Quantum motion of two trapped ions in one dimension

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We develop models for the motion of two trapped ions in one dimension, including both harmonic trapping forces and the Coulomb interaction between the ions. Mathematical and physical consistency dictates that the divergence of the Coulomb interaction at small distances be tempered with a soft core. A split-operator method is used to analyze numerically the energies and eigenstates of the motion of the two ions. Classification and closed-form expressions are also presented for the energies and the eigenstates in the limits when the equilibrium distance due to the Coulomb repulsion is either much smaller or much larger than the amplitude of the zero-point motion of the ions. Implications of the results for the properties of two identical ions with Bose-Einstein or Fermi-Dirac statistics are discussed.

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I. INTRODUCTION

The long-standing effort on spin-polarized hydrogen [1] and more recent developments in laser assisted manipulation of atoms [2] are now approaching the point where the effects of the statistics of the atoms, for instance Bose condensation, become observable. What kinds of experiments will be done and what kinds of new phenomena will be met with cannot be anticipated at the moment, but it is time for theorists to start sharpening their tools in "quantum field theory of cold atoms" [3]. Some initial steps have already been taken [4], but more methods and concepts in atomic degeneracy, and transparent examples on degeneracy, are needed.

The particular case we have in mind is an offshoot of a recent experiment of Eichmann *et al.* [5], in which interference fringes were seen in the light scattered from two trapped ions. We wonder under what circumstances quantum statistics of the ions might affect the results, at least as a matter of principle. Quantum statistics, of course, will only be significant if the occupation numbers of individual quantum states are at least of the order of unity. The point here is that the entire set of quantum numbers, internal *and* center-of-mass degrees of freedom for both ions, needs to be specified in order to discuss atomic degeneracy in a meaningful way.

The present paper is our first step toward the analysis of the degenerate version of the interference experiments analogous to those of Eichmann *et al.* [5]. We study the motion of two harmonically bound ions, taking into account the Coulomb repulsion between them, but in the main body of the paper we ignore the internal degrees of freedom altogether.

A full description of the interference experiment would involve the motion of the ions and the internal degrees of freedom with the added constraint of symmetrization of the state vectors, and the quantized light field as well. In view of the many facets of the problem, one should take advantage of as many simplifications as possible. In the present paper we therefore seek to analyze the motion of the ions in one dimension. It is not advisable simply to drop two dimensions, because the $1/r$ divergence of the Coulomb repulsion between the ions is mathematically more severe in one dimension than in three dimensions. In Sec. II we discuss a physical way out of this dilemma. We then introduce the model interaction used in the rest of the paper.

In Sec. III we present our numerical method for finding the eigenvalues and eigenvectors of the Hamiltonian describing the coupled motion of the ions. Section IV contains the core of our results. The Coulomb interaction tends to push the ions apart. Distinct physical regimes emerge according to whether the classical equilibrium distance between the ions would be much larger or much smaller than the amplitude of the zero-point motion. We analyze these cases separately. The intermediate regime when the equilibrium distance and the amplitude of the zero-point motion are comparable is harder to treat, but a few numerical results will be shown.

Further discussions are contained in Sec. V. We describe briefly the complete state of the ions, including all degrees freedom. We ponder on a qualitative principle that surfaces from our analysis: the effects of statistics are significant only if the ions are *operationally* indistinguishable. Finally, we consider the prospects of degeneracy experiments with trapped ions. On the basis of the present work they admittedly appear bleak. We speculate about possible ways to circumvent this problem.

II. ONE-DIMENSIONAL MOTION

We consider two identical ions $\alpha = 1, 2$ with mass m and charge q. We start with the three-dimensional motion under a quadratic binding potential. The coordinates and momenta of the ions in the principal-axis directions of the trap are denoted by $\{x_\alpha^i\} \equiv \mathbf{x}_\alpha$ and $\{p_\alpha^i\} \equiv \mathbf{p}_\alpha$, with $i = 1, 2, 3$. If the oscillation frequencies of the ions in the trap in the absence of the mu-

tual Coulomb interactions were ν_i, the total Hamiltonian reads

$$H = \frac{1}{2m}(\mathbf{p}_1^2 + \mathbf{p}_2^2) + \frac{m}{2}\sum_{i,\alpha}\nu_i\, x_\alpha^i x_\alpha^i + \frac{q^2}{4\pi\epsilon_0|\mathbf{x}_1 - \mathbf{x}_2|}. \tag{1}$$

We reduce the model to one dimension right away. A quasi-one-dimensional motion would naturally ensue if the restoring forces were much softer in one principal-axis direction than in the two orthogonal directions, say, $\nu_1 \ll \nu_{2,3}$, and if furthermore the quantum energies in the 2 and 3 directions, $\hbar\nu_{2,3}$, were much larger than any other relevant energies of the physical situation. Then the 2 and 3 components of the motion are neither excited nor deexcited during the evolution, but are effectively frozen. We assume that the transverse components of the motion remain in the ground states $|0\rangle_2$ and $|0\rangle_3$. The Hamiltonian for the degree of freedom 1 is then

$$H(1) = {}_3\langle 0|_2\langle 0|H(1,2,3)|0\rangle_2|0\rangle_3. \tag{2}$$

Interestingly, when the transverse frequencies are taken to be equal, $\nu_2 = \nu_3 = \nu_\perp$, the expectation value may be carried out analytically. We write all of our results in terms of the length and energy scales of the quantum harmonic oscillator (HO) in the direction 1,

$$\alpha = \left(\frac{\hbar}{m\nu_1}\right)^{1/2}, \qquad \epsilon = \hbar\nu_1. \tag{3}$$

For the Hamiltonian $\mathcal{H} = H(1)/\epsilon$ we have

$$\mathcal{H} = -\tfrac{1}{2}\left(\frac{\partial^2}{\partial\xi_1^2} + \frac{\partial^2}{\partial\xi_2^2}\right) + \tfrac{1}{2}(\xi_1^2 + \xi_2^2) + V(\xi_1,\xi_2). \tag{4}$$

Here

$$\xi_{1,2} = \frac{x_{1,2}^1}{\alpha} \tag{5}$$

are the scaled coordinates in the direction 1 for the ions 1 and 2,

$$V(\xi_1,\xi_2) = \frac{V_0}{b}\exp\left[\frac{(\xi_1-\xi_2)^2}{\pi b^2}\right]\operatorname{erfc}\left(\frac{|\xi_1-\xi_2|}{b\sqrt{\pi}}\right) \tag{6}$$

is the effective one-dimensional interaction between the ions,

$$V_0 = \frac{q^2}{4\pi\epsilon_0\alpha\,\epsilon} \tag{7}$$

is the Coulomb interaction energy in units of the HO energy ϵ for two ions at the HO characteristic distance α from one another,

$$b = \left(\frac{\nu_1}{\pi\nu_\perp}\right)^{1/2} \tag{8}$$

is essentially the ratio of the length scales of the transverse and longitudinal harmonic oscillators, and $\operatorname{erfc}(x)$ stands for the usual complement of the error function [6].

At large distances the interaction V behaves like the Coulomb potential,

$$V(\xi_1,\xi_2) \sim \frac{V_0}{|\xi_1-\xi_2|}, \quad |\xi_1-\xi_2| \to \infty. \tag{9}$$

However, the divergence of the Coulomb interaction is absent,

$$V(\xi,\xi) = \frac{V_0}{b}. \tag{10}$$

In fact, as may be seen from Fig. 1, the interaction V is overall approximated quite well by the transparent form

$$\tilde{V}(\xi_1,\xi_2) = \frac{V_0}{\sqrt{(\xi_1-\xi_2)^2 + b^2}}. \tag{11}$$

In Sec. II we have basically carried out two tasks. First, trivially, we have introduced the HO model and scalings. Second, we have successfully reduced the Coulomb interaction to act in one dimension. In one dimension the divergence of the unmodified $1/r$ interaction is much more drastic than in three dimensions. For instance, in one dimension perturbation theory with the $1/r$ interaction fails on mathematical divergences. The simple solution is to adopt a Coulomb potential with a softened core, such as V from Eq. (6) or $\tilde{V}$ from Eq. (11). The same trick [7], for similar reasons, is now in widespread use in one-dimensional simulations of high-intensity photoionization of an atom.

Our physical motivation for the soft core, frozen motion in the transverse directions, is strictly valid only in the limit $b \to 0$. However, in what follows we not only disregard this condition, but also model the Coulomb interaction with the heuristic form $\tilde{V}$.

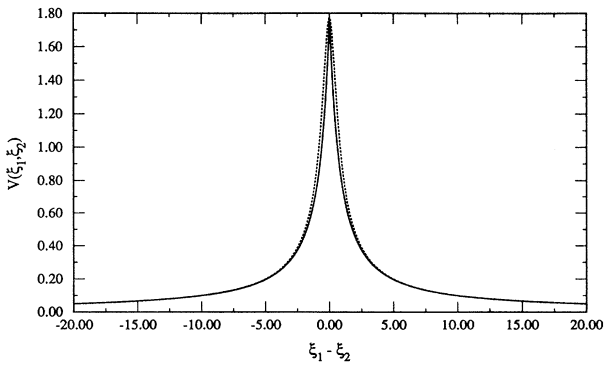

FIG. 1. Comparison of the "exact" one-dimensional potential V (solid line) and our simplified model $\tilde{V}$ (dashed line). Here the potential strength is $V_0 = 1$, and the core size parameter equals $b = 1/\sqrt{\pi}$.

III. NUMERICAL METHODS

We study the eigenvalues and eigenstates of the motion of the two ions numerically by integrating the time-dependent Schrödinger equation in imaginary time using the split-operator method [8,9].

Formally, let us assume that we had the exact time stepping operator for the imaginary time $-i\tau$,

$$T(\tau) = e^{-\tau\mathcal{H}}, \tag{12}$$

at our disposal. Let us denote the eigenvalues and the corresponding eigenstates of $\mathcal{H}$ in the ascending order of energy as ϵ_i and $|i\rangle$, $i = 0, 1, \ldots$. Suppose further that at the present stage k of the iteration we already know the eigenstates $|i\rangle$, $i = 0, \ldots, k$, and that we have selected a (possibly random) state vector $|\psi\rangle^{k+1,0}$. For $m = 0, 1, \ldots$, we now define the iteration

$$|\psi'\rangle = \left(1 - \sum_{j=0}^{k} |j\rangle\langle j|\right) |\psi\rangle^{k+1,m}, \tag{13a}$$

$$|\psi''\rangle = T(\tau)|\psi'\rangle, \tag{13b}$$

$$|\psi\rangle^{k+1,m+1} = \frac{|\psi''\rangle}{\sqrt{\langle\psi''|\psi''\rangle}}. \tag{13c}$$

If the mth iterate wave function is

$$|\psi\rangle^{k+1,m} = \sum_{i=0}^{\infty} a_i |i\rangle, \tag{14}$$

then the $(m+1)$th iterate wave function becomes

$$|\psi\rangle^{k+1,m+1} = \frac{\sum_{i=k+1}^{\infty} a_i \exp[-\tau(\epsilon_i - \epsilon_{k+1})]|i\rangle}{\sqrt{\sum_{i=k+1}^{\infty} |a_i|^2 \exp[-2\tau(\epsilon_i - \epsilon_{k+1})]}}. \tag{15}$$

It is clear that, if the eigenvalue ϵ_{k+1} is not degenerate, then every step m of the iteration amplifies the $|k+1\rangle$ component of the wave function at the expense of the other components. Finally we have the results

$$\lim_{m\to\infty} |\psi\rangle^{k+1,m} = |k+1\rangle, \tag{16}$$

$$\lim_{m\to\infty} -\frac{\ln\left[{}^{k+1,m}\langle\psi|T(\tau)|\psi\rangle^{k+1,m}\right]}{\tau} = \epsilon_{k+1}. \tag{17}$$

Given the eigenvectors and eigenvalues up to k, the iteration neatly spews out the $(k+1)$th eigenvector and eigenvalue. If the iteration is already close to converging and the dominant impurity is a small fraction of the state $|k+2\rangle$, we find using Eq. (15) relations such as

$$\| |\psi\rangle^{k+1,m+1} - |k+1\rangle\| \simeq \frac{\| |\psi\rangle^{k+1,m+1} - |\psi\rangle^{k+1,m}\|}{\exp[\tau(\epsilon_{k+2} - \epsilon_{k+1})]}, \tag{18a}$$

$$\exp[\tau(\epsilon_{k+2} - \epsilon_{k+1})] \simeq \frac{\| |\psi\rangle^{k+1,m+1} - |\psi\rangle^{k+1,m}\|}{\| |\psi\rangle^{k+1,m+2} - |\psi\rangle^{k+1,m+1}\|}. \tag{18b}$$

Our numerical implementation of the algorithm goes as follows. Let ξ_i and π_i denote the canonically conjugate coordinates and momenta of the ions; then we approximate the time stepping operator $T(\tau)$ as

$$T(\tau) = e^{-(\tau/2)f(\boldsymbol{\xi})}\, \mathcal{F}^{-1}\, e^{-\tau g(\boldsymbol{\pi})}\, \mathcal{F}\, e^{-(\tau/2)f(\boldsymbol{\xi})}. \tag{19}$$

Here $\mathcal{F}$ denotes the Fourier transform $\boldsymbol{\xi} \to \boldsymbol{\pi}$, and

$$f(\boldsymbol{\xi}) = \tfrac{1}{2}(\xi_1^2 + \xi_2^2) + \frac{V_0}{\sqrt{b^2 + (\xi_1 - \xi_2)^2}},$$
$$g(\boldsymbol{\pi}) = \tfrac{1}{2}(\pi_1^2 + \pi_2^2). \tag{20}$$

We naturally discretize the position variables $\xi_{1,2}$, and use the fast Fourier transformation to implement the Fourier transformation operator $\mathcal{F}$. In the imaginary world of infinite-precision arithmetics the step (13b) has to be done only once and the normalization (13c) is not needed at all, but for numerical stability we proceed in practice exactly as in Eqs. (13). However, instead of Eq. (17), we obtain the energy directly as the expectation value of the Hamiltonian, using Fourier transforms to calculate the kinetic energy. Useful convergence criteria may be extracted from Eqs. (18).

Three remarks about our particular split-operator algorithm are due. First, we do the ξ space evolution last (and first). In the pure Coulomb case with $b = 0$ the wave function should be zero at $\xi_1 = \xi_2$ in order to avoid an infinite Coulomb energy. Our algorithm would enforce this condition, which we count as a bonus. Second, there are higher-order versions of the split-operator method that are arguably advantageous for the integration of the Schrödinger equation in real time [10]. We have tried these in our imaginary-time case, but they proved violently unstable.

Third, in an attempt to avert convergence problems with degenerate states we ran into a bizarre example of the perils of numerical computations. We tried to modify the algorithm so that, in addition to the steps of Eqs. (13), we had a choice of symmetrizing or antisymmetrizing the state vector with respect to the exchange of the ions. Thus modified, the algorithm should have produced symmetrized or antisymmetrized state vectors. Instead, the computations ran amok. The reason turned out to be accumulation of round-off errors. Even if we start with a real initial guess for the wave function, round-off errors gradually generate an imaginary part. When symmetrization was added, round-off errors began to accumulate catastrophically. We included another step to remove the imaginary part into the algorithm, which restored flawless function.

The finite value of τ and the discretization of space both cause truncation errors in the results. In our calculations we typically use $\tau = 0.01$. To choose the spatial discretization we first pick the number of spatial points for the two-dimensional grid representing the

one-dimensional motion of both ions, typically $N = 64$ for each dimension, then calculate the discretization step $\Delta\xi$ in such a way that the ensuing discretization step in momentum space satisfies $\Delta\pi = \Delta\xi$. If there were no Coulomb interaction in the Hamiltonian (4), by the symmetry of the HO such a choice would be optimal. Coulomb interactions complicate matters, but we may nonetheless reach a ten-digit accuracy in energy eigenvalues with very modest numerical effort.

IV. RESULTS

In Sec. IV we analyze the results from both the numerical calculations and our supporting considerations. The size of the core b notwithstanding, there is basically one parameter V_0 in the problem. To gain additional insight into the meaning of V_0 we consider the classical dynamics of the ions, temporarily assuming the pure Coulomb interaction with $b = 0$. In this case there are two obvious equilibrium positions of the ions, either $\xi_1 = \ell_0/2$, $\xi_2 = -\ell_0/2$, or $\xi_1 = -\ell_0/2$, $\xi_2 = \ell_0/2$, with

$$\ell_0 = (2V_0)^{1/3}. \tag{21}$$

The parameter ℓ_0 is the equilibrium distance between the ions, expressed in units of the HO length scale α. The cases $V_0 \ll 1$ and $V_0 \gg 1$ mean that the classical equilibrium distance between the ions is, respectively, much smaller or much larger than the quantum-mechanical length scale of the HO characterizing the trapping potential. The role of quantum effects is expected to be quite different in these two limits. Accordingly, our treatment is divided into subsections with $V_0 \ll 1$, $V_0 \gg 1$, and arbitrary V_0.

A. Case $V_0 \ll 1$

We start from the extreme case $V_0 = 0$ with no Coulomb interaction at all. We are then left with a two-dimensional HO. The energy spectrum is written in our dimensionless units as

$$E_{n_1,n_2} = n_1 + n_2 + 1, \qquad n_1, n_2 = 0, 1, \ldots. \tag{22}$$

The possible energies and their degeneracies are $E(N) = N + 1$, $g(N) = N + 1$, with $N = 0, 1, \ldots$. The lowest degenerate manifolds are of the form

$$\begin{aligned} N = 0: &\quad \{|0,0\rangle\}, \\ N = 1: &\quad \{|1,0\rangle, |0,1\rangle\}, \\ N = 2: &\quad \{|2,0\rangle, |1,1\rangle, |0,2\rangle\}. \end{aligned} \tag{23}$$

Here the quantum numbers inside the kets refer to the oscillator quantum numbers of ions 1 and 2, as in $|n_1, n_2\rangle = |n_1\rangle_1 |n_2\rangle_2$.

So far, we have ignored quantum statistics and written two-ion kets in total disregard of the symmetry or antisymmetry under the exchange of the particles. This is rectified easily. We write symmetric and antisymmetric manifolds of states, such as

$$\begin{aligned} N = 0: &\quad \{|0,0\rangle\}_S, \\ N = 1: &\quad \{\tfrac{1}{\sqrt{2}}(|1,0\rangle + |0,1\rangle)\}_S, \{\tfrac{1}{\sqrt{2}}(|1,0\rangle - |0,1\rangle)\}_A, \\ N = 2: &\quad \{\tfrac{1}{\sqrt{2}}(|2,0\rangle + |0,2\rangle), |1,1\rangle\}_S, \\ &\qquad \{\tfrac{1}{\sqrt{2}}(|2,0\rangle - |0,2\rangle)\}_A. \end{aligned} \tag{24}$$

It is clear from this example that for even N there are $N/2$ antisymmetric state vectors; for odd N the number of both symmetric and antisymmetric state vectors is $(N + 1)/2$.

Let us now turn on a small Coulomb interaction with $V_0 \ll 1$. Our numerical calculations show that for generic parameters V_0 and b the degeneracy of each manifold is completely lifted. The Hamiltonian remains invariant under the exchange of particle labels, so the proper state vectors are still either symmetric or antisymmetric. But not only are the state vectors different for bosons and fermions, so are the energies.

To appreciate the remaining complication, consult Fig. 2. It shows one antisymmetric (a) and one sym-

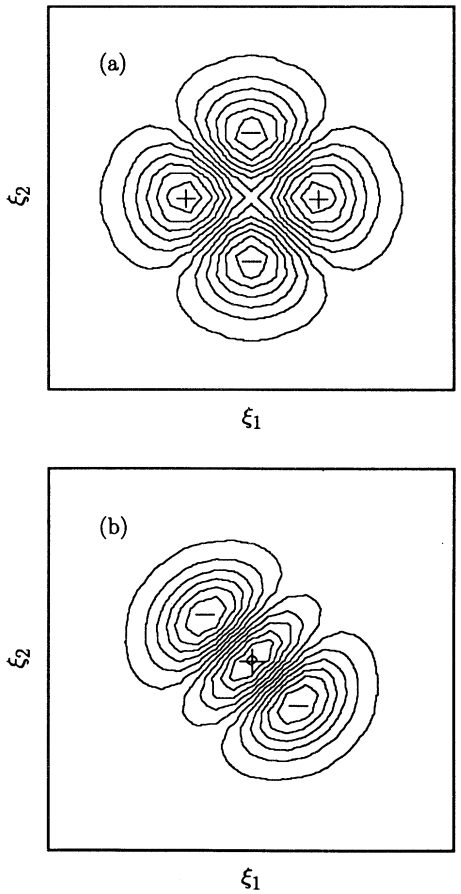

FIG. 2. Contour plot of an antisymmetric (a) and symmetric (b) wave function from the $N = 2$ manifold for the model potential $\tilde{V}$ with $V_0 = 0.1$ and $b = 1$. Plus and minus signs indicate signs of the wave function.

metric (b) wave function from the $N = 2$ manifold for $V_0 = 0.1$ and $b = 1$. Considering the well-known forms of the HO wave functions, the identification of the antisymmetric wave function as $\frac{1}{\sqrt{2}}(|2,0\rangle - |0,2\rangle)$ is straightforward. However, the symmetric wave function clearly is neither one of those listed in (24).

Now, a linear combination of any two symmetric wave functions is also symmetric, and the wave functions in (24) simply do not happen to coincide with those linear combinations that make the approximate eigenfunctions of the Hamiltonian including the Coulomb interaction. Degenerate perturbation theory is the method to resolve this kind of situations. We diagonalize the interaction $\tilde{V}$ separately in each degenerate N manifold. The required matrix elements of $\tilde{V}$ between the unperturbed states as in (23) are obtained numerically from two-dimensional integrals.

The resulting decompositions and energies of the few lowest symmetric and antisymmetric states are tabulated in Table I. A few conclusions survive to any accuracy we have been able to push the computations. First, the expansion coefficients in the wave functions are square roots of simple fractions, as shown in the table. Second, there is a pattern in the energies. These conclusions seem to hold for an arbitrary value of the parameter b, not just $b = 1$ as in Table I. Some underlying symmetry evidently permeates our model, but the nature of the symmetry remains a puzzle.

Summing up, we have enumerated the symmetries and the classes of near degeneracy of the energy eigenstates of the two-ion motion in the limit when the Coulomb interaction is a small perturbation, and given a few state vectors as concrete examples. The energies of the states and the dimensions of the near-degenerate manifolds depend on the symmetry of the state vectors, i.e., on the quantum statistics of the ions.

TABLE I. Energies and state vectors of the lowest-energy eigenstates of the motion of two ions in one dimension obtained using degenerate perturbation theory for the soft-core Coulomb interaction $\tilde{V}$ with the core parameter $b = 1$. The states are listed in order of increasing energy. The notation N_Σ indicates the multiplet N with unperturbed energy $N+1$, and the subscript $\Sigma = \pm$ specifies a symmetric or antisymmetric state vector. ΔE is the perturbation-induced deviation from the multiplet energy, tabulated in units of V_0. The column labeled $|\psi\rangle$ lists the coefficients of the product states $|N,0\rangle$, $|N-1,1\rangle$, ..., $|0,N\rangle$ in the normalized state vector.

N_Σ	$\Delta E/V_0$	$\lvert\psi\rangle$
0_+	0.789640	1
1_-	0.564891	$\frac{1}{\sqrt{2}}, -\frac{1}{\sqrt{2}}$
1_+	0.789640	$\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}$
2_+	0.507195	$\frac{1}{2}, -\frac{1}{\sqrt{2}}, \frac{1}{2}$
2_-	0.564891	$\frac{1}{\sqrt{2}}, 0, -\frac{1}{\sqrt{2}}$
2_+	0.789640	$\frac{1}{2}, \frac{1}{\sqrt{2}}, \frac{1}{2}$
3_-	0.452516	$-\sqrt{\frac{1}{8}}, \sqrt{\frac{3}{8}}, -\sqrt{\frac{3}{8}}, \sqrt{\frac{1}{8}}$
3_+	0.507195	$\sqrt{\frac{3}{8}}, -\sqrt{\frac{1}{8}}, -\sqrt{\frac{1}{8}}, \sqrt{\frac{3}{8}}$
3_-	0.564891	$\sqrt{\frac{3}{8}}, \sqrt{\frac{1}{8}}, -\sqrt{\frac{1}{8}}, -\sqrt{\frac{3}{8}}$
3_+	0.789640	$\sqrt{\frac{1}{8}}, \sqrt{\frac{3}{8}}, \sqrt{\frac{3}{8}}, \sqrt{\frac{1}{8}}$

B. Case $V_0 \gg 1$

In the opposite limit when the Coulomb interaction is large, $V_0 \gg 1$, two observations immediately emerge from our computations. (i) Energy eigenstates come in near-degenerate doublets, one state symmetric and the other antisymmetric. (ii) Doublet energies are closely matched by the formula

$$E = E_0' + n_1 + \sqrt{3}\, n_2, \qquad n_1, n_2 = 0, 1, \ldots . \tag{25}$$

The $\sqrt{3}$ is the giveaway. If the ions are in near equilibrium under the Coulomb interaction, the classical small-vibration frequencies are 1 and $\sqrt{3}$. Equation (25) obviously describes the stationary Coulomb energy corresponding to the equilibrium, plus the quantized energy of small vibrations.

We first build on the observation about the mode frequencies. We take the soft-core interaction $\tilde{V}$ with the range b. Straight from Newtonian mechanics we obtain equilibrium distance l, equilibrium energy E_0, and frequencies $\nu_\pm$ of the small-vibration modes as

$$l = \sqrt{\ell_0^2 - b^2}, \quad E_0 = \frac{3\ell_0^2 - b^2}{4}, \qquad \nu_+ = 1, \quad \nu_- = (\ell/\ell_0)\sqrt{3}. \tag{26}$$

Here $\ell_0 = (2V_0)^{1/3}$ is the equilibrium distance for the pure Coulomb interaction, as before. In the common-motion vibration mode + the ions oscillate in phase, in the breathing mode − in opposite phases. We finally write a prediction for the two-ion energies as

$$E_{n_+,n_-} = E_0 + (n_+ + \tfrac{1}{2})\nu_+ + (n_- + \tfrac{1}{2})\nu_-, \qquad n_+, n_- = 0, 1, \ldots . \tag{27}$$

The quality of our model may be evaluated by inspecting Table II. We present side by side the values from Eq. (27) and the average energy of the two states in the numerically obtained doublets. For these data we use the parameters $b = 1$ and $V_0 = 32$, whence $\ell_0 = 4$. We present seven significant digits, at which resolution the doublet splitting can only be detected for a few pairs n_+, n_- included in Table II. The analytical formula produces about four usable digits. There is a pattern in the difference between the analytical and the numerical results that could probably be exploited to find more accurate approximate formulas, but we have not followed up on this lead.

We next consider the state vectors of the ions. First take a near equilibrium with the ion 1 (2) around the position $\ell/2$ ($-\ell/2$). Denoting the deviations from the equilibrium by $\eta_{1,2}$, we have

$$\xi_1 = \ell/2 + \eta_1, \quad \xi_2 = -\ell/2 + \eta_2. \tag{28}$$

TABLE II. Energies of a few lowest motional states of the two-ion system in the case when the Coulomb interactions is large. The soft-core potential $\tilde{V}$ is assumed, with the parameters $V_0 = 32$ and $b = 1$. The first column lists the quantum numbers n_+, n_- characterizing the doublet of states. E_T is the theoretical prediction from Eq. (27), and $\bar{E}_N$ is the average of the doublet energies from the numerical calculations.

n_+, n_-	E_T	$\bar{E}_N$
0,0	13.08853	13.09732
1,0	14.08853	14.09732
0,1	14.76558	14.78747
2,0	15.08853	15.09732
1,1	15.76558	15.78747
3,0	16.08853	16.09732
0,2	16.44263	16.48853
2,1	16.76558	15.78747
4,0	17.08853	17.09732
1,2	17.44263	17.48853

On the other hand, the normal coordinates of the small vibrations may be defined as

$$\eta_\pm = \tfrac{1}{\sqrt{2}}(\eta_1 \pm \eta_2). \tag{29}$$

One may trivially solve $\eta_\pm = \eta_\pm(\xi_1, \xi_2)$ from Eqs. (28) and (29). Now, the quantum representation of a small-vibration mode is a HO. Given the wave functions $u^\pm_{n_\pm}(\eta_\pm)$ corresponding to $n_\pm$ HO quanta in the oscillators with the frequencies $\nu_\pm$, we have a wave function of the two-ion system,

$$\begin{aligned} U^{+\ell}_{n_+,n_-}(\xi_1,\xi_2) &= u^+_{n_+}(\eta_+)u^-_{n_-}(\eta_-) \\ &= u^+_{n_+}(\tfrac{1}{\sqrt{2}}(\xi_1+\xi_2))\, u^-_{n_-}(\tfrac{1}{\sqrt{2}}(\xi_1-\xi_2-\ell)). \end{aligned} \tag{30}$$

We could equally well have started from the equilibrium in which the ion 1 (2) dwells around $-\ell/2$ ($\ell/2$). The corresponding wave function $U^{-\ell}_{n_+,n_-}$ is obtained by simply replacing ℓ with $-\ell$ in Eq. (30).

It is this possibility of choosing between the two wave functions $U^{\pm\ell}_{n_+,n_-}$ that underlies the twofold near-degeneracy of the ionic states. Simply put, if the ions were distinguishable, exchanging them would give two different but physically equivalent situations.

However, since the Hamiltonian is invariant under the exchange of the particles, quantum mechanics tells us that the eigenstates may always be chosen either symmetric or antisymmetric under the exchange of the particle labels. The two wave functions $U^{\pm\ell}_{n_+,n_-}$ do not satisfy this requirement, but suitable linear combinations thereof do. We write our final ansatz for the two-ion wave functions as

$$\begin{aligned} U^\pm_{n_+,n_-}(\xi_1,\xi_2) &= \tfrac{1}{\sqrt{2}}[U^{+\ell}_{n_+,n_-}(\xi_1,\xi_2) \pm (-1)^{n_-}U^{-\ell}_{n_+,n_-}(\xi_1,\xi_2)] \\ &= \frac{u^+_{n_+}(\frac{1}{\sqrt{2}}(\xi_1+\xi_2))}{\sqrt{2}}\{u^-_{n_-}(\tfrac{1}{\sqrt{2}}(\xi_1-\xi_2-\ell)) \pm u^-_{n_-}(\tfrac{1}{\sqrt{2}}(\xi_2-\xi_1-\ell))\}. \end{aligned} \tag{31}$$

The superscript $\pm$ refers to the exchange symmetry.

We have compared several numerically obtained wave functions with the predictions from Eq. (31). The analytical wave functions $U^\pm_{n_+,n_-}$ were always in excellent agreement with the numerical results.

The splittings of the doublets remain to be discussed. We are on loose ground here. It is easy to show that no quadratic (hence, solvable) Hamiltonian can have the degenerate eigenstates $U^\pm_{n_+,n_-}$, and so we have been unable to develop a systematic perturbation theory.

Nonetheless, some qualitative insights have emerged from numerical computations. In our example cases in the limit $V_0 \to \infty$ the antisymmetric state always was the higher one in energy. Based on the asymptotic form of the HO wave functions we surmise that the asymptotic form of the doublet splitting should be

$$\Delta E_{n_+,n_-} = E^-_{n_+,n_-} - E^+_{n_+,n_-} = K_0\, e^{-K_1\ell^2}, \quad \ell \to \infty, \tag{32}$$

where $K_{0,1} = K_{0,1}(\ell, b, n_+, n_-)$ should be slowly varying functions of ℓ. In Fig. 3 we correspondingly plot $\log_{10}(\Delta E_{0,0})$, the ten-base logarithm of the splitting of the ground-state doublet, as a functions of ℓ^2. The three

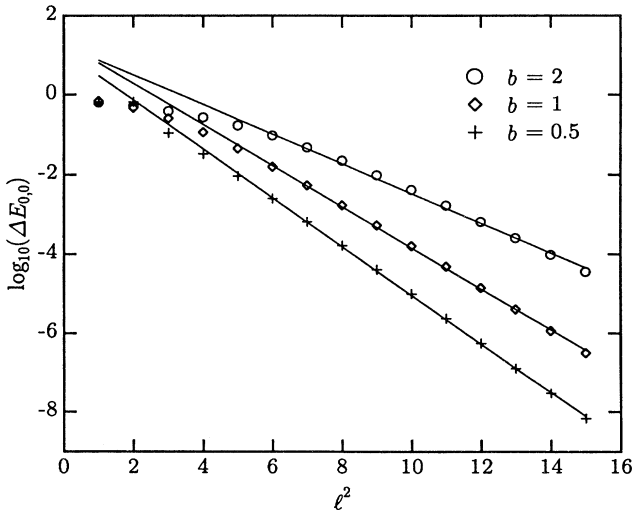

FIG. 3. Ten-base logarithm of the splitting of the ground-state doublet $n_+ = 0, n_- = 0$ as a function of the square of the classical equilibrium distance ℓ^2 for the soft-core potential $\tilde{V}$. Data are displayed for $b = 0.5$, $b = 1$, and $b = 2$, choosing $V_0 = V_0(\ell, b)$. Solid lines are linear least-squares fits to each data set for $\ell^2 \geq 5$.

data sets are for $b = 0.5$ (pluses), $b = 1$ (diamonds), and $b = 2$ (circles). The asymptotic form of Eq. (32) is verified. A linear least-squares fit to the numerical data with $\ell^2 \geq 5$ is also shown for each choice of b. The corresponding values of the parameters are $K_0 = 12.3$, $K_1 = 1.41$ for $b = 0.5$, $K_0 = 20.8$, $K_1 = 1.19$ for $b = 0.5$, and $K_0 = 17.6$, $K_1 = 0.86$ for $b = 2$. The parameters K_0 and K_1 have stubbornly resisted prediction, but at least we may see that, to the order of magnitude, $K_1 \sim 1$.

All told, we have characterized both the energies and the state vectors of the two-ion states in the limit when the Coulomb interaction dominates and pushes the ions far apart compared with the motional amplitudes of the ions. Energy eigenstates come in doublets, one state symmetric and one antisymmetric under the exchange of the ions. The energy spectrum of the motional states would be the same for bosons and fermions, except for a correction that is exponentially small in the equilibrium separation between the ions.

C. Case of arbitrary V_0

In the intermediate region $\ell \sim 1$ there is little hope for a transparent classification of energies and eigenstates of two-ion motion, but they may still be studied numerically as needed.

In Fig. 4 we plot the variation of the energies of a few of the lowest eigenstates as a function of the interaction strength V_0, with $b = 1$ fixed, for the soft-core potential $\tilde{V}$. Symmetric and antisymmetric eigenstates, respectively, are represented by solid and dashed lines. One may follow the continuous development of the pattern of motional energies from the limit $V_0 = 0$ to the other extreme $V_0 \to \infty$. Higher up in the energy we have also found states with the same symmetry that cross when the parameter V_0 is varied. It appears from our numerical calculations that these are true crossings, not avoided crossings.

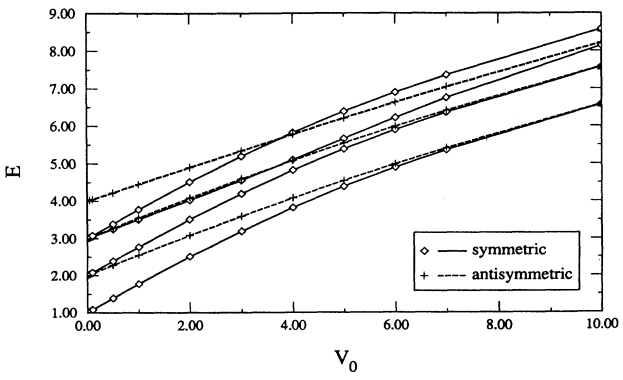

FIG. 4. Variation of the energies of the two-ion motional states with the strength of the Coulomb interaction for the potential $\tilde{V}$, given that $b = 1$ is fixed. Solid (dashed) lines follow symmetric (antisymmetric) states.

V. DISCUSSION

We have been able to classify and characterize the eigenvalues and eigenstates of energy of the motion of two ions in two asymptotic limits, when the classical equilibrium distance due to the Coulomb interaction is either much smaller or much larger than the amplitude of the quantum-mechanical zero-point motion. In the intermediate regime one may at least resort to numerical computations.

Our analysis pertains to one-dimensional motion of the ions. To this end, we have reduced the Coulomb interaction from three dimensions to one dimension in a manner solidly rooted in physics. Besides, we have resorted to a simplified model for the interaction. Numerical values such as in Tables I and II only apply to quite specific cases; their best use may be in comparisons with numerical schemes that a reader may want to set up. It is the qualitative understanding that we really were after.

One might ponder on generalizations to three dimensions. Let us first consider the case when all three trapping frequencies are different, a likely state of affairs in real experiments. In the limit of small Coulomb interactions, degenerate perturbation theory should again be the proper tool. Computation of the matrix elements of the Coulomb interaction may be tedious, but we do not anticipate any qualitatively new considerations. In the opposite limit of large Coulomb interactions one may set up the small-vibration energies and state vectors exactly analogously to one dimension.

However, in the case of precisely degenerate trap frequencies, the trap has rotational invariances and conserved components of total angular momentum. Degenerate states may remain even after the Coulomb interaction is included, and zero small-vibration frequencies are encountered. In this paper we do not attempt an analysis of such situations.

In the regime when the separation of the ions owing to the Coulomb interaction is smaller than the amplitude of the zero-point motion, the energy spectrum of symmetric and antisymmetric states is quite different. In the opposite case the energy spectrum is the same (except for small corrections) for symmetric and antisymmetric states. In the latter case system properties that probe the energy spectrum, e.g., heat capacity, do not directly depend on the statistics of the ions.

This observation suggests an operational meaning of distinguishability. For small Coulomb interactions mere quantum fluctuations may put both ions in the same region of space. If one carries out two measurements, each of which finds an ion in some region of space, one cannot tell if it was the same ion twice or two different ions. The case of large equilibrium separation stands in pointed contrast. If a measurement finds an ion twice in the neighborhood of the equilibrium position $+\ell/2$, it is intuitively plausible that it *was* the same ion all along. Even though the ions are indistinguishable, in effect one can distinguish them: one is at $+\ell/2$, the other at $-\ell/2$. We have here a hint of an intriguing notion: If there is an operation that may distinguish between particles, there are manifest properties of the system that are indepen-

dent of particle statistics. Indistinguishability is not a property of the particles alone, but of the physical system as a whole. The ions are indistinguishable if one *cannot* distinguish them.

Crystalline matter is an everyday example. Technically speaking the ions (atoms, molecules) that fill the crystal structure should impose their quantum statistics on the system, but in ordinary condensed matter the ions stay put and one need not consider exchange symmetries. Our case of large Coulomb interaction offers an accurate analog. The ions make a minicrystal with two degrees of freedom, and two "phonon" modes—and the energy spectrum of phonons is independent of the statistics of the ions.

It is tempting to speculate on another related notion. Depending on the strength of the Coulomb interaction, there is an intermediate regime in which the effects of quantum statistics vary continuously. Elementary textbook examples of Bose-Einstein and Fermi-Dirac statistics suggest that the statistics is a matter of yes or no, black or white. We think that, even at zero temperature, physics may present the whole scale of gray: If the particles may be distinguished with ambiguity, then the statistics shows partly.

So far we have considered only the mechanical motion of the ions. As concerns optical interactions, the internal degrees of freedom have to be included as well. Indistinguishability of the particles dictates that the state vector is either symmetric or antisymmetric when the particle labels are swapped, for both the motional and the internal states. Except for special cases such as an internal level with zero angular momentum, the state vector for the two-ion motion may quite well be either symmetric or antisymmetric for both bosons and fermions. It is then up to the exchange symmetry of the internal degrees of freedom to uphold the proper overall symmetry. A rich phenomenology could be expected when the coupling of a light field, internal degrees of freedom, two-ion motion, and exchange symmetry are simultaneously taken into account.

Our final item is the experiments. The condition that the spectrum of the two-ion motional states shows degeneracy effects $V_0 \leq 1$ may also be written

$$\hbar\nu_1 \geq \frac{m}{m_e} R, \tag{33}$$

where m and m_e are the masses of the ion and the electron, and $1R$ is one Rydberg, 27 eV. It is clear that this condition is far beyond the reach of the present ion trap techniques, which produce radio frequencies for ν_1. Furthermore, the condition (33) implies that, for any atomic ion, the vibration frequency ν_1 would be larger than the classical orbital frequency of any electron. The separation of the internal degrees of freedom and the motion of the ions, the cornerstone of our analysis, is then impossible.

It seems safe to conclude that conventional ion trap techniques will never lend themselves to comparisons of the motional energy spectra of fermions and bosons. However, the possibility that some optical experiments might be sensitive to wave-function symmetries remains to be investigated. An alternative path to experiments could open up with neutral atoms in optical or magnetic traps. For instance, interactions between magnetic dipoles might provide a repulsion analogous to the Coulomb interactions in an ion trap. If workable modifications of our ion trap scheme are discovered along these lines, or otherwise, the general methods and concepts we have introduced should still prove useful.

ACKNOWLEDGMENTS

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