Double wells, scalar fields and quantum phase transitions in ions traps

A. Retzker, R. Thompson, D. Segal, and M.B. Plenio
Institute for Mathematical Sciences, Imperial College London, SW7 2PE, UK and QOLS, The Blackett Laboratory, Imperial College London, Prince Consort Rd., SW7 2BW, UK
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Since Hund’s work on the ammonia molecule \cite{1}, the double well potential has formed a key paradigm in physics. Its importance is further underlined by the central role it plays in the Landau theory of phase transitions \cite{2}. Recently, the study of entanglement properties of many-body systems has added a new angle to the study of quantum phase transitions of discrete and continuous degrees of freedom, i.e., spin \cite{3,4} and harmonic chains \cite{5,6}. Here we show that control of the radial degree of freedom of trapped ion chains allows for the simulation of linear and non-linear Klein-Gordon fields on a lattice, in which the parameters of the lattice, the non-linearity and mass can be controlled at will. The system may be driven through a phase transition creating a double well potential between different configurations of the ion crystal. The dynamics of the system are controllable, local properties are measurable and tunnelling in the double well potential would be observable.

The development of ion trap technology enables precise control of the internal and external degrees of freedom in strings of ions \cite{7}. This motivated proposals for the realization of massive scalar fields in ion traps \cite{8,9}. These suggestions employed the longitudinal degrees of freedom only, leading to significant restrictions both in the accessible field theories, their mass etc, as well as the extraction of local properties of the system. We note that critical behavior is not experimentally accessible in such systems. More recently the use of radial modes in ion traps for the simulation of spin systems \cite{10,11} and Bose-Einstein condensation of phonons \cite{12} has been proposed.

Here we suggest the use of the radial degrees of freedom of the ions for the creation of a scalar field whose mass we may adjust freely by varying the radially confining potential. Crucially, in this way we have access to non-linear fields if we allow the system to approach its configurational phase transition where it changes from a linear to a zig-zag structure. While this transition is well known at the classical, high-temperature, level, \cite{13,14,15,16,17} at zero temperature it realizes a quantum phase transition in the quantum field describing the system. Furthermore, at zero temperature the groundstate of the zig-zag structure is degenerate (see Fig.1) and thus realizes a double well structure. Parameters such as the width and depth of the double well depend on the distance from the phase transition point and may thus be controlled precisely thanks to the high degree of control within reach in ion trap experiments. This approach compares favorably to the artificial creation of an electromagnetic double-well potential for a single ion by applied electric fields, as this would require field gradients and a degree of control that are not likely to be accessible in the foreseeable future. The crucial aspect of our proposal is the fact that the presence of several ions in the string leads to the automatic creation of a well controlled double well potential.

We will demonstrate that the above QPT may be characterized by the potential seen by a single normal mode, namely the mode of lowest frequency. Then the realization of a QPT requires the ability to experimentally adjust the potential perceived by the normal mode,

\begin{equation}
V(x) = V(0) + \frac{1}{2}a(\omega)x^2 + \frac{1}{4}b(\omega)x^4 + \frac{1}{6}c(\omega)x^6 + \ldots, \quad (1)
\end{equation}

where $x$ is the degree of freedom of the ‘important’ normal mode and $\omega$ is the external trap potential frequency analogous to the control parameter in the Landau theory. A second order transition occurs when $a(\omega) = 0$ and $b(\omega) > 0$. A first order transition occurs when the symmetry is broken by a cubic term.

In the remainder of this paper we first discuss the entanglement structure of the system in both the linear and the non-linear regimes, i.e. next-to or away from the phase transition. Then we present the non-linear Hamiltonian that is accessible experimentally and show how it enables the creation and full control of a double well

\[\omega_x > \omega_c\]

\[\omega_x = \omega_c\]

\[\omega_x < \omega_c\]

FIG. 1: The geometric transition between a linear formation and a 2D zigzag potential. The rotational symmetry has to be broken by the electrode structure. By controlling the potential a double well structure could be realized for which the ground state is a superposition of the two zig zag configurations.
potential. Finally, we discuss carefully possible measurement schemes to verify our predictions.

The Hamiltonian — In this work we consider chains of ions of mass $m$ that are subject to external confining potentials in the radial (x-y) plane and axial (z) direction as well as their mutual electrostatic repulsion. The external potentials are harmonic and we will assume that the confining potential in the y-direction is much stronger than in the x-direction, resulting in an essentially two-dimensional problem. This may be achieved both in linear ion traps and Penning traps [19]. Thus the Hamiltonian for $N$ ions is of the form

$$H = \sum_{i=1}^{N} \left[ \frac{\dot{\xi}_i^2}{2m} + \frac{1}{2} m \omega_x^2 \xi_i^2 + \frac{1}{2} m \omega_z^2 \xi_i^2 \right] + \sum_{i,j=1}^{N} \frac{\epsilon}{4\pi\epsilon_0} \sqrt{\frac{1}{(\tilde{x}_i - \tilde{x}_j)^2 + (\tilde{z}_i - \tilde{z}_j)^2}}$$

(2)

where $\tilde{x}_i$ is the distance of the i-th ion from the axis, $\tilde{z}_i$ is the position on the axis and we have fixed the strength of the confining potential in the axial direction. All the numerical results in this work assume $\omega_z = 1$ $MHZ$. One may now determine the equilibrium arrangement of the electrostatic problem posed here. There is a critical value $\omega_c$ ($\omega_c \approx 3N\omega_z/(4\sqrt{\log N})$ for $N \gg 1$ [18]) of the external confining potentials $\omega_x$ for which we observe a transition from a linear chain ($\omega_x \geq \omega_c$) to a zig-zag configuration ($\omega_x < \omega_c$) as shown in fig. 1. In the former case the equilibrium positions in the axial direction do not depend on $\omega_x$, while they become functions of $\omega_x$ in the latter. We will be interested in the regime of small displacements $\tilde{x}_i$ when the coupling between radial and axial modes may be neglected [20]. Assuming the system is cooled close to its ground state, we may then replace the operators $\hat{\xi}_i$ by their equilibrium positions which we denote by $x_i$. Then we perform a fourth order Taylor expansion of the potential to obtain the effective Hamiltonian

$$H_{\text{eff}} = \frac{1}{2m} \sum_{i=1}^{N} \dot{x}_i^2 + \frac{1}{2} \sum_{i,j=1}^{N} \gamma_{ij} \dot{x}_i \dot{x}_j + \sum_{i=1}^{N} b_i \dot{x}_i^4$$

(3)

where $\gamma_{ii} = \omega_x^2 \sum_j \frac{g_{ij}^2}{2m\pi\sigma_0 |x_i - z_j|}$, $b_i = \frac{1}{4} \sum_j \frac{g_{ij}^2}{4m\pi\sigma_0 |x_i - z_j|}$, and for $i \neq j$ we have $\gamma_{ij} = \frac{g_{ij}^2}{2m\pi\sigma_0 |x_i - z_j|}$, $\kappa_{ij} = \frac{9g_{ij}^2}{16\pi\sigma_0 |x_i - z_j|}$, $\kappa_{ij} = \frac{-3g_{ij}^2}{8\pi\sigma_0 |x_i - z_j|}$, the coupling to axial modes which exists in third and fourth order has been omitted. While for $\omega_x \gg \omega_c$, the contribution of the non-linear terms is small, this lowest order expansion of the Hamiltonian shows that by lowering $\omega_x$ we decrease $\gamma_{ii}$ leading to an increase of $\langle \dot{x}_i^2 \rangle$ and thus of the contribution of the non-linear terms. Eventually, for $\omega_x = \omega_c$ this will lead to a phase transition between a linear chain and a zig-zag configuration. Further decreasing $\omega_x$ results in more complex spatial configurations [16].

Scalar quantum field with an adjustable mass — The Hamiltonian [43] describes a non-linear scalar field theory on a lattice whose effective mass may be adjusted via the free parameter $\omega_x$ [21]. At the point of phase transition between the linear chain and the zig-zag formation (fig. 1) the field becomes massless corresponding to a critical field. The behavior of the entropy of single sites as well as its scaling with the size of blocks of sites for critical and non-critical lattice field theories has been of recent interest. While for non-critical systems an area law holds [22], the block entanglement diverges at the critical point at least in Gaussian 1-D models [4]. Here we explore these questions numerically for the full non-linear Hamiltonian [3] that may be realized in ion traps and, in order to gain intuition, for a version of it that is linearized about the equilibrium positions in the linear and the zig-zag cases.

We begin with the linearized model for a chain of ions, i.e., the regime where $\omega_x \gg \omega_c$, and expand $\tilde{x}_i$ and $\tilde{p}_i$ for the radial motion at site $i$ into normal modes of frequency $\omega_n$ with annihilation and creation operators $a_n, a_n^\dagger$. Here $\tilde{x}_i = \sum_n b_n \langle \tilde{n} e^{-i\omega_n t} + a_n^\dagger \tilde{n} e^{i\omega_n t} \rangle \sqrt{\hbar/2m\omega_n}$ and $\tilde{p}_i = -i \sum_n b_n \sqrt{\hbar m\omega_n}/2 \langle \tilde{n} e^{-i\omega_n t} - a_n^\dagger \tilde{n} e^{i\omega_n t} \rangle$, where $b_n$ are the normal mode coefficients of the crystal. Then $\langle \dot{\tilde{x}}^2_i \rangle = \frac{1}{2} \sum_n (b_n^2) \hbar/2m\omega_n$ and $\langle \tilde{p}^2_i \rangle = \frac{1}{2} \sum_n (b_n^2)^2 \hbar m\omega_n$. At the phase transition between the linear and the zig-zag configuration one normal mode becomes massless, i.e. its frequency $\omega_n$ vanishes. In a linearized model the massless mode leads to diverging $\langle \hat{\xi}_i^2 \rangle$. Since $\langle \hat{p}_i^2 \rangle$ remains finite the entropy, which is a function of $\langle \hat{\xi}_i^2 \rangle \cdot \langle \hat{p}_i^2 \rangle$, diverges [23]. Only sites that have vanishing amplitude in the zero mode would have a finite $\langle \hat{\xi}_i^2 \rangle$.

For $\omega_x < \omega_c$, the system possesses two nearly degenerate ground states and a double well potential for a large crystal is realized (Fig. 1). Here the restriction to a 2-dimensional setting is essential as otherwise the potential has a ’Mexican hat’ structure allowing for continuous rotations rather than forming a double well potential. For $\omega_x \ll \omega_c$ we then expect that the system will possess slightly more than one bit of entropy per site arising from the binary choice of location for each ion. The excess is due to the entropy available to the ion within each potential well.

At the transition point the entropy of a single ion of the harmonic chain diverges logarithmically. The entropy of a harmonic oscillator near the transition point satisfies $S_1(\omega_x) = \log(\sqrt{\langle \hat{\xi}_i^2 \rangle \langle \hat{p}_i^2 \rangle} / \hbar) \approx \log(|b_n| \sqrt{\langle \hat{p}_i^2 \rangle})/(2\hbar m\omega_n))$. Since, the lowest normal mode frequency, $\omega_0 = \omega_x^2 - \omega_c^2$, we find

$$S_1(\omega_x) \approx -\frac{1}{4} \log(\omega_x^2/\omega_c^2 - \omega_c^2/\omega_c^2) = -\frac{1}{2} \log \omega_0/\omega_c.$$  

(4)

For a small number of ions in the linearized model analytical results for the entropy may be derived. For $\omega_x > \omega_c$
and two ions the entropy is $S_2 = -\frac{1}{4} \log(\omega_x^2/\omega_z^2 - 1) + \log \left(\frac{1}{\sqrt{5}}\right) + 1 + O\left(\frac{1}{\omega_z^2}\right)$ while for the middle ion in a three ion chain $S_3 = -\frac{1}{4} \log(\omega_x^2/\omega_z^2 - \frac{1}{4}) + \log \left(\sqrt{2/5}/3\right) + 1 + O\left(\frac{1}{\omega_z^2}\right)$. 

Following the discussion of the linearized models, we now analyze numerically the phase transition between the linear chain and the zig-zag configuration for the non-linear Hamiltonian (3) for three ions. The transition between the two phases is a second order transition and the linearized models discussed above, where the order parameter is the displacement of the equilibrium position from the axis as indicated by the Landau theory. A full numerical calculation using Hamiltonian (3) without any externally applied non-linearities is shown in Fig. 2. Far from the transition point $\omega_x \gg \omega_c$, there is excellent agreement between the full numerical calculation and the linearized models discussed above. When approaching the transition the linearized models predict diverging single site entropies while the full Hamiltonian (3) yields a finite maximum value and then, for $\omega_x \ll \omega_c$, the entropy approaches unity i.e. an EPR state between one ion and the rest. The inset shows the comparison between the full numerics and the results of treating the low normal mode as decoupled, i.e., the red line results from the full numerics for three ions and the blue line is obtained by considering only the zero mode and then convolving the other modes to get the $x_1$ distribution. In order to compare the results we have checked the equation $\langle x_1^2 \rangle = \frac{1}{b}(\langle x_0^2 \rangle + 2\langle x_{zm}^2 \rangle + 3\langle x_{n}^2 \rangle)$, i.e., the $x_1$ deviation as a function of the normal mode deviations. The correspondence is perfect except at the transition point where $\sqrt{\langle x_1^2 \rangle}$ is 32nm and the decoupled normal mode result gives 38nm. For three ions the coefficient for the quartic term is $b = 3 \times 10^{-4} J \cdot m^{-4}$ which limits the energy gap to $\approx 50 k\text{Hz}$. As can be seen from Fig. 2 the nonlinear coupling between the different normal modes is negligible. As the number of ions increases the distances between the ions decreases; this raises the minimal energy gap and reduces the maximal entanglement. In this region the chain becomes highly non linear; this enables the observation of features peculiar to nonlinear systems like solitons and quantum and classical discrete breathers.

After this discussion of the critical entanglement properties at the phase transition between the linear chain and the zig-zag formation we now move to the discussion of the second main feature of this system.

**Double well potential** – The formation of double well potentials in ion traps through the application of external potentials has been considered in the past as an interesting system for the exploration of the classical-quantum boundary and as a system in which to preform atom interferometry. A number of groups are currently working towards scaling up ion trap quantum information processing to larger numbers of qubits following the general approach suggested by [25]. A key step in this approach is to separate two ions that are initially close together in a particular trapping zone of an array of miniature traps, so that they end up in separate trapping zones. This is done by raising the potential on a small ‘separation’ electrode. This electrode needs to be very small in order to allow for the production of a steep gradient in the potential between the ions. During the separation protocol the trap transiently moves through a double well configuration. The separation of a pair of ions in this way has been reported using a separation electrode with an axial dimension of 100μm [26]. A new generation of traps with smaller dimensions is currently under development worldwide but problems with anomalously high heating rates in these very small traps have yet to be solved. A theoretical study of relevance to this problem indicates that higher field gradients may be generated with relatively large electrodes that provide a dc octupole moment along with the usual a.c. radial quadrupole [27]. Traps based on these ideas have yet to be tested. Despite these advances in the experimental ability to realize double well potentials for ions with a measurable tunneling rate is still not within reach. However, as we have explained above, the zig-zag configuration gives rise to degenerate ground states separated by a tunnel barrier, thus providing a natural double well potential requiring no externally applied fields. As only the harmonic trapping potential needs to be controlled, precise control of the depth and separation of the effective double well potential and measurable tunneling rates should be achievable. This moves the realization of double well experiments in ion crystals within the reach of current experimental technology.

We will now discuss various possibilities to control the
parameters of the double well, to rotate the two-level system formed by the double well potential across the entire Bloch sphere and to measure coherence and tunneling rates in the double well potential. In the vicinity of the transition point the low normal mode alone controls the transition. Therefore by controlling the parameters of the Hamiltonian \( \mathfrak{H} \) and thus the values of \( a \) and \( b \) in Eq.1, a double well structure with a distance between the two minima is \( 2(-a/b)^{1/2} \) and the width of the wave function of \( (\hbar / (2\sqrt{-ma}))^{1/2} \) is created. The double well is created at the stage when each well is deep enough to accommodate one level, i.e. \( \frac{1}{4}a_0^2 \approx \hbar \sqrt{2a} \) (the depth is of the order of one excitation). Which means \( a \gtrsim 2^{5/3}(\hbar^2b^2/m)^{1/3} \). For the zig-zag configuration for three to ten ions \( \sqrt{\omega_x^2 - \omega_z^2} \) varies between 76kHz to 155kHz and for the square configuration it is 36kHz.

Such double wells can be created for the zig-zag configurations. In order to make the transition between the single well and the double well adiabatic, the transition rate should be slower than the minimal energy gap. The energy gap that should be considered is of the order of the energy gap of the quartic potential. The ground state in the Gaussian approximation is \( \propto \hbar^{1/3}h^{1/3} \) and the energy gap is approximately \( \left( \frac{3}{4} \right) \frac{3!}{4!} \hbar^{4/3}b^{1/3} \). In the zig zag configuration the minimal energy gap varies from 80kHz for three ions to 200kHz for seven ions. High energy gaps increase the robustness of the system to decoherence at the transition point.

Double wells can also be realized in the transition between 2D and 3D. This transition may be more suitable for Penning trap crystals which are not heated by micromotion. The zig zag transition could be realized both in Paul traps and in Penning traps after axialization. In the case of four ions, for \( \omega_x / \omega_z < 0.822 \) the stable configuration is two dimensional in the \( x-y \) plane (Fig.3(a)). For \( 0.822 < \omega_x / \omega_z < 1.27 \) a tetrahedron shown in Fig.3(b) is the stable configuration. In the square configuration \( b = 5 \times 10^{-4} \cdot m^{-4} \) thus the energy gap is 36kHz and the local potential is 140kHz at the optimal double well point.

The tunneling rates and the minimal energy gap increase with the number of ions. For three ions in the zig zag configuration the optimal point is at \( \omega_x = \omega_z - 3kHz \), where distance between the configurations is 180nm and the tunneling rate is 26.7kHz. For seven ions the optimal point is at \( \omega_x = \omega_z - 5.7kHz \) the distance between the configurations is \( \approx 1\mu m \) and the tunneling rate is 55kHz. For the square configuration the optimal point is at \( \omega_x = \omega_z - 1kHz \) and the distance is \( \approx 300nm \). For the zigzag configuration the tunneling rates vary from 3kHz for three ions to 4.5kHz for seven ions and 1kHz for the square configuration Fig.3(a). The distance at the optimal point varies between 30nm to 40nm and 20nm for four ions.

Having created a double well potential in the way described above the manipulation of its quantum state may be achieved in two ways. The first approach maps the external degree of freedom into the electronic one employing a Hamiltonian \( \eta \Omega (\sigma_+^{\text{atom}} |L-R\rangle \langle L+R| + \sigma_-^{\text{atom}} |L+R\rangle \langle L-R|) \). This is achieved employing a laser driving an electronic transition with a detuning equalling the energy gap between \( |L-R\rangle \) and \( |L+R\rangle \) and is possible since in the regime where each well supports one localized state and the spatial separation is less than \( \mu m \), one laser can make the transitions as long as the operation rate is slower than the energy gap \( \eta (70kHz) \) for three ions). Thus the manipulation of the external degree of freedom is achieved by mapping it onto the electronic degree of freedom, followed by its manipulation employing an on-resonance laser and the subsequent mapping back onto the external degree of freedom.

For larger separation two lasers could create Raman transitions between the \( |L\rangle \) and \( |R\rangle \) (the ground states of the wells) states using an excited state \( |C\rangle \) of the system whose wave function extends across both wells and whose energy is thus well above the gap between the two lowest lying states of the double well potential. The Raman transition could be created using the internal degrees of freedom of the ion, by using the three state \( \uparrow |L\rangle \longleftrightarrow \uparrow |C\rangle \longleftrightarrow \uparrow |R\rangle \). Raman transitions for double well systems were suggested in [31,52,33]. For this purpose an asymmetry between the two potential wells should be introduced in order to distinguish between the right and the left well which will break the symmetry between left and right. In order for the cubic term(\( ax^3 \)) to
create an energy gap of $1kHz$, $\alpha$ should be of the order of $10^{-10}\frac{m}{V}$. This will require application of $10V$ voltage for electrode size of $1nm$. A cubic term can be created using a trap geometry shown in Fig. 3.

The manipulation of the external degree of freedom may also be achieved by applying a radio frequency drive, i.e., by applying a time varying potential $V_0 \cos \omega t$. This will create the effective $\sigma_x$ or $\sigma_y$ rotations. Another way to create only one of these rotations is by adding a small cubic interaction which will add a phase shift between the $|L\rangle$ and $|R\rangle$ states.

An alternative approach to the manipulation of the state of the double well system exploits the fact that we are able to control the state of a single well potential. Thus by moving back and forth across the phase transition between single well and double well potential adiabatically we can generate any desired state in the double well potential by controlling the state in the single well potential. The state $|0\rangle$ of the single well would change adiabatically to $|L\rangle - |R\rangle$ in the double well while the state $|1\rangle$ evolves into $|L\rangle + |R\rangle$. Due to the non-linear term - $bx^4$, the minimal gap would not vanish in this process and thus the transition can be carried out at a sufficiently high rate while remaining approximately adiabatic. Thus, in order to move adiabatically from one phase to the other, the rate should be less than the minimal energy gap but higher than the decoherence rate (Fig. 3(c)). Arbitrary measurements on the double well may be achieved by combining unitary rotations implemented as explained above with measurements of the presence or absence of the system in the left or right well.

In the following we show a specific example of the transition between the two phases. For four ions, in the transition between a 2D and a 3D structure, the adiabatic condition is restrictive at the transition point $\omega_0 = 0$, at which the potential is $V = \frac{1}{4}bx^4$. For this transition the the minimal energy gap between the ground state and the first excited state is $50kHz$. This implies that the adiabatic sweeping could be relatively fast and create a small number of excitations. Fig. 3 shows the overlap of the state at a specific time of the transition, with the instantaneous ground state. The faster the rate the smaller the overlap. Fig. 3(d) shows the Rabi flipping for four ions between the different states in Fig. 3(b). It can be seen that a few cycles could be measured. Another way to measure the state is to change the system adiabatically to the state where the distance between the two wells is larger than one wavelength and then to measure, the $|L\rangle$ and $|R\rangle$ states using lasers.

The realization of the double well described here could open the way to interferometry at the Nano-scale. Ion traps have already been used as a measurement apparatus at the nanoscale [34]. Double wells for single atoms and BEC’s have been used for precise measurement in interferometry experiments. Using the Ion trap double well, measurements of non linear electric fields on the nanoscale should be possible. Measurements via interferometry should be more precise than the single well measurements. Moreover since linear fields are not seen by the ion trap, this procedure could measure cubic fields while completely eliminating the linear contribution. This double well could also measure magnetic field gradients. The initial state of the internal degrees of freedom can be initialized in a superposition of two levels and the phase induced by the magnetic fields can be measured by the population of the excited state.

The ideas presented here may be realized in linear Paul traps as well as Penning traps. Linear ion traps will exhibit micro-motion when ions are displaced from the trap axis. Nevertheless, for small deviations as discussed here, micromotion and the resulting decoherence effects
will not be significant. The advantage of the Penning trap is that it does not suffer from micro-motion, and thus the crystal may be less fragile to decoherence. However, observations need to take place in a rotating frame in which the effect of the magnetic field is cancelled \[24\].

**DISCUSSION**

We have suggested a realization of a non-linear Klein-Gordon field on a lattice with adjustable parameters. For a small number of ions the crystal may be cooled to the ground state and entanglement properties may be measured to a high precision. We have demonstrated that by crossing the quantum phase transition between a linear and a zig-zag configuration a fully controllable double well potential may be achieved with available technology. This demonstrates the potential of this system for the study of complex quantum many body phenomena. By controlling the nonlinear terms for example, highly non-linear excitations, such as kinks and breathers, can be created. Furthermore, rapidly driving the system through the phase transition, the Kibble mechanism may be observed \[36\], due to the ability of addressing and measuring individual ions with high precision.

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