Entanglement of compound atom-ion quantum systems: 
Effects of finite temperature and ion motion

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We consider a quantum Bose gas confined in a double well potential in interaction with a trapped ion and investigate the impact of two relevant sources of imperfections in experiments on the system dynamics that were not considered previously: Ion motion and thermal excitations of the bosonic ensemble. Particularly, their influence on the entanglement generation between the spin state of the moving ion and the atomic ensemble is analysed. We find that the detrimental effects of the ion motion on the entanglement protocol can be mitigated by properly choosing the double well parameters as well as timings of the protocol. Furthermore, thermal excitations of the bosons affect significantly the system’s tunnelling and self-trapping dynamics already at moderate temperatures, i.e. thermal occupation of a few double well quanta reduces the protocol performance of about 10%. Hence, we conclude that finite temperature is the main source of decoherence in such junctions and we demonstrate the possibility to entangle the condensate motion with the ion vibrational state.

I. INTRODUCTION

The newly attained experimental controllability for generating and manipulating atomic quantum mixtures affords a new playground to study many-body quantum physics. Some examples are: the formation and spread of correlations, mediated interactions and polarons [1][3]. Of particular interest is the generation of genuine quantum correlations that are of relevance for applications such as metrology [14] and sensing [13] as well as for fundamental research related, e.g., to the classical-to-quantum transition [16]. Within the plethora of compound atomic quantum systems recently realised in the laboratory (Bose-Fermi mixtures, spinor condensates, etc.), atom-ion systems constitute a rather unique platform because of the long-ranged interspecies interaction – on the order of a few hundred nanometers – compared to ultracold neutral matter, where the interaction range is on the order of a few nanometers. The competing effects owed to the different length and energy scales involved in the system enable one to study, as a paradigmatic example, the polaron strong-coupling regime more naturally [17]. They also give rise to novel phenomena like density bubbles [18][19] and the formation of mesoscopic molecular ions [20][21], to just mention a few (we refer to Refs. [22][25] for comprehensive overviews on the subject). In all these instances, the crucial role played by correlations beyond mean-field theory is the primary feature of such multi-length and multi-energy scale physics.

Among the cornucopia of systems exhibiting macroscopic quantum behaviour, atomic Josephson junctions (JJ) have acquired special attention in the last few years and offer unique prospects to study out-of-equilibrium dynamics in a very controllable manner. For example, measurements of high-order correlation functions [24] and quantum transport [27][29] can be carried out. In the former case, the system turns out to be a special-purpose quantum simulator of the so-called sine-Gordon model, which is a relevant integrable model for interacting quantum field theories, that enables access to non-perturbative information about different interesting quantities such as correlation functions or excitation spectra [30]. Furthermore, it has been theoretically shown that the tunnelling dynamics in bosonic JJs (BJJ) can be controlled with an impurity like a trapped ion enabling, e.g., the engineering of tailored entangled states between the atomic internal degrees of freedom and the motional states of a Bose-Einstein condensate (BEC) [31][32]. Particularly, it has been shown that by accurately choosing the atom-ion scattering length, it is possible to induce macroscopic self-trapping, namely suppression of tunnelling through the barrier. Such a phenomenon was predicted to occur only by controlling the relative phase between the condensates in the two wells and the interspecies interactions [35]. Hence, such a capability would allow for the generation of large many-particle–impurity states useful, e.g., for inferring scattering properties of the compound system via interferometric measurements as well as for information processing tasks [37][39]. Moreover, such ion-controlled BJJ can be viewed as building block of quantum simulators of condensed-matter [40][47] and lattice gauge models [38].

In previous studies of such controlled junctions, the following systems were investigated in detail: For the case of a single atom and single ion in the presence of micromotion and imperfect ion ground state cooling [39], it was

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found that a large ion-atom mass ratio and a minimal atom-ion separation considerably reduce the detrimental effects of the ion micromotion, similar to what has been pointed out in Refs. [40–42]. Many bosons interacting with a static ion in the framework of the two-mode Bose-Hubbard [31] and with numerical ab-initio simulations [32] have also been investigated. In particular, Ref. [32] has confirmed that within the execution time of the ion-BEC entanglement protocol, mean-field theory describes very accurately the self-trapping dynamics, whereas the two-mode approximation [33] with time-dependent orbitals describes the tunnelling regime very precisely. Specifically in the tunnelling regime, a natural population analysis (i.e. computation of the eigenvalues \( \lambda_j \) of the one-body density matrix) shows that a second orbital becomes populated up to 5% (i.e. \( \lambda_2 \leq 0.05 \)), while at most 95% of the atoms are in the condensate mode (i.e. \( \lambda_1 \geq 0.95 \)). Hence, the occupancy of a second orbital is indeed small, that is, mean-field and Bogoliubov theory are quite good descriptions of the system dynamics. Therefore, up until now, the system was investigated only when (a) the ion was tightly trapped so that its motion could be neglected and (b) at zero temperature. While (a) could be justified to some extent if the ion trap frequency is much larger than the atom trap frequency, (b) is much harder to attain, as in experiments, thermal fluctuations are unavoidable. Hence, the present study aims to include these effects in the description of the ion-controlled BJJ. Towards that end, we derive equations of motion for the compound atom-ion systems by starting from a many-particle wave function ansatz that is simpler than that of ab-initio methods at zero temperature [44–46], where all correlations are taken into account. More precisely, in our ansatz we shall assume that, regardless of the ion motional state, the bosonic quantum state can be described by a product state that relies upon the occurrence of correlations between the ion and the bosonic ensemble, which are the key ingredients for the observation of entanglement between the two subsystems. In this way, as we shall see later, we can include thermal fluctuations in the Bose gas by employing the truncated Wigner (TW) method [47–49].

This paper is organised as follows: In Sec. II, we outline the general theoretical model, while in Sec. III, we investigate the problem of many weakly interacting bosons for cases interacting with a static and a moving ion. Here the goal is to investigate the impact of ion motion and Bose gas finite temperature on the entanglement between the ion internal spin state and the motional state of the BJJ, assuming the ion to be in the ground state of its trap. In Sec. IV, we investigate the entanglement between the ion and BJJ motional states, i.e. without ion internal spin, and we analyse its performance at zero temperature in detail. Finally, in Sec. V, we draw our conclusions and briefly discuss future research directions.

II. THEORETICAL FRAMEWORK

In this section we introduce the microscopic many-particle Hamiltonian, together with the interactions involved in the problem, as well as the corresponding energy scales. Then, we outline the entanglement protocol we would like to implement that we shall investigate against ionic motion and finite temperature of the Bose gas. All this will form the basis for the subsequent analyses.

A. Hamiltonian

We consider a trapped ion and an ensemble of bosonic atoms confined in a double well, such that both subsystems can be treated in one-dimension (1D), i.e. their transverse motions are frozen to the corresponding ground state of their traps, as shown pictorially in Fig. 1. Hence, the full Hamiltonian of the compound quantum system at ultralow temperatures is given by

\[
\hat{H} = \sum_{j=1}^{N} \left[ \frac{\hat{p}_j^2}{2m} + V_{dw} (z_j) + \sum_{\xi = \uparrow, \downarrow} V_{\text{at}}^{\xi} (z_j - Z) |\xi\rangle \langle \xi| \right] + g \sum_{j < i} \delta (z_j - z_i) + \frac{\hat{P}^2}{2M} + \frac{M \omega_0^2}{2} Z^2. \tag{1}
\]

Here \( \hat{P} \) (\( \hat{p}_j \)) and \( Z \) (\( z_j \)) denote the momentum operator and the spatial coordinate of the ion (\( j \)-th atom), \( \omega \) is the ion secular trap frequency, if the ion is confined in a Paul trap [50], or the frequency of an optical trap [51–53]. Moreover, \( M \) (\( m \)) denotes the mass of the ion (atomic boson) and \( g = 2\hbar \omega \lambda_1 a_s / (1 - 1.4603a_s/\lambda_1) \) the effective atom-atom interaction in a waveguide [54]. Here \( \omega_0 \) is the frequency of the atom transverse trap (typically a few tens of \( \omega_0 \) – see also below Eq. [2]), \( a_s = \sqrt{2\hbar/(ma_\perp)} \) the width of the atomic waveguide, and \( a_\perp \) being the 3D s-wave atom-atom scattering length.

For the double well potential we consider the following simple analytical expression [43]

\[
V_{\text{dw}} (z) = \frac{b}{q^4} (z^2 - q^2)^2, \tag{2}
\]

where \( b \) denotes the inter-well barrier height and \( 2q \) is the distance between the two minima of the double well potential (see also Fig. 1). At the minima, i.e. at \( z = \pm q \), by Taylor expanding to second order the above outlined expression for the double well potential, the potential can be approximated by a harmonic potential with frequency \( \omega_0 = \sqrt{8b/mq^2} \) (see dashed line in Fig. 1).

Finally, the atom-ion polarisation potential is given by

\[
V_{\text{at}} (z - Z) = -C_4 / (z - Z)^4 \tag{3}
\]

with \( C_4 = \alpha e^2 / 2 \) (see Ref. [55] for a discussion on the validity of the 1D interaction). Here \( \alpha \) is the static polarisability of the atom and \( e \) is the ion electric charge.
Equation (6) represents the atom-ion interaction at long-range distances, thus not depending on the internal state of the ion. However, at short-range, typically below a few nanometers, the atom and ion electronic configurations matter. Since such a reliance on the internal state is generally not known, as accurate energy potentials are extremely difficult to obtain, its impact on the atom-ion wave function is accounted for by so-called scattering short-range phase shifts, which are used as boundary conditions for solving the stationary Schrödinger equation [55]. In this sense, the state-dependence of the atom-ion potential (6) on the electronic configurations has to be understood. Furthermore, the interaction (6) is characterised by typical energy and length scales that are denoted as: $R^* = \sqrt{\alpha^2\mu/h^2}$ and $E^* = [\hbar^2/2\mu(R^*)^2]$ with $\mu$ being the reduced mass. While one could employ quantum defect theory [55] for solving both the time-independent and time-dependent Schrödinger equation, for the sake of numerical convenience we shall use the following model potential replacing (6):

$$V_{\text{ai}}(z - Z) = v_0^\xi e^{-\gamma^\xi(z - Z)^2} - \frac{1}{(z - Z)^4 + 1/\bar{\xi}^4},$$

with $\xi = \downarrow, \uparrow$ denoting the internal spin state of the ion. As discussed in detail in Ref. [56], the parameter $v_0^\xi$ is fixed to a relatively large number (in units of $E^*$) in order to ensure that the atom wavefunction at the ion location is close to zero. On the other hand, the parameters $\gamma^\xi$ and $\bar{\xi}^\xi$ are chosen in such a way that the scattering phase shifts at large distances of the 1D atom-ion scattering problem at zero energy, map to the corresponding ones obtained with quantum defect theory, from which the reliance of the short-range phases, $\varphi_c$ and $\varphi_o$, on the model potential parameters is determined.

Hence, a certain pair of model parameters $(\gamma^\xi, \bar{\xi}^\xi)$ does correspond to a specific pair of short-range phases $(\varphi_c, \varphi_o)$, thus to a particular ion spin configuration $\xi = \uparrow, \downarrow$. Specifically, as model parameters we have chosen $v_0^\xi = 29(R^*)^{-4}$ and $\gamma^\xi = 10\gamma_{\text{min}}(\varphi^\xi = 80(R^*)^{-4}$ and $\gamma^\uparrow = \gamma_{\text{min}}$) with $\gamma_{\text{min}} = 4\sqrt{10}\bar{\xi}$, which correspond to the quantum defect parameters $\varphi^\xi_c = 0.23\pi$, $\varphi^\xi_o = -0.45\pi$ ($\varphi^\uparrow_c = 0.23\pi$, $\varphi^\uparrow_o = 0.3\pi$). In both cases, we have set $v_0^\xi = 3\bar{\xi}^\xi$. We note that the short-range phases are related to the corresponding even and odd 1D atom-ion scattering lengths. These can be tuned either by means of magnetic Feshbach resonances or by the transverse external potential of the atom and the ion [55, 57, 58]. In the case where the atom-ion entanglement is controlled by the ion motion (see Sec. IV), we have used only the pair corresponding to the spin state $| \downarrow \rangle$.

To conclude, we rescale the Hamiltonian in the following units: $R^* = \sqrt{\alpha^2\mu/h^2}$ and $E^* = [\hbar^2/2\mu(R^*)^2]$, where we have replaced the reduced mass with the mass of the boson. For instance, for $^{87}$Rb we have $R^* \approx 375.31$ nm and $E^*/\hbar \approx 0.41$ kHz. We prefer to make this choice, especially for the numerical simulations of the static ion case, since in this way the factor $\mu/m$ that otherwise would appear in the kinetic and trapping energies is removed.

### B. Entanglement protocol

Our objective is to generate entanglement between either the internal or motional state of the ion and the motional state of the atomic ensemble. In particular, we are interested in quantum states of the kind

$$|\Phi\rangle = \alpha|\psi_L\rangle|\eta_0\rangle + \beta|\psi_R\rangle|\eta_1\rangle,$$

(5)

where $\alpha, \beta \in \mathbb{C}$ with $|\alpha|^2 + |\beta|^2 = 1$, and $|\eta_n\rangle$ with $n \in \mathbb{N}$ denotes either the eigenstate of the ion harmonic trap, i.e. the usual harmonic oscillator state ($n = 0$ the ground state, $n = 1$ the first excited state, etc.), or the ion internal state $|\eta_1\rangle \equiv \uparrow, |\eta_0\rangle \equiv \downarrow$. Besides, the atomic states $|\psi_{L,R}\rangle$ with $\langle \psi_{L,R}\rangle |\psi_{L,R}\rangle = 1$ denote the states of the left and right well of the interacting bosonic ensemble, respectively. These states are linear combinations of the lowest energy symmetric and antisymmetric states of the double well potential. In the many bosons case, such states are obtained by imaginary propagation of the GPE [59, 61]. In trapped ion experiments, superposition states $\alpha|\eta_0\rangle + \beta|\eta_1\rangle$ of internal states can be generated by controlling their detuning with respect to the atomic transition and the light-ion interaction strength, i.e. Rabi frequency. On the other hand, iononic motional state superpositions can be attained by laser pulses in Raman configuration [50]. To this end, at the initial time, the ion and the atomic ensemble are assumed to be noninteracting, which is attained by choosing a sufficiently large inter-well separation $q$ or, alternatively, by a large bar-
rier height $b$. Here, however, we choose to control dynamically $q$. In this situation, assuming that the atomic bosons are initially prepared in the left well (see also Fig. [1]), the quantum state of the compound system is simply the tensor product $|\Phi\rangle = |\psi_L\rangle \otimes (\alpha|n_0\rangle + \beta|n_1\rangle)$. By properly choosing the model potential parameters as well as a tailored time dependence of the inter-well separation $q(t)$, it is possible, as we shall see later, to produce entangled states of the form (6). Because of the linearity of the Schrödinger equation (no spin-nonconserving interactions are assumed), however, we can focus simply on two separated processes, namely either $\alpha = 0$ or $\beta = 0$. Thus, after having identified suitable short-range scattering parameters for the atom-ion polarisation potential, together with a proper choice of the function $q(t)$, we can then generate any superposition state.

As already pointed out, the aforementioned dynamical processes are controlled by the inter-well separation, for which we have chosen the particular form:

$$q(t) = \begin{cases} 
q_0 & t < 0 \\
\frac{q_0 - q_{\text{min}}}{2} f(t) + \frac{q_0 + q_{\text{min}}}{2} & 0 \leq t < T_t \\
q_{\text{min}} & T_t \leq t < T' \\
\frac{q_0 - q_{\text{min}}}{2} f(t - T) + \frac{q_0 + q_{\text{min}}}{2} & T' \leq t < T \\
q_0 & t > T 
\end{cases}$$

where $f(t) = \cos(\pi t / T_t)$, $T = 2T_t + T_w$, and $T' = T_t + T_w$. Here $T_t$ is the time for decreasing and increasing the inter-well separation, whereas $T_w$ denotes the “waiting time”, i.e. the time needed to transport the bosons from one well to the other one. Furthermore, the maximum inter-well separation is denoted by $q_0$, whereas $q_{\text{min}}$ is the minimum inter-well separation reached in the dynamics. We note that hereafter we choose $q_{\text{min}}$ in such a way that it is larger than the critical atom-ion separation $q_c = 2|R^*| h / (M \omega)^{1/3}$ below which the effects of micromotion become significantly detrimental [39] [41]. We note, however, that micromotion is not an issue for ion trapping techniques based on optical fields [51] [53] and that for linear Paul traps it is advisable to engineer the double well potential along the longitudinal ion trap axis, where the radiofrequency fields are absent. As a rule of thumb, in order to identify the most suitable parameters defining $q(t)$, we fix $T_t = 12h / E^*$ [42], $q_0 = 5R^*$ and $b = 5.5E^*$, which ensure that initially the Bose gas and the ion do not interact, while $T_w$ varies within the range $10 - 90h / E^*$ and $q_{\text{min}}$ within the range $2 - 3R^*$. In this way, the entanglement, i.e. the fidelity defined in Eq. (7), for obtaining the desired entangled state at time $T_f$ is larger than 95%. The parameters quoted above would correspond to $(q_0 \simeq 383.25, q_{\text{min}} \simeq 153.30 - 229.95) \text{ nm}$, $(T_t \simeq 0.02, T_w \simeq 0.01 - 0.12) \text{ ms}$ for the atom-ion pair $^7\text{Li} / ^{174}\text{Yb}^+$, and $(q_0 \simeq 1.88, q_{\text{min}} = 0.75 - 1.13) \mu\text{m}$, $(T_t \simeq 4.65, T_w \simeq 3.87 - 34.86) \text{ ms}$ for $^{87}\text{Rb} / ^{171}\text{Yb}^+$, which are experimentally realistic [27] [29] [63] [67]. On the other hand, for the critical atom-ion separation, assuming $\omega = \omega_0$, we have for example: $q_c = 169.67 \text{ nm}$ for $\omega = 2\pi \times 7.27 \text{ kHz}$ and $^7\text{Li} / ^{174}\text{Yb}^+$, whereas $q_c = 572.83 \text{ nm}$ for $\omega = 2\pi \times 0.77 \text{ kHz}$ and $^{87}\text{Rb} / ^{171}\text{Yb}^+$.

Finally, the performance of the protocol is assessed by computing the Uhlmann fidelity defined as [68] [69]

$$F(t) = \text{Tr}[\sqrt{\rho_G \sigma(t) \sqrt{\rho_G}}].$$

Here $\rho_G$ is density matrix of the goal state we aim at, i.e. $\rho_G = |\psi_{L,R}\rangle \langle \psi_{L,R}|$, whereas $\sigma(t)$ is the density matrix of the system at time $t$ obtained by simulating the many-body quantum dynamics with the protocol outlined above. In particular, we use the one-body density matrix of the quantum state of the Bose gas. We also note that for pure states the Uhlmann fidelity reduces to the absolute value of the overlap integral between the evolved state $|\psi(t)\rangle$ and the goal state, that is

$$F_{L,R}(t) = |\langle \psi_{L,R}| \psi(t) \rangle|.$$  

### III. Entanglement Generation with the Ion Internal State

In this section we investigate the impact of finite temperature of the Bose gas and the ion motion on the entanglement protocol when the ion internal degree of freedom controls the tunnelling of the bosons through the barrier, as suggested in Refs. [31] [32]. Hence, here we assumed that the ion is prepared, and possibly kept, in the ground state of its ( secular) trap.

#### A. Zero temperature

To begin with, we consider the case of a static ion, whose dynamics is well described by the Gross-Pitaevskii equation (GPE)

$$i\hbar \frac{\partial \psi}{\partial t} = \left[ \frac{\hat{p}^2}{2m} + V_{\text{dw}}(z) + V_{\text{at}}(z) + g(N - 1)|\psi|^2 \right] \psi,$$

where $\psi = \psi(z,t)$ is the condensate wavefunction normalised to unity, $N = 50$, and $g = 0.004 E^*/R^*$. At the mean-field level, the tunnelling and the self-trapping processes can be characterised by the single parameter

$$\Lambda = \frac{U N}{2J},$$

where $U = g \int |\psi_L(z)|^4 dz$ is the onsite energy and $J$ is tunnelling rate. Upon the initial conditions, one can identify a critical value of $\Lambda$ above which self-trapping occurs. For instance, for the trap parameters $b = 5.5E^*$ and $q_{\text{min}} = 2.55R^*$ we have $\Lambda_c = 2$. Particularly with
the ion, we have $\Lambda = 0.54$ for $(\varpi^+, \gamma^+)$, i.e. tunnelling, $\Lambda = 5.97$ for $(\varpi^-, \gamma^+)$, i.e. the BEC is self-trapped. This confirms that the BJJ can be indeed controlled by a single trapped ion.

We have analysed the performance of the protocol by computing the Uhlmann fidelity by varying $T_w$ and $q_{\min}$, but for fixed $T_t = 12\hbar/E^*$ and $q_0 = 5\bar{R}$. The result of this investigation is summarised in Fig. 2(a) for the tunnelling process only, since for the other pair of model potential parameters, regardless of $T_w$ and $q_{\min}$, the bosonic ensemble remains essentially in its original starting well, namely we have always macroscopic self-trapping. As it can be seen, there are revivals dependent on the waiting time and the minimal separation between the wells. This indicates that there is a certain flexibility in the choice of the trapping and timing parameters. In order to gain insight about the origin of the revivals along the waiting time $T_w$ at fixed $q_{\min}$, however, we have performed a Fourier analysis which is summarised in Fig. 2(b). We compared the numerically extracted oscillation frequency via Fourier transform, $\Omega_{FT}$, with the one obtained within the mean-field two-mode approximation $[33, 70]$, $\Omega_{mf}$, the plasma frequency $\Omega_p$, the Uhlmann fidelity shown in Fig. 2(a) are not precisely adiabatic, we cannot attribute the oscillations of $F$ to a single frequency mode. Nonetheless, we note that for large values of $q_{\min}$, $\Omega_{mf}$ or $\Omega_p$ as they are very similar – is the dominating one, whereas for small values of $q_{\min}$ the plasma frequency $\Omega_p$ seems to prevail over the other two modes. To conclude this analysis, in Fig. 3 we show, as an example, the (normalised) density evolution of the two processes, i.e. tunnelling and self-trapping, whose fidelity is in both cases larger than 99%, thus proving the feasibility of the protocol.

![FIG. 2. (a) Uhlmann fidelity at the final time $T$ for a BEC interacting with a static ion as a function of the waiting time $T_w$ and minimal well separation from the barrier $q_{\min}$ for the model parameter pair $(\varpi^+, \gamma^+)$, which corresponds to the tunnelling regime. The barrier height is set to $b = 5.5\bar{E}^*$. (b) Oscillation frequency of the Uhlmann fidelity shown in panel (a), i.e. along its vertical axis, for various minimal separations $q_{\min}$: $\Omega_p$ is the plasma frequency, $\Omega_{FT}$ is the frequency of the oscillations of panel (a) obtained via Fourier transform, $\Omega_R$ is the frequency of the Rabi weakly interacting regime, $\Omega_{\text{ms}}$ is the frequency obtained with the two-mode mean-field model. The continuous lines are merely a guide to the eye.]

![FIG. 3. Temporal evolution of the atomic density (normalised to unity) for the pair $(\varpi^+, \gamma^+)$ (a) and for the pair $(\varpi^-, \gamma^+)$ (b) during the entanglement process for a BEC and a static ion. Here, $q_{\min} = 2.55\bar{R}$, $b = 5.5\bar{E}^*$, and $T_w = 32\hbar/E^*$, which correspond to $\omega_0 \simeq 2\pi \times 7.27$ kHz for $7\text{Li}$ atoms and to $\omega_0 \simeq 2\pi \times 0.77$ kHz for $^{87}\text{Rb}$ atoms. The frequency $\omega_0$ is computed at $q = q_0$, that is, when initially atom and ion do not interact.]

Now, the natural question is: How does the ion motion influence the BJJ and specifically the entanglement between the ion internal degree of freedom and the motional state of the BEC? In order to answer this question, we first have to define a proper ansatz for the correlated BEC-ion wave function and derive equations of motion that take into account the ion motion coupled to the quantum Bose gas. Towards that end, we introduce the ansatz

$$|\Psi(t)\rangle = \sum_{n=0}^{n_{\mathsf{c}}} c_n(t)|\Phi_n(t)\rangle|\phi_n\rangle,$$

where $|\Phi_n(t)\rangle$ denotes the wave function of $N$ bosons when the ion state is in the $n$-th harmonic oscillator state $|\phi_n\rangle$, whereas $\sum_{n=0}^{n_{\mathsf{c}}} |c_n(t)|^2 = 1$ with $n_{\mathsf{c}}$ being a cutoff, i.e. we truncate the ion Hilbert space by considering its most relevant portion. The complex numbers $c_n$ reveal the degree of entanglement between the Bose gas and the ion (i.e. the Schmidt number [69]), namely if $c_0 = 1$ and $c_{\neq 0} = 0$, then the compound quantum system is not entangled. In general, solving the dynamics of the compound quantum system for time-dependent $c_n$ and $|\Phi_n\rangle$ can be very involved. The previous study [32] on the static ion approximation shows that it is very reasonable to make the ansatz $|\Phi_n(t)\rangle = \prod_{j=1}^{n_{\mathsf{c}}} |\varphi_{n_{\mathsf{c}}}^{(j)}(t)\rangle$, namely assume no correlations between the bosons, at least for times shorter than a few tens of $\hbar/E^*$ like in Fig. 3. Thus, by employing the so-called Dirac-Frenkel variational principle [71, 72], we can derive the corresponding equations of motion for $c_n(t)$ and $|\varphi_{n_{\mathsf{c}}}^{(j)}(t)\rangle$, which are outlined in Eqs. (A20-A21) in the appendix. By solving these equations, we can then obtain the corresponding one-body density matrix for the bosons as well as the density matrix of the ion from the full density matrix $\hat{\rho} = |\Psi\rangle \langle \Psi|$. The $N$-body density matrix is given by

$$\hat{\rho}_{\mathsf{BG}} = \text{Tr}_I(\hat{\rho}) = \sum_n |c_n|^2 \rho_{\mathsf{BG}}^{(n)},$$

where $\rho_{\mathsf{BG}}^{(n)} = |\Phi_n\rangle \langle \Phi_n|$ is the density matrix of the
bosonic ensemble when the ion is in the $n$-th motional state of the trap. Thus, $\hat{\rho}_{BG}$ is the weighted average over the motional states of the ion. The one-body density matrix of the Bose gas is then obtained by tracing out $N-1$ bosons, which yields

$$\hat{\rho}_{BG} = \text{Tr}_{N-1}(\hat{\rho}_{BG}) = \sum_n |c_n|^2 \langle \varphi_n | \varphi_n \rangle.$$

(13)

On the other hand, the ion density matrix is given by

$$\hat{\rho}_I = \text{Tr}_{BG}(\hat{\rho}) = \sum_{n,n'=0}^\infty c_n c_{n'}^* \langle \varphi_{n'} | \varphi_n \rangle^N \langle \phi_{n'} | \phi_n \rangle.$$

(14)

Hence, the fidelity of each of the two processes is determined by replacing $\hat{\sigma}$ in Eq. (1) with $\hat{\rho}_{BG}$ of Eq. (13) and by the ground state occupancy of the ion. In other words, the total fidelity is defined as

$$\mathcal{F} = F|c_0|^2.$$

(15)

We note that while the states $|\varphi_n\rangle$ are normalised to unity, they are in general not orthogonal to each other.

We have analysed the effect of the ion motion on the entanglement protocol for different ion trap frequencies. The findings are illustrated in Fig. 4 where we have chosen to rescale the ion trap frequency in units of the double well characteristic frequency $\omega_0$. We see that the larger the ion trap frequency is, the better the static ion approximation. In particular, for the self-trapping regime (STR) (circles) this holds already for moderated trap frequencies, i.e. larger than (approximately) 30 $\omega_0$, whereas for the tunnelling regime (TR) (squares) the ion trap has to be much tighter in order to attain the static ion limit. This can be explained by the fact that for shallower ion traps the ion wavefunction plays a major role in the tunnelling dynamics of the bosons, because of the long-range atom-ion interaction. This effect is completely neglected in the static ion limit, where the reliance of the tunnelling rate on the ion is only due to the atom-ion short-range phases, i.e. the short-range part of the atom-ion potential. On the other hand, for the STR it turns out that the $\Lambda$ parameter (10) is only marginally affected by the ion wavefunction, that is, it is still above $\Lambda_{tr}$, thus ensuring the self-trapping condition, unless $\omega \leq 10 \omega_0$ as we found from a numerical analysis. We note that in that scenario a Markovian description of the ion dynamics in the framework of quantum master equations [14] would not hold, as the correlation functions of the bosonic bath would decay on the time scale of the ion’s dynamics.

Finally, in Fig. 5 we display the time evolution of the occupations $|c_n|^2$, that is, the population of the vibrational states of the ion trap [see also Eq. (11)]. In the panels (a-c) $|c_n|^2$ is shown for the TR, while in panels (d-f) it is shown for the STR. First of all, we note the appearance of peaks for ion vibrational states higher than the ground state [see panel (b)-(c) and (e)-(f)]. We attribute these peaks to the occurrence of several avoided crossings in the single-atom and single-ion energy spectrum as a function of the well separation $q$, as shown in the panel (g) of Fig. 5 as well as in a detailed analysis in Ref. [39]. As it can be seen, the larger the ion trap frequency is, the smaller the contribution of energetically higher trap states. As we already pointed out, for shallower ion traps, the ion wavefunction is broader and, because of the long-range atom-ion polarisation potential, the interaction occurs over a longer time. Thus, not only does the ion modify the tunnelling rate of the bosons, but also the atoms significantly affect the ion motion by causing population of additional vibrational states. Hence, the condition for which the ion is kept in the ground state is no longer satisfied, and, as a consequence, the total fidelity $\mathcal{F}$ decreases. Therefore, the static ion approximation is reasonably good for both processes if the ion trap frequency is roughly larger than 100 $\omega_0$ (see also Fig. 4), when we choose particular values of the trap and timing parameters. By properly choosing those parameters, however, as shown in Fig. 6 for a particular set of trap and timing parameters, we find that both STR and TR are still possible with quite good fidelities (above 90%) even at shallow ion traps (cfr. Fig. 4 for $\omega/\omega_0 = 18.8$). At the same time, the ion is almost in the ground state of its trap, i.e. $\min_{t} \{|c_0(t)|^2\} \geq 0.96$.

In summary, while the ion trap plays a non negligible role on the Josephson dynamics, the entanglement protocol is attained efficiently by an accurate search of parameters.

### B. Finite temperature

We proceed further with our analysis by investigating the impact of thermal fluctuations of the Bose gas on the correlated BEC-ion quantum state. To this end, we employ the truncated Wigner method [47]. This method, which belongs to the family of so-called classical fields...
methods \cite{73,74}, consists of generating a stochastic ensemble of initial matter-wave fields that are then propagated by means of the time-dependent GPE. Contrary to the usual GPE, which describes the evolution of the condensate wavefunction only, in the TW method the wave function describes the entire matter-wave field, i.e. both the condensed and non-condensed part. By averaging over a sufficiently large sample of stochastic fields, one can compute quantities like one-body and two-body density matrices that can be then used to obtain observables of interest, e.g. correlation functions. Furthermore, in the TW method the temperature of the gas is set initially by choosing a thermal state at temperature $T$. In the particle-number-conserving Bogoliubov approach \cite{75,76} that we adopt here, the thermal state is a canonical ensemble in which the many-body Hamiltonian is replaced by the quadratic Bogoliubov Hamiltonian \cite{48}. Within this approach the number of noncondensed atoms has to be small compared to $N$, thus implying that relatively low temperatures can be treated. At the same time $k_B T/(\hbar \omega_0) > 1$ has to be fulfilled, that is, the temperature cannot be too low as well. For further details on the method, see Ref. \cite{49,77}.

We begin our analysis by investigating the static ion limit. In this scenario, the standard TW method can be straightforwardly employed \cite{78}, since the atom-ion polarisation potential appears in the GPE \cite{9} as an additional external potential for the bosons. In this new setting, as a goal state, i.e. the density matrix $\hat{\rho}_G$, we use the initial one-body density matrix of the Bose gas at temperature $T$ when the two subsystems are well separated, i.e. the ion does not interact with the quantum gas, i.e.

$$\rho_G(z, z') = \langle z|\hat{\rho}_G|z'\rangle = \langle \varphi_0^L(z)|\varphi_0^R(z')\rangle_W - n_q \delta_{z,z'}.$$  \hspace{1cm} \hspace{1cm} (16)

Here $n_q = 1/(2\Delta z)$ mimics the $\delta$-function on a spatial grid ($\Delta z$ is the grid spacing chosen in the numerics), $\delta_{z,z'}$ is the Kronecker’s delta, and $\langle \varphi_0^L(z)|\varphi_0^R(z')\rangle_W$ represents the statistical average over the $N_s$ stochastic fields distributed according to the Wigner representation of the N-body density matrix of the Bose gas \cite{79}. Note, however, that in this context the one-body density matrix is normalised to $N + \mathcal{M}/2$ with $\mathcal{M}$ being the number of Bogoliubov modes used in the expansion of the noncondensed matter field (see Refs. \cite{48,49} for further technical details). Thus, in order to make a meaningful comparison with the zero temperature case, we do first normalise to unity the density matrices, e.g. $ho_G(z, z') \rightarrow \rho_G(z, z')/(N + \mathcal{M}/2)$. This state, however, differs from $\rho_G = |\psi_L,R\rangle|\psi_L,R\rangle$. Nonetheless, we do note that for the purpose of the entanglement generation we do not necessarily require being in the condensate mode, but in some motional state of the gas, e.g. a thermal state, either localised in the left or right well. Finally, the time-evolved density matrix $\sigma(z, z', t = T)$ is determined similarly to $\rho_G(z, z')$. The result of this study is summarised in Fig. 7, where on the left panel we show the Uhlmann fidelity for the tunnelling process at $k_B T = 3.2 \hbar \omega_0$ as a function of the
separation and waiting time, while in the right panel the Uhlmann fidelity as a function of the temperature \( T \) is shown. First, we see that the fidelity shows also at finite temperature the same dependence on \( q_{\text{min}} \) and \( T_w \), as in Fig. 2 left panel. Notwithstanding, the maximum of the fidelity is not anymore unity, but about 0.93. Hence, this indicates a strong impact of the gas temperature on the tunnelling dynamics. Second, the temperature affects almost equally the TR and the STR (i.e. almost the same slope in the right panel), even though the fidelity of the TR is worse than for the STR, as atoms do cross the barrier, and therefore do interact with the ion more strongly than in the STR. In contrast to imperfect ion ground state cooling (see Fig. 9 in Ref. [39]), however, the entanglement scheme is more resilient to thermal excitations in the Bose gas, thus enabling one to obtain the desired state at finite temperature still reasonably well.

We continue the analysis by including the motional degree of freedom of the ion. When the ion is moving, however, the quantum dynamics of the combined system does not simply obey the GPE, as we have seen in the previous subsection, and therefore the TW method has to be revisited. Initially, however, when the Bose gas and the ion do not interact, the stochastic ensemble of classical fields can be generated as in the standard approach, that is, by using the same prescription we used for the static ion limit, as outlined in Ref. [38]. The initial ensemble of stochastic fields is then propagated accordingly to Eq. (A21) instead of Eq. (9), where the ion and condensate motion are correlated. We justify this approach by the fact that we have assumed for each ionic motional state a condensate-like wave function, i.e. a product state, as for the GPE. Thus, in the same spirit of the original formulation of the TW method for single species, we apply it to the compound atom-ion quantum system for (partially) uncorrelated [38], but interacting, bosons. In this new framework, the one-body density matrix can be computed by using Eq. (13) as

\[
\rho_{BG}(z, z') = \langle z | \hat{\rho}_{BG} | z' \rangle = \sum_n \langle |c_n|^2 \rangle_W \langle (\varphi_n^*(z) \varphi_n(z'))_W - n_q \delta_{z,z'} \rangle
\]

(17)

where \( \langle \varphi_n \rangle \langle \varphi_n \rangle \) has been replaced by the term in the parenthesis in the last line of Eq. (17) in coordinate space representation. This expression is a weighted average over the vibrational states of the ion with weight \( \langle |c_n|^2 \rangle_W \), which is the statistical average over the \( N_s \) values of \( |c_n|^2 \) (for each \( n \)) as a consequence of the \( N_s \) stochastic fields generated initially. Similarly to Eq. (16), \( \langle \varphi_n^*(z) \varphi_n(z') \rangle_W \) represents the statistical average over the same \( N_s \) stochastic fields. Note also that \( \rho_{BG}(z, z') \) is a \( N \times N \) hermitian matrix with \( N \) being the number of grid points.

Now, since Eq. (A21) determines the time evolution of the single-particle orbitals of the bosons by assuming them of \( O(1) \)-norm, contrarily to the usual particle-number-conserving Bogoliubov approach of TW [38] [49], where the stochastic fields have \( O(N) \)-norm, we proceed as follows:

(i) We first generate \( N_s \) stochastic fields of \( O(N) \)-norm as in the original TW method.

(ii) We propagate the \( N_s \) stochastic fields accordingly to modified Eqs. (A20) [A21], where their \( O(N) \)-norm is taken into account (see appendix A.3).

(iii) We compute the resulting Uhlmann fidelity at the final time \( T \).

In this way we can consistently use the equations of motion Eq. (A21), which, together with Eq. (A20), preserve unitarity, as well as utilise the prescription of Ref. [38] for generating the initial sample of stochastic fields for the whole bosonic matter-wave field.

We have applied the above outlined ‘recipe’ in order to investigate the impact of finite temperature on the Uhlmann fidelity for the case of a moving ion, as discussed previously. In particular, we have considered an ion trap frequency of \( \omega = 81 \omega_0 \) in interaction with \( N = 50 \) bosons with coupling strength \( g = 0.004 E^\ast R^\ast \). We have analysed the TR only and found that, for example, for \( k_B T = 1.6 h \omega_0 \) it is about 0.94, i.e. very similar to the static ion case [cfr. panel (b) of Fig. 7]. Hence, the combination of both ion motion and finite temperature of the Bose gas does not render the performance of the entanglement protocol worse. Thus, this indicates that finite temperature is indeed the major source of imperfections and quite cold atomic ensembles are required for a successful implementation of the protocol.
IV. ENTANGLEMENT GENERATION WITH THE ION MOTIONAL STATE

In this section we investigate the possibility to entangle the Bose gas with the motional states of the ion. Particularly, we investigate the zero temperature scenario. Similarly to the mean-field analysis, we look for a suitable entanglement process by fixing $T_w = 5\hbar/E^*$ and $q_0 = 5\bar{R}^*$, but by varying the $T_w$ within the range $5 - 10.8\hbar/E^*$ and $q_{min}$ within the range $2.2 - 2.8\bar{R}^*$. Moreover, we consider $N = 10$ atomic bosons with an interaction strength $g = 0.02E^*\bar{R}^*$. In this way we have the same $gN/(E^*\bar{R}^*) = 0.2$ as in Sec. III A, but at the same time we reduce the complexity of the numerical simulation of the equations of motion (A28). Furthermore, the ion trap frequency has been chosen as $\omega = 12.8\omega_0$, and the barrier height as $b = 5.5E^*$.

In this new scenario, the entanglement protocol is defined in such a way that when the ion is in the vibrational ground state ($n = 0$), the one-body density matrix of the bosons is $\tilde{\rho}_G = |\psi_R\rangle\langle\psi_R|$, while when the ion is in the first excited state ($n = 1$) of the trap, the goal state is $\tilde{\rho}_G = |\psi_L\rangle\langle\psi_L|$. The results of this analysis are depicted in Figs. 8 and 9. Interestingly, when the ion is in the ground state, then the ion motional state is almost unperturbed (the ion Uhlmann fidelity is generally larger than 0.98, not shown). On the other hand, when the ion is in the first excited state ($n = 1$), then the ion motion is substantially affected by the coupling to the bosonic ensemble. Similarly to the peaks we have observed in Fig. 5, we attribute this difference to the arise of avoided crossings for excited vibrational states of the ion that cause admixture with excited motional states of both the ion and the bosons. Specifically, for the chosen trap frequencies, the set of parameters $T_w = 10.8\hbar/E^*$ and $q_{min} = 2.42\bar{R}^*$ are ‘optimal’, that is, $F_R(T) \simeq 0.97$, $F_L(T) \simeq 0.92$ for the bosonic ensemble, while $F_{n=0}(T) \simeq 0.997$ and $F_{n=1}(T) \simeq 0.93$ for the ion. We have performed a similar analysis for $N = 50$ and $g = 0.004E^*\bar{R}^*$ and found that it is still possible to identify suitable parameters for generating the entanglement, but, particularly when the ion is prepared initially in the first excited state, the parameter range is narrower and precise control of the double well position and waiting time is required. We note, however, that additional shaping of the transport function $q(t)$ could be attained by means of optimal control techniques [31,32]. Those methods do not only allow for enhanced performance of the entanglement protocol, but also for increased robustness against experimental imperfections of the manipulated time-dependent functions [33].

In conclusion, we have demonstrated that one can indeed produce entangled states of the form $\alpha |n = 0\rangle\langle n = 0| + \beta |n = 1\rangle\langle n = 1|$, for specific values of $q_{min}$ and $T_w$ and for any initial superposition $\alpha |n = 0\rangle + \beta |n = 1\rangle$ of the ion motional states with $\alpha, \beta \in \mathbb{C}$.

V. CONCLUSIONS AND OUTLOOK

We have investigated the quantum dynamics of a degenerate atomic Bose gas in a double well potential coupled to a trapped ion. Contrarily to previous studies concerning the same setup [31,32], we have analysed in detail the impact of the ion motion on the dynamics of the ultracold quantum gas as well as the impact of finite temperature of the gas on the entanglement protocol. We have found that, upon the tightness of the ion trap, different vibrational states of the ion motion can be populated. This is particularly true for the tunnelling regime, as the atoms interact more frequently with the ion as they pass through the barrier, whereas for the self-trapping regime, even shallower ion traps do not affect significantly the bosonic dynamics in the well. We have also found that thermal excitations on the top of the condensate can have a detrimental effect on the protocol. Notwithstanding, a suitable entanglement scheme can be attained, if we do
not aim at populating a single mode of the bosonic field (i.e., the condensate mode) as well as if the ion is not strictly kept in the ground state. Indeed, entanglement between two quantum systems can be also attained for mixed states \[84\]. In addition to this, we have demonstrated the possibility to realise an entanglement protocol between the ion and the bosonic ensemble motions, and therefore beyond the two-body schemes proposed in previous studies \[34, 89\]. This alternative pathway to entangle many-particle systems with the quantised motion of an ion is particularly appealing. Indeed, recent experiments \[55, 58\] on the ion spin dynamics have shown that ionic spin-relaxation, which is caused by large second-order spin-orbit interactions \[59\], occurs after a few Langevin collisions. Hence, this is indeed a fundamental drawback for the recently proposed entanglement schemes based on ionic spin-dependent short-range interactions. On the other hand, the experimentally observed strong spin-exchange processes \[55\] could be exploited to develop alternative entanglement schemes.

Another interesting aspect of our work is the application of the truncated Wigner method for simulating a Bose gas at finite temperature in the presence of an impurity. We have applied the method \textit{ad hoc} and seen that it provides a good description of the dynamics at nonzero temperature, and therefore enabled us to make quantitative predictions on the entanglement fidelity. It would be definitely interesting to better understand the applicability of our strategy to other problems involving an impurity in a thermal bath. This would have relevant applications in current research on impurity physics with atomic quantum gases, e.g., in order to better understand the role of finite temperature effects on the polaron formation, especially in view of its coherence properties, which are typically analysed in the framework of the (Markovian) quantum master equation formalism \[42, 90\].

Finally, a natural extension of the present work concerns the replacement of the quantum Bose gas with an ensemble of spin-polarised fermionic atoms, since experiments combining trapped ytterbium ions with fermionic lithium atoms are becoming available \[86, 91\]. Apart from the generation of entangled atom-ion states, an interesting question in this regard is how the ion can modify the junction transport properties. For example, can an ion stop the atomic flow through the barrier, particularly when the system is a superfluid, or can \(\mu m\)-sized density bubbles in the Fermi gas be formed, similarly to an ion embedded in a strongly correlated Tonks-Girardeau atomic gas \[19\]? Besides this, another intriguing research direction is the generation of correlated quantum dynamics induced by time-dependent modulation of the atom-ion interaction via laser fields that couples to Rydberg states \[55, 62\], as conducted in recent pioneering experiments \[63, 64\]. Here, interesting questions on thermalisation of closed systems and energy exchange between subsystems could be especially addressed.

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Appendix A: Appendixes

In this appendix we derive the equations of motion for a Bose gas in an external trap (e.g., a double well) interacting with an ion confined in a harmonic trap, as we discussed in Sec. III A. In doing so, we shall provide all steps of the derivation in a pedagogical manner, given the fact that the approach based on the Dirac-Frenkel variational principle that we adopt here might not be so familiar and that the technicalities of the derivation of the corresponding equations of motion are usually skipped. In addition to this, we also discuss briefly the actual numerical implementation.

1. Hamiltonian

Let us consider the one-dimensional Hamiltonian describing \(N\) interacting bosons of mass \(m\) in interaction with an impurity of mass \(M\) such as an ion:

\[
\hat{H} = \sum_{j=1}^{N} \left[ \frac{\hat{p}_j^2}{2m} + V_{\text{ext}}(z_j) + V_{\text{ai}}(z_j - Z) \right] + g \sum_{j<i} \delta(z_j - z_i) + \frac{\hat{P}_z^2}{2M} + \frac{M\omega^2}{2} Z^2.
\]

(A1)

Here \(\hat{p}_j = -i\hbar \partial_{z_j}\) is the momentum operator of the \(j\)-th boson, \(V_{\text{ext}}(z_j)\) is an external confining potential for the bosons, \(V_{\text{ai}}(z_j - Z)\) describes the interaction between the bosons and the impurity atom, \(\hat{P}_z = -i\hbar \partial_{Z}\) is the impurity’s momentum operator, and \(\omega\) the impurity trap frequency. Here \(\partial_{Z}\) denotes the first partial derivative with respect to \(Z\).

The Hamiltonian rescaled with respect to the length
\[ H = \sum_{j=1}^{N} \left[ -\frac{\partial^2}{\partial z_j^2} + \tilde{V}_{\text{ext}}(\tilde{z}_j) + \tilde{V}_{\text{at}}(\tilde{z}_j - \bar{Z}) \right] + \frac{g}{2} \sum_{k \neq j} \delta(\tilde{z}_j - \tilde{z}_k) + \tilde{H}_i, \]

with \( \tilde{z}_j = z_j/\tilde{R}^* \), \( \tilde{V}_{\text{ext}}(\tilde{z}_j) = V_{\text{ext}}(\tilde{z}_j)/\tilde{E}^* \), etc., and

\[ \tilde{H}_i = -m \frac{\partial^2}{\partial \bar{Z}^2} + \frac{m}{\bar{M}} \left( \frac{\tilde{R}^*}{\ell_i} \right)^4 \bar{Z}^2, \]

where \( \ell_i = [\hbar/(M\omega)]^{1/2} \), and \( \tilde{H}_i|\phi_n\rangle = \tilde{E}_n|\phi_n\rangle \).

2. Many-body state ansatz

The general many-body quantum state for such a compound system, which takes into account all correlations, is given by

\[ |\Psi\rangle = \sum_{n=0}^{\infty} c_n|\Phi_n\rangle|\phi_n\rangle, \tag{A4} \]

with \( \sum_{n=0}^{\infty} |c_n|^2 = 1 \). In practice we truncate the impurity Hilbert space in such a way that only the first \( n_i + 1 \) states are relevant. In order to proceed further, we make the assumption that the bosons are accurately described by the tensor product state \( |\Phi_n\rangle = \prod_{j=1}^{N} |\varphi_{n,j}\rangle \). We would like to underscore that while within such kind of mean-field approximation we neglect correlations between bosons when the impurity is in the \( n \)-th motional state, bosonic correlations can occur when the ion is occupying simultaneously different motional states. Under these conditions, the total system state is given by

\[ |\Psi\rangle = \sum_{n=0}^{n_i} c_n \prod_{j=1}^{N} |\varphi_{n,j}\rangle|\phi_n\rangle, \tag{A5} \]

with \( \langle \varphi_n|\varphi_n\rangle = 1 \ ∀n \). We note, however, that the single-particle states (i.e. orbitals) \( |\varphi_n\rangle \) are in general nonorthogonal, while we consider an orthonormal and time-independent basis for the impurity states \( |\phi_n\rangle \). In this formulation, the coefficients \( c_n \) and the orbitals \( |\varphi_n\rangle \) are the only time-dependent functions.

3. Derivation of the equations of motion

In order to obtain differential equations for \( c_n \) and \( |\varphi_n\rangle \) we employ the so-called Dirac-Frenkel variational principle \[^{[71,72]}\]

\[ \langle \delta \Psi | \partial_{\tau} - \tilde{H} |\Psi\rangle = 0, \tag{A6} \]

with \( \tau = (\tilde{E}^*/\hbar) \ t \). Here, \( \delta \Psi \) denotes the variation of the total wavefunction with respect to the free parameters \( c_n \) and \( \varphi_n \), while we ignore any variation of the ion’s states \( \phi_n \), as we have chosen them to be time-independent.

Towards that end, we begin with the computation of the vector state \( \langle \delta \Psi | \), which is simply given by

\[ \langle \delta \Psi | = \sum_{n=0}^{n_i} \delta c_n^* \prod_{j=1}^{N} |\varphi_{n,j}\rangle|\phi_n\rangle + c_n^* \prod_{j=1}^{N} \langle \delta \varphi_{n,j} | \langle \varphi_{n,j} | \phi_n \rangle \tag{A7} \]

whereas for the time derivative of the state we obtain

\[ \dot{|\Psi\rangle} = \sum_{n=0}^{n_i} \dot{c}_n \prod_{j=1}^{N} |\varphi_{n,j}\rangle|\phi_n\rangle + \sum_{n=0}^{n_i} c_n \prod_{j=1}^{N} |\varphi_{n,j}\rangle|\varphi_{n,j}\rangle \tag{A8} \]

Now, let us assess the two scalar products involved in Eq. (A6). To this aim, we start with the scalar product between the above outlined state variation and the time derivative of the many-body state, which yields

\[ \langle \delta \Psi | \dot{|\Psi\rangle} = \sum_{n=0}^{n_i} \delta c_n^* \left[ \dot{c}_n + Nc_n \langle \varphi_n | \varphi_n \rangle \right] \]

\[ + N \sum_{n=0}^{n_i} \langle \delta \varphi_n | \left[ c_n^* \dot{c}_n | \varphi_n \rangle + |c_n|^2 \right. \]

\[ \times \left. \left( |\varphi_n\rangle + (N - 1) \langle \varphi_n | \varphi_n \rangle |\varphi_n\rangle \right) \right]. \tag{A9} \]

We then compute the second scalar product in Eq. (A6), which is a sort of expectation value of the many-body Hamiltonian that gives the following result:
\[
\langle \delta \Psi | \hat{H} | \Psi \rangle = \sum_{n=0}^{n_i} \delta c_n \left[ c_n N \langle \varphi_n | H_0 | \varphi_n \rangle + \frac{\bar{g}}{2} N(N-1) c_n \langle \varphi_n, \varphi_n | \delta (\bar{z} - \bar{y}) | \varphi_n, \varphi_n \rangle + c_n \bar{E}_n \right]
\]

\[+ \sum_{n=0}^{n_i} c_n \langle \varphi_n, \phi_n | \bar{V}_{ai} | \phi_{n'}, \varphi_{n'} \rangle \langle \varphi_{n'} | \varphi_{n'} \rangle^{N-1} \bigg]\]

\[+ \sum_{n=0}^{n_i} \left| c_n \right|^2 N(N-1) \left| \langle \varphi_n | H_0 | \varphi_n \rangle \right| \langle \varphi_n, \varphi_n | \delta (\bar{z} - \bar{y}) | \varphi_n, \varphi_n \rangle + \sum_{n=0}^{n_i} \left| c_n \right|^2 \left| \langle \varphi_n | H_0 | \varphi_n \rangle \right| \langle \varphi_n, \varphi_n | \delta (\bar{z} - \bar{y}) | \varphi_n, \varphi_n \rangle
\]

\[+ \sum_{n=0}^{n_i} \left( \langle \varphi_n | V_{ai} | \phi_{n'} \rangle \langle \phi_{n'} | \phi_{n'} \rangle^{N-1} + (N-1) \langle \varphi_n, \phi_n | \bar{V}_{ai} | \phi_{n'}, \phi_{n'} \rangle \langle \phi_{n'}, \phi_{n'} | \phi_{n', \phi_{n'}} \rangle^{N-2} \right) \langle \varphi_{n'}, \varphi_{n'} \rangle,
\]

(A10)

with \( H_0 = -\partial^2 + \bar{V}_{\text{ext}} \). Let us note the appearance of the factor \( \langle \varphi_n | \varphi_{n'} \rangle^{N-1} \) with \( k = 1, 2 \). This is a direct consequence of the product ansatz \( \psi_n^a \) we made for the ensemble of bosons. Upon the “strength” of the orthogonality between the orbitals \( \varphi_n(\bar{z}) \) and \( \varphi_{n'}(\bar{z}) \) and the number of bosons, terms in the Eq. \( \text{(A10)} \) in which such overlaps appear will be large or small, thus strongly influencing the correlated impurity-gas quantum dynamics.

Now that we have all ingredients, we can insert the results of Eqs. \( \text{(A9)} \) and \( \text{(A10)} \) into Eq. \( \text{(A6)} \) in order to obtain the following equations of motion for the expansion coefficients

\[
i \left\{ c_n^\ast \partial_t c_n + \left| c_n \right|^2 \left[ \hat{\varphi}_n + (N-1) \langle \varphi_n, \varphi_n | \varphi_n, \varphi_n \rangle \right] \right\} =
\]

\[\frac{\left| c_n \right|^2}{\left| c_n \right|^2} \left( H_0 + (N-1) \langle \varphi_n | H_0 | \varphi_n \rangle + \frac{\bar{g}}{2} \left[ (N-1) \langle \varphi_n | \delta (\bar{z} - \bar{y}) | \varphi_n \rangle + (N^2 - 3N + 2) \langle \varphi_n, \varphi_n | \delta (\bar{z} - \bar{y}) | \varphi_n, \varphi_n \rangle + \bar{E}_n \right] \right) \langle \varphi_n, \varphi_n | \varphi_n, \varphi_n \rangle
\]

\[+ \sum_{n=0}^{n_i} c_n^2 c_{n'} \left( \langle \varphi_n | V_{ai} | \phi_{n'} \rangle \langle \phi_{n'} | \phi_{n'} \rangle^{N-1} + (N-1) \langle \varphi_n, \phi_n | \bar{V}_{ai} | \phi_{n'}, \phi_{n'} \rangle \langle \phi_{n'}, \phi_{n'} | \phi_{n', \phi_{n'}} \rangle^{N-2} \right) \langle \varphi_{n'}, \varphi_{n'} \rangle.
\]

(A12)

In order to arrive at the above outlined equations, we note that we made use of the following identities

\[
\langle \varphi_n | \delta (\bar{z} - \bar{y}) | \varphi_n \rangle = \left| \varphi_n(\bar{z}) \right|^2,
\]

(A13)

\[
\langle \varphi_n, \varphi_n | \delta (\bar{z} - \bar{y}) | \varphi_n, \varphi_n \rangle = \int d\bar{z} \bar{\varphi}_n(\bar{z})^4.
\]

(A14)

Now, by substituting in Eq. \( \text{(A12)} \) the time derivative \( \partial_t \)

\[\langle \varphi_n | \partial_t | \varphi_n \rangle = i \langle \varphi_n | \partial_t | \varphi_n \rangle + \hat{H}_{\text{gg}}[\varphi_n] | \varphi_n \rangle - \langle \hat{H}_{\text{gg}}[\varphi_n] | \varphi_n \rangle
\]

\[+ \sum_{n=0}^{n_i} c_n^2 c_{n'} \left( \langle \varphi_n, \phi_n | \bar{V}_{ai} | \phi_{n'}, \varphi_{n'} \rangle (N-1) \langle \varphi_n | \varphi_n \rangle
\]

\[+ \langle \varphi_n | V_{ai} | \phi_{n'} \rangle \langle \phi_{n'} | \phi_{n'} \rangle^{N-2} \right) \langle \varphi_{n'}, \varphi_{n'} \rangle,
\]

(A15)

where \( \hat{H}_{\text{gg}}[\varphi_n] = -\frac{\partial^2}{\partial \bar{z}^2} + \bar{V}_{\text{ext}} + \bar{g} (N-1) | \varphi_n \rangle^2 \) and \( \langle \hat{H}_{\text{gg}}[\varphi_n] | \varphi_n \rangle = \langle \varphi_n | \hat{H}_{\text{gg}}[\varphi_n] | \varphi_n \rangle \). With these definitions,
we can rewrite Eq. (A11) as

\[
\hat{c}_n = N c_n \left( H_{gp}^n [\varphi_n / \sqrt{2}] - i \langle \varphi_n | \hat{\varphi}_n \rangle \right) 
+ \sum_{n' = 0}^{n} C_{n'} C_{n''} N \langle \varphi_n, \phi_{n'} | \bar{V}_{ai} | \phi_{n''}, \varphi_{n''} \rangle \langle \varphi_{n'}, \varphi_{n''} \rangle N^{-1} \tag{A16}
\]

where \( H_{gp}^n [\varphi_n / \sqrt{2}] = H_0 + \frac{\tilde{g}}{2} (N - 1) |\varphi_n|^2 \). To further simplify the above outlined equations of motion, we first perform a unitary transformation on the coefficients, that is, \( c = \hat{U} c' \) with \( c' \equiv (c_0, c_1, \ldots, c_n)^T \) (similarly for \( C \)), where

\[
\hat{U} = \begin{pmatrix}
    e^{-i \eta_n (t)} & 0 & \cdots \\
    0 & e^{-i \eta_1 (t)} & \cdots \\
    \vdots & \ddots & \ddots \\
    0 & \cdots & e^{-i \eta_{n-1} (t)}
\end{pmatrix} \tag{A17}
\]

\[
i \hat{\psi}_n = H_{gp}^n [\psi_n] |\psi_n\rangle + \sum_{n' = 0}^{n} \frac{C_{n'} C_{n''}}{|C_n|^2} \left\{ (N - 1) \langle \psi_{n'}, \phi_{n'} | \bar{V}_{ai} | \phi_{n''}, \psi_{n''} \rangle \langle \psi_{n'}, \psi_{n''} \rangle N^{-2} + \langle \phi_{n'} | \bar{V}_{ai} | \phi_{n''} \rangle \langle \psi_{n'}, \psi_{n''} \rangle N^{-1} \right\} |\psi_n\rangle 
- \sum_{n' = 0}^{n} \frac{C_{n'} C_{n''}}{|C_n|^2} N \langle \psi_{n'}, \phi_{n'} | \bar{V}_{ai} | \phi_{n''}, \psi_{n''} \rangle \langle \psi_{n'}, \psi_{n''} \rangle N^{-1} + \frac{\tilde{g}}{2} (N - 1) |\psi_n|^2 \right\} |\psi_n\rangle. \tag{A21}
\]

In summary, we have derived coupled differential equations for the coefficients \( \langle A20 \rangle \) and for the orbitals \( \langle A21 \rangle \) that have to be solved numerically for given initial conditions. These equations, within the accuracy of the product ansatz for the bosons we made at the beginning, which is well justified for the purposes of our study, provide a sufficiently good description of the compound quantum system dynamics.

Finally, we note that Eqs. \( \langle A20 \rangle \langle A21 \rangle \) are valid for zero temperature and for functions \( \psi_n (x) \) normalised to unity. These equations, however, can be also utilised for the finite temperature TW method as described in Sec. IIIIB, but the following replacements are required:

\[
\langle \psi_n | \psi_{n'} \rangle N^{-1} \rightarrow \langle \psi_n | \psi_{n'} \rangle N^{-1} \tag{A22}
\]

in Eq. \( \langle A20 \rangle \), while in Eq. \( \langle A21 \rangle \)

\[
\langle \psi_n | \psi_{n'} \rangle N^{-k} \rightarrow \langle \psi_n | \psi_{n'} \rangle N^{-k-1} \tag{A23}
\]

for the terms in which \( \langle \psi_n, \phi_{n'} | \bar{V}_{ai} | \phi_{n'}, \psi_{n''} \rangle \) appears with \( k = 1, 2 \),

\[
\langle \psi_n | \psi_{n'} \rangle N^{-1} \rightarrow \langle \psi_n | \psi_{n'} \rangle N^{-1} \tag{A24}
\]

By applying this unitary transformation we obtain

\[
i \hat{C}_n = \sum_{n' = 0}^{n} C_{n'} e^{-i \eta_n (t)} N \langle \varphi_{n'}, \phi_{n'} | \bar{V}_{ai} | \phi_{n}, \varphi_{n} \rangle \times \langle \varphi_{n}, \varphi_{n} \rangle N^{-1}, \tag{A18}
\]

\[
\eta_n (t) = N \int_0^t d\tau (H_{gp}^n [\varphi_n / \sqrt{2}] - i \langle \varphi_n | \hat{\varphi}_n \rangle + \bar{E}_n / N) = NF_n (t). \tag{A19}
\]

By defining \( |\psi_n\rangle := |\varphi_n e^{-iT_n (t)}\rangle \), we have

\[
i \hat{C}_n = \sum_{n' = 0}^{n} C_{n'} N \langle \psi_n, \phi_{n'} | \bar{V}_{ai} | \phi_{n'}, \psi_{n'} \rangle (\psi_n |\psi_{n'}\rangle N^{-1}. \tag{A20}
\]

Since \( |\varphi_n\rangle = e^{iT_n (t)} |\psi_n\rangle \), we can use Eq. \( \langle A15 \rangle \) in order to get a differential equation for the quantum state \( |\psi_n\rangle \), which is given by the following expression

\[
\frac{d |\psi_n\rangle}{dt} = H_n |\psi_n\rangle \tag{A25}
\]

for the term in which \( \langle \phi_{n'} | \bar{V}_{ai} | \phi_{n'} \rangle \) appears, and

\[
\langle |\psi_n\rangle^2 \rangle \rightarrow \langle |\psi_n\rangle^2 \rangle \tag{A25}
\]

for the terms in which \( \bar{g} \) appears (this also applies for \( H_{gp}^n [\psi_n] \)). Note that for states normalised to unity the equations \( \langle A20 \rangle \langle A21 \rangle \) are unchanged. Instead the appearance of the norm \( \langle |\psi_n\rangle |\psi_n\rangle \) is essential in the TW, where the generated stochastic fields have a norm of the order \( O(N) \).

4. Numerical procedure

We have implemented numerically the equations \( \langle A21 \rangle \) in the following way: First, we have computed the wavefunction of the condensate by using the imaginary time propagation algorithm for the GPE \( G \) by using as trial functions the single-particle ground and first excited states of the double-well potential \( [60] \). These states are degenerate when the separation \( 2q \) between the wells is sufficiently large. The distance \( q \) has been chosen in such a way that the atom-ion interaction is essentially negligible at \( 2q_0 \), and therefore \( \langle A21 \rangle \) reduce to \( \langle 9 \rangle \). In this way, the left and right condensate wavefunctions are obtained
by linear combination of the symmetric and antisymmetric solutions of the imaginary time propagation. For the latter we used a time step \( \Delta t_{\text{im}} = 10^{-4} \hbar / \bar{E}_r \). Once the initial left condensate wavefunction has been determined, we have expanded the state onto the eigenstates \( |m\rangle \) of the double-well potential (i.e. \( H_0 \)) at \( q = 3.5 \bar{R}^* \) as

\[
|\psi_n\rangle = \sum_{m=0}^{n_a} B^n_m(t)|m\rangle.
\] (A26)

Here, we have truncated the Hilbert space in such a way that we safely consider the first \( n_a + 1 \) eigenstates only. Thus, by inserting (A26) into (A20) we obtain:

\[
i \dot{C}_n = N \sum_{m'=0}^{n_a} C_{m'} \left[ \sum_{m,m'=0}^{n_a} (B^n_m)^* B^n_{m'} \langle m,n|\bar{V}_{\text{int}}|n',m'\rangle \times \left( \sum_{m=0}^{n_a} (B^n_m)^* B^n_{m'} \right)^{N-1} \right].
\] (A27)

Finally, by substituting (A26) into (A21) and by multiplying \( \langle m\rangle \) from the left hand side, we obtain the following final equations of motion of the new expansion coefficients:

\[
i B^n_m = \left[ E^n_0(m) + \frac{\bar{q}}{2}(N-1)B^n_m + \frac{\bar{E}_n}{N} \right] B^n_m - \sum_{m'}\langle m|V^{q=\text{cons}}_{\text{ext}} - \bar{V}_{\text{ext}}(t)|m'\rangle \left( \sum_{m=0}^{n_a} (B^n_m)^* B^n_{m'} \right)^{N-1} B^n_{m'}
\]

\[
+(N-1) \frac{C^n_s}{|C^n_s|^2} \left[ \sum_{m'=0}^{n_a} C_{m'} \left( \sum_{m,m'=0}^{n_a} (B^n_m)^* B^n_{m'} \langle m,n|\bar{V}_{\text{int}}|n',m'\rangle \right) \left( \sum_{m=0}^{n_a} (B^n_m)^* B^n_{m'} \right)^{N-1} \right]
\]

\[
+ \frac{C^n_s}{|C^n_s|^2} \left[ \sum_{m'=0}^{n_a} C_{m'} \left( \sum_{m,m'=0}^{n_a} (B^n_m)^* B^n_{m'} \langle m,n|\bar{V}_{\text{int}}|n',m'\rangle \right) \left( \sum_{m=0}^{n_a} (B^n_m)^* B^n_{m'} \right)^{N-1} \right]
\]

\[
-N \frac{C^n_s}{|C^n_s|^2} \left[ \sum_{m'=0}^{n_a} C_{m'} \left( \sum_{m,m'=0}^{n_a} (B^n_m)^* B^n_{m'} \langle m,n|\bar{V}_{\text{int}}|n',m'\rangle \right) \left( \sum_{m=0}^{n_a} (B^n_m)^* B^n_{m'} \right)^{N-1} \right] B^n_{m'}.
\] (A28)

Here \( H_0|m\rangle = E^n_0(m)|m\rangle \), \(|n\rangle \equiv |\phi_n\rangle \) and \( V^{q=\text{cons}}_{\text{ext}} \) is the added and subtracted double-well potential at a constant value \( q = 3.5 \bar{R}^* \). To solve the above outlined differential equations we have chosen a time step of at least \( \Delta t_{\text{re}} = 10^{-2} \hbar / \bar{E}_r \) and used standard routines for integrating coupled differential equations in MATLAB.

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