. (4b) in the following section.

Using the dimensionless variable ξ and constant σ defined by

$$\xi = \alpha r, \qquad \alpha = \left(\frac{m\nu}{2\hbar}\right)^{1/2}, \qquad \sigma = \frac{e^2}{4\pi\varepsilon_0}\left(\frac{2m}{\hbar^3\nu}\right)^{1/2} \tag{5}$$

we obtain Eq. (4b) in the simplified form

$$\frac{d^2\psi_r}{d\xi^2} + \left(\frac{2E_r}{\hbar\nu} - \xi^2 - \frac{\sigma}{\xi}\right)\psi_r = 0 \tag{6}$$

This dimensionless expression is helpful for analyzing the orders of magnitude of each term. In usual experiments [8], the ion's mass is probably 10 times the proton's mass m_p and the motion frequency is on the order of 10^7 Hz. Then Eqs. (5) give $\xi \approx 10^8\, r$ [m] and $\sigma \approx 10^7$ such that the sum of the two negative terms in Eq. (6) is always greater than 10^5 for any value of distance r between the two ions. This implies that the positive energy term $2E_r/(\hbar\nu)$ in Eq. (6) must be taken as quite large value. We will verify this assertion by exactly solving Eq. (6). We guess the solution of Eq. (6) in the form

$$\psi_r = Au(\xi)\xi \exp\left(-\frac{1}{2}\xi^2\right), \qquad u = \sum_{i=0}^{\infty} C_i\xi^i \tag{7}$$

with A is the normalization constant and C_i are constant coefficients. Substituting these into Eq. (6), we obtain the equation

$$\frac{d^2u}{d\xi^2} + 2\left(\frac{1}{\xi} - \xi\right)\frac{du}{d\xi} + \left(\frac{2E_r}{\hbar\nu} - 3 - \frac{\sigma}{\xi}\right)u$$
$$= \sum_{i=0}^{\infty}\left[i(i+1)\,C_i\xi^{i-2} - \sigma C_i\xi^{i-1} + \left(\frac{2E_r}{\hbar\nu} - 3 - 2i\right)C_i\xi^i\right] = 0 \tag{8}$$

To make the solution a finite series, we truncate the series in Eqs. (7) and (8) at $i = l$ for $l = 1, 2, \ldots$. After the truncation, equating the sum of coefficients of ξ^l, ξ^{l-1}, and ξ^{l-j-2} (for $j = 0, 1, 2, \ldots, l-1$) to zero, respectively, leads to the following equations for the coefficients C_i:

$$2E_r/(\hbar\nu) - 3 - 2l = 0, \qquad -\sigma C_l + 2C_{l-1} = 0$$
$$\text{for} \quad l = 1, 2, \ldots \tag{9a}$$

$$(l-j)(l-j+1)C_{l-j} - \sigma C_{l-j-1} + 2(j+2)C_{l-j-2} = 0$$
$$\text{for} \quad j = 0, 1, \ldots, l-1 \tag{9b}$$

and $C_j = 0$ for $j < 0$. These are overdetermined linear equations with the number of coefficients C_i being less than that of the equations. They therefore have solutions only for a set of special energy values

$$E_r = E_{rl} = (l + 3/2)\hbar\nu_l \qquad \text{for} \quad \nu = \nu_l, \quad l = 1, 2, \ldots \tag{10}$$

and constant $\sigma = \sigma_l$. For example, in the case $l = 1$ of Eqs. (9) we have the equations

$$2E_{r1}/\hbar\nu_1 - 5 = 0, \qquad -\sigma_1 C_1 + 2C_0 = 0, \qquad 2C_1 - \sigma_1 C_0 = 0$$

with the solutions $C_0 = 1$, $C_1 = 1$ and the special energy values $E_{r1} = 2.5\hbar\nu_1$, $\sigma_1 = 2$. Note that $\sigma_l > 0$ in Eqs. (5). When $l = 2$, Eqs. (9) give the four equations

$$2E_{r2}/(\hbar\nu_2) - 7 = 0, \qquad -\sigma_2 C_2 + 2C_1 = 0,$$

$$2C_1 - \sigma_2 C_0 = 0, \qquad 6C_2 - \sigma_2 C_1 + 4C_0 = 0$$

Under the conditions $E_{r2} = 3.5\hbar\nu_2$ and $\sigma_2 = \sqrt{20}$ they have the solutions $C_0 = 1$, $C_1 = \sqrt{5}$, and $C_2 = 1$. We have obtained, by means of a similar analysis, the constant σ_l and solutions of Eqs. (9) up to $l = 7$. The application of Eqs. (5) and (10) produces the corresponding frequencies and energies. For the cases $l \geq 3$, any l is associated with $N > 1$ sets of solutions. In Table I we show the detailed data for a set of the coefficients C_i, constant σ_l^2, frequencies ν_l, and energy E_{rl}.

Although the energies and frequencies here are too high for usual experiments [6–8], Table I displays several interesting results: (1) The constant $\sigma_l = \sigma(l)$ depends on the quantum number l of the relative motion, so that Eqs. (5) give the frequency $\nu_l = \nu[\sigma(l)]$ as a function of l. (2) The energy and frequency decrease with increasing l value. We estimate that the quantum number l corresponding to a frequency of 10^7 Hz is greater than 100. Thus the energy given in Eq. (10) is quite large, as asserted above. (3) The lower level corresponds to the state of relative motion with larger quantum number $l > 100$, where the quantum effect is not evident. The main quantum characteristics of the system come from the COM motion for the frequency $\nu < 10^{10}$ Hz. If the frequency is fixed, the quantum number l is also fixed. Therefore the quantization of the energy is due solely to the COM mode in this case.

Table I. Coefficients in Solutions (7) and the Corresponding Quantities

l	C_0	C_1	C_2	C_3	C_4	C_5	C_6	C_7	$\sigma^2{}_l$	ν_l (Hz)	E_{rl} (J)
1	1.0	1.0							4.0	3.8×10^{20}	1.0×10^{-13}
2	1.0	2.2	1.0						20.0	7.5×10^{19}	2.8×10^{-14}
3	1.0	3.7	3.7	1.0					54.7	2.7×10^{19}	1.3×10^{-14}
4	1.0	5.3	8.0	4.2	0.8				112.4	1.3×10^{15}	7.5×10^{-15}
5	1.0	7.2	15.7	14.2	5.5	0.8			208.8	7.2×10^{18}	4.9×10^{-18}
6	1.0	9.3	27.0	34.1	20.9	6.1	0.7		347.6	4.3×10^{18}	3.4×10^{-15}
7	1.0	11.5	41.8	68.6	58.0	14.0	−0.6	−0.1	529.8	2.8×10^{18}	2.5×10^{-15}

Applying the result to Eqs. (7), we get the wave function of relative motion

$$\psi_{rl} = A_l\left(\sum_{i=0}^{l} C_i\xi^i\right) \xi \exp\left(-\frac{1}{2}\xi^2\right) \qquad \text{for} \quad l > 100 \tag{11}$$

The wave function and energy of the COM motion governed by Eqs. (4) are

$$\psi_c = \psi_{cnl} = B_{nl}H_n(\alpha_{cl}x_c)\exp(-\tfrac{1}{2}\alpha_{cl}^2x_c^2) \tag{12}$$

$$E_c = E_{cnl} = (n + \tfrac{1}{2})\hbar\nu_l \qquad \text{for} \quad n = 0, 1, 2, \ldots; \quad l > 100 \tag{13}$$

where B_{nl} is constant and $H_n\,(\alpha_{cl}x_c)$ is the Hermitian polynomial with

$$\alpha_{cl} = \sqrt{m_c\nu_c/\hbar} = \sqrt{2m\nu_l/\hbar} = 2\alpha, \qquad \nu_c = \nu_l \tag{14}$$

Combining Eq. (3) with Eqs. (11) and (12), we obtain the exact energy eigenstate

$$\psi = \psi_{nl} = N_{nl}H_n\,(\alpha_{cl}x_c)\left(\sum_{i=0}^{l} C_i\xi^i\right)\xi \exp\left[-\frac{1}{2}\,(\alpha_{cl}^2x_c^2 + \xi^2)\right] \tag{15}$$

with $N_{nl} = A_lB_{nl}$ being the normalization constant. The total energy of the system is

$$E_{nl} = E_{cnl} + E_{rl} = (n + l + 2)\hbar\nu_l \qquad \text{for} \quad n = 0, 1, 2, \ldots; \quad l > 100 \tag{16}$$

This solution represents superposition and entanglement among the pure phonon states of two harmonic oscillators. In the case $n = 0$, $l = 1$, substituting Eqs. (2), (5), (14) and $H_0 = 1$, $C_0 = C_1 = 1$ into Eq. (15) yields the exact solution as an evident entangled state

$$\begin{aligned}\psi_{01} &= N_{01}[1 + \alpha(x_2 - x_1)]\,\alpha(x_2 - x_1)\exp\left[\frac{-1}{2}\,\tilde{\alpha}^2(x_1^2 + x_2^2)\right] \\ &= \frac{1}{\sqrt{6}}\,(|0\rangle_1|1\rangle_2 - |1\rangle_1|0\rangle_2 + |0\rangle_1|2\rangle_2 + |2\rangle_1|0\rangle_2 - \sqrt{2}|1\rangle_1|1\rangle_2)\end{aligned} \tag{17}$$

under the condition $\sigma_1 = 2$. Here $|j\rangle_i$ denotes that ion i is in the state $|j\rangle$; by

$$\begin{aligned}|0\rangle_i &= (\tilde{\alpha}/\sqrt{\pi})^{1/2}\exp(-\tfrac{1}{2}\tilde{\alpha}^2x_i^2), \qquad \tilde{\alpha} = \sqrt{2}\alpha \\ |1\rangle_i &= \sqrt{2}\tilde{\alpha}x_i|0\rangle_i, \\ |2\rangle_i &= \sqrt{2}(\tilde{\alpha}^2x_i^2 - \tfrac{1}{2})|0\rangle_i\end{aligned} \tag{18}$$

we mean several lower pure states of the harmonic oscillator i. In fact, for any l, say $l > 100$, making use of the expansion form of the Hermitian polynomial, we can rewrite Eq. (15) as

$$\psi_{nl} = \begin{cases} N_{nl}[a_n(|0\rangle_1|1\rangle_2 - |1\rangle_1|0\rangle_2) + b_n(|0\rangle_1|2\rangle_2 + |2\rangle_1|0\rangle_2) + O_n(|1\rangle)] \\ \qquad \text{even } n \\ N_{nl}[b'_n(|0\rangle_1|2\rangle_2 - |2\rangle_1|0\rangle_2) + O'_n(|1\rangle)] \\ \qquad \text{odd } n \end{cases} \tag{19}$$

where a_n, b_n, and b'_n are constants and $O_n(|1\rangle)$, $O'_n(|1\rangle)$ are the higher exited states without $|0\rangle_i$. Noticing Eq. (14) and $\tilde{\alpha} = \sqrt{m\nu_l/\hbar} = \sqrt{m\ \nu'_l/\hbar}$ in Eqs. (5), we see that the frequency of pure states really is $\nu'_l = \nu_l = \nu_c$, with ν_c being the frequency of the COM mode. That is, Eqs. (15) and (19) are superpositions of the entangled states among various pure states of the harmonic oscillator with mass m and frequency ν_l, which is equal to the corresponding frequency of COM motion. For a single ion confined in the trap, it will oscillate with frequency $\nu = \nu_c$. However, the frequencies ν'_l and ν_c are commensurable, which is required for operation of the quantum gates [5].

In the state ψ_{nl}, ion i possesses $(n + l + 2)$ possible states $|j\rangle_i$ for $j = 0, 1, \ldots, (n + l + 1)$. Although the entanglements and superposition of the states make the quantum system so evasive, using the projection postulate [16] in quantum mechanics allows one to arrive at a simple entangled state by the action of a measurement. For instance, suppose the system is initially in any state of Eqs. (19). Now we measure the state $|0\rangle_1$ of ion 1; then Eqs. (19) mean that the state ψ_{nl} has been projected either onto $D_n|0\rangle_1|1\rangle_2 + D'_n|0\rangle_1|2\rangle_2$ for even n or onto $|0\rangle_1|2\rangle_2$ for odd n instantaneously, where D_n and D'_n are constants. The state ψ_{nl} will not be purified to a pure singlet unless the ions undergo collective measurement [17]. Experimental realization of the measurement is a difficult task. But the COM mode has been cooled to the ground state [4] with $n = 0$ by the Raman transition [8] with level difference $\hbar\nu_c$. For a given frequency ν_l the mode of *the relative motion cannot be cooled*, since the quantum number l is fixed by the function $\nu_l = \nu(l)$. In the case $n = 0$, Eq. (15) gives the exact COM ground state, which is still the entanglement and superposition among the pure phonon states, representing a mixed mode involving the COM and relative motions. Because heating of the non-COM mode can be substantially suppressed [8], such entangled ground states are important for transferring quantum information between the two ions.

We have constructed an exact solution of the quantum gate system with two trapped ions. It describes the entanglements and superposition among the pure states of two harmonic oscillators. In the presence of laser cooling, the system can transit to an entangled ground state of COM mode. However, for a given trapping frequency the relative motion cannot be laser-cooled.

Extending the results to a string of N two-level ions stored in a linear trap [4], we expect the existence of a similar exact solution, which is the superposition of entangled states among pure states of the N oscillators. By laser cooling one can arrive at an entangled ground state, as in the two-ion case. Taking the direct product between this state and an internal state vector as the initial state, then the quantum logic operations on the ions will lead to entanglement between the external and internal states. These problems need further exploration for realizing quantum computation.

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