Dynamical formation of polarons in a Bose-Einstein Condensate: A variational approach

L. A. Peña Ardila
Institut für Theoretische Physik, Leibniz Universität, 30167 Hannover, Germany

We investigate the non-equilibrium dynamics of an impurity coupled to a Bose-Einstein condensate, comparing systematically with recent experimental results (arXiv:2005.00424). The dynamics of the impurity is tracked down by using a time-dependent variational coherent ansatz. For weak coupling between the impurity and the bath, analytical expressions for the time-dependent overlap (or contrast) are derived, matching quite well with previous findings obtained within a Master Equation Approach (MEA). For strong coupling instead, the variational ansatz provides a good quantitative description of the polaron dynamics, in particular, in signaling the transition from the few to the many-body correlated regime where polarons are expected to form.

PACS numbers:

I. INTRODUCTION

One of the most challenging problems in current quantum science and technology has to do with providing a complete description of a many-body system. Besides the large number of degrees of freedom, interactions and correlations makes the problem even harder to be tackled. The concept of quasiparticle arises as an alternative for mapping this complex problem into a more tractable one. In fact, quasiparticles are crucial for understanding phenomena ranging from atomic, nuclear, to high-energy physics. One of the most famous paradigms of quasiparticles relies on Pekar and Landau's original proposal of the polaron concept [1]. When an electron travels through a material, it gets dressed by the low-energy excitations of the lattice (phonons), forming a polaron with renormalised energy and mass [2]. Polarons give insight into transport properties in semiconductors [3], electrical conduction in polymer chains [4], spin transport in organic materials [5, 6] and superconductivity [7]. Moreover, they can be used as a "probe" for highly correlated quantum many-body environments as well, for instance, ³He impurities immersed into ⁴He superfluids [8].

Ultra-cold quantum gases offer a pristine platform where interaction between atoms can be tuned at will [9, 10], allowing for the possibility to create polarons by immersing atomic impurities in quantum gases. Here, we do not rely on a lattice, but the mechanism is analogous. The impurity gets dressed by the low-energy excitations of the quantum gas instead. Polarons can be created in a Bose-Einstein condensate (Bose polarons) [11–15] or in a degenerate Fermi gas (Fermi polarons) [16–22]. Albeit research on transport properties using polarons in quantum gases is still premature, these quasiparticles can be used for probing quantum [23] and thermal effects [24] as well as topological invariants [25, 26] in the host bath. However, the precise nature of the dopant is fundamental as the many-body environment can be probed using impurities, rather than polarons [27] and hence, it is relevant to understand the time scales of polaron formation. Contrary to the condensed matter scenario, the shortest response to collective excitations in ultracold quantum gases are on the order of microseconds enabling current state-of-the-art Ramsey techniques to measure these time scales with high precision. Thus, the non-equilibrium dynamics of polaron in quantum gases has attracted a lot of attention both in theory and experiments. In the former case, the dynamics have been investigated using field-theory, renormalization group, time-dependent variational and perturbative approaches [28–37], whereas recent experiments shed light on quasiparticle formation and the non-equilibrium dynamics of impurities which are quantified by using Ramsey interferometry protocols [20, 38, 39].

In this work we use a time-dependent variational method [30, 40] to study the real-time evolution of an impurity embedded in a Bose-Einstein condensate. The non-equilibrium dynamics is tracked down by measuring the time dependent overlap, namely the probability to find the polaron at a certain time with respect to its initial non-interacting state, |ψ(0)|. Formally the overlap is defined as $S(t) = \langle \psi(0) | \exp[-iHt] | \psi(0) \rangle$. Within the variational approach this quantity is derived for arbitrary times and coupling strength, which means that one can go beyond the truncated Bogoliubov-Fröhlich Hamiltonian that is accurate only in the weakly interacting regime.

The article is organized as follows. In Sec.II we describe the model and we introduce the full Hamiltonian of the system. By using a low-energy truncation, we obtain the Bogoliubov-Fröhlich Hamiltonian which enables a "system plus reservoir" description in terms of a MEA. In Sec.III we review this perturbative formalism and introduce the observable of interest, i.e. the contrast. In Sec.IV we use the time dependent variational approach to compute the Euler-Lagrange equations of motion (EoM). In Sec.V the EoM can be solved exactly in the weakly interacting regime and proper benchmark is done with respect to the perturbative approach. In order to do comparisons with experiments, additional decoherence effects must be included in the theory, in Sec.VI we discuss trap dephasing and in Sec.VII decoherence by magnetic-field fluctuations and losses. In Sec.VIII we discuss some results within the experimental available coupling strengths both in the weak and strongly interacting regime. Comparisons yield a good agreement between the theory and the experimental measurements [39]. Finally, conclusions are drawn in Sec. IX.
II. MODEL AND HAMILTONIAN

We consider an ultradilute gas of impurities of mass \( m_I \) immersed in a Bose-Einstein condensate (BEC) of mass \( m_B \) and density \( n \). The Hamiltonian of the system reads

\[
\mathcal{H} = \sum_{p} \Omega_p c_p^\dagger c_p + \sum_{k} \epsilon_k a_k^\dagger a_k \\
+ \frac{1}{2V} \sum_{k,k',q} V_B(q) a_{k+q}^\dagger a_{k'}^\dagger a_{k'} a_{k+q} \\
+ \frac{1}{V} \sum_{k,k',q} V_I(q) a_{k+q}^\dagger a_{k'}^\dagger b'_k b_{k'} ,
\]

(1)

where the operator \( c_p \) (\( c_p^\dagger \)) annihilates (creates) an impurity of momentum \( p \) and energy \( \Omega_p = p^2/2m_I \), whereas \( a_k \) (\( a_k^\dagger \)) annihilates (creates) a boson with momentum \( \hbar k \) and energy \( \epsilon_k = \hbar^2 k^2/2m_B \). Moreover, \( V_B(q) = T_B \) and \( V_I(q) = T_I \) are the Fourier transform of the short-ranged boson-boson and impurity-boson potentials respectively. In addition, we define \( T_\nu = 2\pi \hbar^2 a/m_{red} \) as the zero-energy impurity-bath coupling constant depending on the tunable s-wave scattering length \( a \) and \( m_{red} = m_B^{-1} + m_I^{-1} \) the reduced mass. We perform the Bogoliubov transformation on the bosonic operators, i.e. \( \hat{a}_k = u_k \hat{b}_k - v_k b_{-k}^\dagger \), with amplitudes \( u_k = 1 + v_k^2 = (\epsilon_k + T_B n + \omega_k)/2\omega_k \) and \( v_k = -T_B n/2\omega_k \), bearing the bosonic coupling strength \( T_B = 4\pi \hbar^2 a_B m_B a_B \) and \( a_B \), the s-wave boson-boson scattering length. Moreover, \( \omega_k = \sqrt{\hbar^2 \xi^2 \mp 2} \) is the dispersion relation of the bosonic bath written in terms of the healing length \( \xi = 1/\sqrt{8\pi naB} \). Thus the transformed hamiltonian in the single impurity limit (characterized by its position operator \( \hat{R} \)) yields

\[
\mathcal{H} = \mathcal{H}_F + \frac{T_\nu}{V} \sum_{k,q} V_{k,q}^{(+)} e^{i(k-q)\cdot R} \hat{b}_k^\dagger \hat{b}_q \\
+ \frac{T_\nu}{V} \sum_{k,q} V_{k,q}^{(-)} e^{i(k+q)\cdot R} \left( \hat{b}_k^\dagger \hat{b}_q + \hat{b}_k^\dagger \hat{b}_q \right).
\]

(2)

In order to capture all order of multi-scattering process in the problem, quadratic terms in the Bogoliubov operators must be also included. Moreover, \( V_{k,q}^{(+)} = \frac{1}{2} \left[ W_k W_q \pm (W_k W_q)^{-1} \right] \)

with the coupling matrix \( W_k = \left[ \frac{(\xi k)^2}{(k^2)^2 + 2} \right]^{1/4} \) and \( \mathcal{H}_F \) reads

\[
\mathcal{H}_F = \frac{\hat{p}_I^2}{2m_I} + \sum_{k} \hbar \omega_k \hat{b}_k^\dagger \hat{b}_k + nT_\nu \\
+ \frac{T_\nu}{V} \sum_{k,q} W_k e^{i k \cdot R} \left( \hat{b}_k^\dagger + \hat{b}_q \right).
\]

(3)

The truncated Hamiltonian Eq. (3) is known as the Bogoliubov-Fröhlich Hamiltonian which provides the ground-state properties of a single impurity weakly interacting with the low-energy excitations of the quantum gas. This process is represented by the scattering of an impurity with a single-excitation of the condensate. However, this Hamiltonian is inaccurate for strong coupling, which is characterized by high energy multi-scattering process featuring a transition from low-energy excitations to bare bosons and thus the formation of many-body bound states once the resonance is crossed [15, 30]. Hence, beyond-Fröhlich terms in Eq. (2) are needed for arbitrary coupling strength in order to describe the physics properly.

Lee-Low-pines (LLP) transformation. – To simplify the problem further, one can translate the impurity-bath system into a new set of coordinates by evoking the celebrated LLP canonical transformation \( \mathcal{H} = \hat{U}^\dagger \mathcal{H} \hat{U} \) where \( \hat{U} = \exp \left\{ i \sum \hat{b}_k^\dagger \hat{b}_k \right\} \) [30, 40, 41]. The transformed Hamiltonian depends on the total momentum of the system, \( \hat{U}^\dagger \hat{P} \hat{U} = \hat{P} - \sum \hat{b}_k^\dagger \hat{b}_k \). The Hamiltonian Eq. (2) in the new reference frame reads

\[
\mathcal{H} = T_\nu n + \frac{1}{2m_I} \left( \hat{P} - \sum \hat{b}_k^\dagger \hat{b}_k \right)^2 \\
+ \frac{T_\nu}{V} \sum_{k,q} V_{k,q}^{(+)} \left( \hat{b}_k^\dagger \hat{b}_q + \hat{b}_q \hat{b}_k \right) \\
+ \frac{T_\nu}{V} \sum_{k,q} V_{k,q}^{(-)} \left( \hat{b}_k^\dagger \hat{b}_q + \hat{b}_q \hat{b}_k \right).
\]

(4)

In the new impurity frame of reference, the total momentum commutes with the transformed Hamiltonian and is a conserved quantity. Hence the bare impurity degrees of freedom are fully eliminated and the expectation value of the impurity momentum can be set to zero, which is consistent with the polaron ground-state of the system. One more detail that should be taken with care in the Hamiltonian Eq. (4) is the renormalization of the impurity-boson coupling strength as the contact interaction potential is modeled by a nonphysical \( \delta \)-potential in real space. From the Lippmann-Schwinger equation the zero-energy coupling constant and the s-wave scattering length are related via

\[
T_\nu = \frac{m_{red}}{2\pi \hbar^2 a} - \frac{1}{V} \sum_{k} \frac{2m_{red}}{\hbar^2 k^2}.
\]

(5)

III. MASTER EQUATION APPROACH

At \( t = 0 \) the total density matrix of the whole system can be factorized as the product of the density matrix of a small subsystem (impurities) and the host reservoir (bath). In the spirit of the Born approximation, when the interaction system-bath is turned on, correlations play an important role giving place to decoherence of the polaron and hence the
density matrix of the system displays deviations on the order of the system-reservoir coupling strength [42]. This situation can be described accurately within a MEA, provided that interactions (impurity-bath) are weak enough [33]. In fact, Eq. (3) follows a system-reservoir kind of Hamiltonian. In order to characterize the coherence of the system we study the time-dependent overlap (also known as Ramsey overlap), 

\[ S(t) = \langle 0 | \hat{c}(t) \rho_f(t) | 0 \rangle, \]

where \( \rho_f(t) \) is the reduced density matrix of the impurity obtained explicitly with the MEA. In reference [33] a detailed derivation of \( \rho_f(t) \) is presented. Moreover, \( \hat{c}(t) \) depicts the impurity operators and |0\rangle is the vacuum of phonons. Thus within the Fröhlich model, the decoherence for an uniform system yields [33]

\[ S^h(t) = \exp \left[ -\frac{i}{\hbar} E_{pol}^F t + i \frac{1}{8} \frac{a_B}{a_0} F(t/t_n) \left( \frac{a}{a_B} \right)^2 \right], \]  

with \( t_n = m/(8\pi \hbar n a_B) \) and the function \( F(t) = t + i (it + 3) (\frac{1+i}{2}) \sqrt{\pi t} \exp (it/2) \text{erfc} \left( \frac{1+i}{2} \sqrt{t} \right) \). The upper index “h” indicates the contrast computed for a homogeneous system and

\[ E_{pol}^F = \frac{8\pi}{(6\pi^2)^{1/3}} (na_B^3) \left[ \frac{a}{a_B} + \frac{a_B}{a_0} \right] \left( \frac{a}{a_B} \right)^2 \frac{\hbar^2 k_n^2}{2m}, \]  

is the polaron energy in the Fröhlich regime. Here \( k_n = (6\pi^2 n)^{1/3} \) and \( \frac{a_B}{a_0} = \frac{3}{\sqrt{3}} \sqrt{\frac{n a_B^3}{32\pi^2}} \). In addition, for short-time, namely \( t \ll \hbar/E_{MF} \) (being \( E_{MF} = T_n n \) the mean-field polaron energy) the contrast yields a particular form

\[ S^0(t) \sim 1 - (i + 1) \left( \frac{t}{\hbar} \right) - i \hbar E_{MF} t, \]  

with the characteristic time scale \( t_\Omega = \frac{m n}{32\pi \hbar n a_n^2} \) which depends on the shape of the impurity-bath potential. Both theoretical approaches addressed in this work assumes a quenched impurity. Universality of the very short-time dynamics and the corresponding time scales are discussed in [39] and they are not within the scope of the present work.

### IV. VARIATIONAL ANSATZ

In this section we employ a time-dependent variational ansatz to study polaron dynamics as previously used in references [30, 35, 40]. On one hand we benchmark the results obtained within a variational ansatz against a MEA. On the other hand the variational formalism enables us to access to the strongly interacting regime ruled by the full Hamiltonian Eq. (4). The ansatz is based on a coherent state product

\[ |\psi_c(t)\rangle = \exp[-i\phi(t)] \hat{O}(t) |0\rangle, \]  

where \( \hat{O}(t) = \exp \left( \frac{1}{\sqrt{\hbar}} \sum_k \beta_k(t) \hat{b}_k - h.c. \right) \) and |0\rangle is the total state at \( t = 0 \) before the impurity-boson interaction is quenched, i.e. an impurity with momentum \( p \) and the vacuum of phonons. Here \( \gamma_k(t) = \{ \beta_k(t), \phi(t) \} \) plays the role of time-dependent variational parameters. The displacement operator \( \hat{O} \) obeys \( \hat{O}(t) b_k \hat{O}(t) = b_k + \beta_k \). These properties are heavily used to compute the equations of motion and expectation values. Note that, the ansatz Eq. (9) is exact in the limit of an immobile impurity and non-interacting bosons. Following [30], the Euler Lagrange equations, \( \frac{d}{dt} \frac{\partial L}{\partial \dot{\gamma}_k} - \frac{\partial L}{\partial \gamma_k} = 0 \), with the Lagrangian density, \( L = \langle \psi_c(t) | i h \dot{\phi} - H | \psi_c(t) \rangle \) and for the manifold of variational parameters \( \gamma_k(t) \) reads

\[ i \hbar \dot{\beta}_k = T_n W_k \left\{ \sqrt{n} + \Gamma(k) \beta_k + \frac{T_n}{2} \left[ W_k \sum_{k'} W_{k'} (\beta_{k'} + \beta^*_k) + \frac{1}{W_k} \sum_{k'} \frac{1}{W_{k'}} (\beta_{k'} - \beta^*_{k'}) \right] \right\} \]  

and

\[ \hbar \dot{\phi} = T_n n + \frac{T_n}{2 \sqrt{n}} \sum_k W_k (\beta_k + \beta^*_k) - \frac{P^2_B}{2 m_B}. \]  

Here \( \Gamma(k) = \omega_k + \Omega_k + \hbar k \cdot P_B/m_I \) and \( P_B = \sum_k \beta_k^* \beta_k \). As mentioned previously and without loss of generality, we restrict to the case of slow motion impurities, i.e. \( \mathbf{P} = 0 \). Moreover, note that \( P_B \) is always zero for all times due to spherical symmetry. Solving the coupled differential equations will allow us to compute quantities of interest such as the contrast

\[ S^0(t) = \langle \psi_c(0) | \psi_c(t) \rangle, \]  

where \( \langle \psi_c(t) \rangle \) is given by Eq. (9). Carrying out the calculation and after some algebra one ends up with a simple expression

\[ S^0(t) = \exp \left[ -i \phi(t) - \frac{1}{2} \sum_k |\beta_k(t)|^2 \right]. \]  

In the stationary case, i.e. \( \dot{\gamma}_k(t) = 0 \), Eq. (10) can be split into a real and an imaginary part and hence one obtains

\[ \begin{pmatrix} \text{Re}[\beta_k] \\ \text{Im}[\beta_k] \end{pmatrix} = \begin{pmatrix} -W_k \sqrt{n} \left( T_n^{-1} + \sum_{k'} W_{k'}^2 \right)^{-1} \end{pmatrix} \]  

Thus the polaron energy in the stationary case can be computed by \( E_{pol} = \langle \psi_{st} | H | \psi_{st} \rangle \) yielding

\[ E_{pol} = \frac{8\pi (na_B^3)^{1/3}}{(6\pi^2)^{2/3}} \left[ \frac{a_B}{a} - \frac{a_B}{a_0} \right]^{-1} \frac{\hbar^2 k_n^2}{2m_B}. \]
Fröhlich Hamiltonian and the EoM are reduced to
\[
\frac{i\hbar}{\sqrt{\nu}} \sum_k W_k (\beta_k + \beta_k^*) = \Gamma(k) \beta_k
\]
\[
\frac{\hbar}{\nu} \frac{1}{\sqrt{2V}} \sum_k W_k (\beta_k + \beta_k^*) \frac{\beta_k}{\nu} = T_v n + T_v \sqrt{\nu} \sum_k W_k (\beta_k + \beta_k^*). \tag{16}
\]

The previous equations can be solved exactly. Notice that, in the mean-field case the solution for the contrast is trivial since \(\beta_k(t) = 0\) and \(\phi(t) = \frac{T_v n}{\hbar} t\), hence the contrast reads
\[
S^h(t) = \exp \left[ -i T_v nt / \hbar \right]. \tag{17}
\]

In order to recover beyond mean-field terms, the strategy is to solve the first equation in Eq. \(16\) for \(\beta_k\). It yields \(\beta_k(t) = \frac{T_v}{\sqrt{\nu}} \sqrt{\nu} W_k \exp \left[ -i \Gamma(k) t / \hbar \right] - 1\) for the initial condition \(\beta_k(0) = 0\) and subsequently this solution is plugged into the \(\phi\)-equation, obtaining thus, \(\phi = \frac{1}{\hbar} \int_0^t ds \left[ T_v n + \frac{T_v}{\sqrt{\nu}} \sum_k W_k (\beta_k(s) + \beta_k^*(s)) \right]\). In addition, one should take into account the proper renormalization of the impurity-boson coupling strength, \(T_v\), by means of Eq. \(5\). After some algebra a closed form for both \(\beta_k(t)\) and \(\phi(t)\) is found. Plugging the previous solutions into the definition of the contrast Eq. \(13\), one finally gets
\[
S^h(t) = \exp \left[ -i E^F_{\text{pol}} t + \frac{\hbar}{2} \sum_k (\frac{\beta_k^*}{\beta_k}) F(t/t_0) \right],
\]
which coincides with the very same expression found by the MEA in Eq. \(6\). The variational approach captures surprisingly the quantitative behaviour of the polaron dynamics out of equilibrium. This conclusion yields interesting consequences. In reference [33] the master equation for the impurity problem was derived upon two strong assumptions. First, the Born approximation, which was genuinely justified on the fact that the impurity weakly perturbs the host medium. Second, for this system a highly degree of Markovianity is expected [31]. Within the MEA at zero temperature, this latter approximation is valid due to the sufficiently large difference in time scales. Thus, the variational approach indirectly justifies the use of the Markovian-approximation in this regime.

VI. TRAP DEPHASING

If we consider the simplest case at the mean-field level, the amplitude of the contrast Eq. \(17\) is one for all times. In order to do proper comparison with the experiments, the contrast must be averaged over a non-homogeneous density profile, i.e. dephasing by the trap. In the mean-field case and using Eq. \(17\) one finds
\[
S(t) = \frac{1}{N_B} \int d^3 \nu(n(r) \frac{t}{\hbar}) \tag{18}
\]
being \(n(r) = v_{TF}(r)\) the condensate density (see Appendix A), whereas the first beyond-mean field correction reads

V. DECOHERENCE-WEAK COUPLING

The coupled system of Eqs. \(10\) and \(11\) are computed using the full Hamiltonian in Eq. \(4\) and should be solved numerically. However, for weak-coupling one can use the truncated

\[
\begin{align*}
S(t) = \frac{1}{N_B} \int d^3 \nu(n(r) \frac{t}{\hbar}) \tag{18}
\end{align*}
\]

being \(n(r) = v_{TF}(r)\) the condensate density (see Appendix A), whereas the first beyond-mean field correction reads

\[
\begin{align*}
F(t/t_0) &= \exp \left[ -i E^F_{\text{pol}} t + \frac{\hbar}{2} \sum_k (\frac{\beta_k^*}{\beta_k}) F(t/t_0) \right],
\end{align*}
\]

which coincides with the very same expression found by the MEA in Eq. \(6\). The variational approach captures surprisingly the quantitative behaviour of the polaron dynamics out of equilibrium. This conclusion yields interesting consequences. In reference [33] the master equation for the impurity problem was derived upon two strong assumptions. First, the Born approximation, which was genuinely justified on the fact that the impurity weakly perturbs the host medium. Second, for this system a highly degree of Markovianity is expected [31]. Within the MEA at zero temperature, this latter approximation is valid due to the sufficiently large difference in time scales. Thus, the variational approach indirectly justifies the use of the Markovian-approximation in this regime.
FIG. 2: (a) Contrast amplitude for $1/k_a a = -5.0$. The experimental points from [39] are represented by orange circles. The blue crosses are the second-order perturbative result Eq. (19) which overlaps fully with the green curve depicting the variational ansatz. The purple dashed line depicts for the short-time behaviour characterised by the time scale $\sqrt{\bar{n}}$ (defined in the mean text). On top of the trap dephasing decoherence, the variational approach also includes decoherence by losses represented by the red dashed line and finally magnetic-field fluctuations depicted by the dashed black line (MFF) (b) zoom-in of Fig. 2(a) in order to distinguish better all theories for short and intermediate times. The MFF fitting experimental parameter here is $\Delta = 1800\text{Hz}$.

$$S(t) = \frac{1}{N_B} \int d^3r \rho(r) S(r, t), \quad (19)$$

with

$$S(r, t) = \exp \left[ -\frac{i}{\hbar} E_F^F \left[ n(r) \right] t + i \frac{a_B}{8} \frac{F(t/t_n(r))}{a_B} \right], \quad (20)$$

containing the inhomogeneity of the condensate in terms of the local time scale $t_n(r) = \frac{m_B}{a_B} \frac{\hbar}{E_F^F}$.

**VII. DEPHASING BY LOSSES AND MAGNETIC FIELD FLUCTUATIONS (MFF)**

Inelastic losses arising from three-body recombination process can strongly influence the contrast and give rise to decoherence by losses. The experimental impurity loss rate as a function of the coupling strength has been measured in [39] using the function $\Gamma_{\text{loss}} = A \exp(\frac{B}{n_{\text{pol}}}) + C$, with fitting parameters $A = 0.1788$, $B = 1.0130$ and $C = 0.0061$. In addition, $\hbar/E_n = 2m/\left(\hbar^{3/2} 6\pi^2 n^2\right)^{2/3}$. On the other hand, the Ramsey interferometry protocol is sensible to magnetic field variations for each experimental measurement and hence MFF is another important source of decoherence [39]. Therefore, the total contrast needs to include also these additional inherent effects from the experiment. Thus, the total contrast is modified as

$$S(t) = \frac{1}{N_B} S^{\text{Loss}}(t) S^{\text{MFF}}(t) \int d^3r \rho(r) S(r, t), \quad (21)$$

with

$$S^{\text{Loss}}(t) = \exp \left[ -\Gamma_{\text{Loss}} t \right]. \quad (22)$$

and

$$S^{\text{MFF}}(t) = \int_{-\infty}^{\infty} d\phi \exp \left[ -i\phi - \frac{\phi^2}{8\pi^2 \Delta^{2/3}} \right], \quad (23)$$

being the decoherence associated to losses and MFF respectively. Instead, $S(r, t)$ is the contrast including only the trap dephasing. From the experiments, one observe that dephasing due to the trap and by losses are the most important contributions on top of the dephasing by collisions. Additional decoherence effects, such as the one due to magnetic field fluctuations (MFF) are quite relevant in the weakly interacting regime and becomes less important for strong coupling, albeit never negligible.

**VIII. RESULTS**

*Weak-coupling.*—The time evolution of the contrast is plotted in Fig. 2. The circles with error bars depict the recent experimental data [39] for a fixed coupling strength $1/k_a a = -5.0$, featuring a typical value in the weakly interacting regime. The computed contrast using the perturbative MEA is shown by the blue crosses (see also Eq. (19)), whereas the variational ansatz calculation including only trap dephasing is represented by the green solid curve. As expected both curves overlap according to our discussion in Sec.V. In addition, the dashed purple line shows the power-law short-time behavior (see also Eq. (8)) valid for $t_d < t \ll t_n = \hbar/E_{MF} \sim 50\mu s$ for this particular coupling strength. Note that, the short time prediction in Fig. 2 represents the initial high energy two-body dynamics [33] which is independent of the host bath interaction, i.e. the impurity does not experience the condensate presence. Therefore decoherence is originated only
by impurity-boson interactions. This regime is preceded by the polaron relaxation and formation stage, where the impurity interact with the condensate excitations and many-body effects start to take place ($t \approx t_n$). Instead, the formation time is expected for times $t \gg t_B \sim 500\mu s$ as revealed by the instantaneous polaron energy defined as $E_{Pol}(t) = \langle \psi_c(t) | H | \psi_c(t) \rangle = \tilde{h} \dot{\phi}$ and plotted in Fig. 1(b). A discussion on the degeneracy time scale $t_d = ma^2/\bar{h}$ can be found in [39, 43]. This time scale is set by the coupling strength and for this particular case is on the order of $t_d = 0.08\mu s$.

For very short-times $t_d < t < t_n$, the mean-field prediction already provides a good qualitatively agreement with respect to the experimental contrast, however the effect of quantum fluctuations (originated from impurity-bath collisions) tends to shift the mean-field contrast amplitude for larger times, following thus the experimental downward trend as shown in Figures 2(a)-2(b), but still far from a fully quantitatively agreement with the experimental data. For intermediate and larger times $t_n > 100\mu s$ the contrast decays faster in the experiment with respect to the theoretical prediction which only includes trap dephasing. In fact, additional decoherence effects which are inherent to the experiment are absent in the theory and need to be included, for instance, decoherence by losses and by MFF [39]. We have included the losses dephasing as well as the MFF decoherence as illustrated in Sec.VII. A quantitatively agreement with respect to the experimental data is reached as shown by the black dashed line in Figures 2(a) and 2(b). The effect of including losses dephasing is more evident in the strongly interacting regime, in contrast to the dephasing due to MFF which is less relevant.

Strong-coupling.—We investigate the time-dependent overlap in the strongly interacting regime, i.e. $-1 < (k_n a)^{-1} < 0$. Here we rely solely on numerical solutions of equations Eq. (10) and Eq. (11) with the experimental parameters associated to each $1/k_n a$ [39], in particular for two characteristic coupling strengths, $1/k_n a = -1$ and at unitarity. In the former case, a very good agreement between the variational results including losses decoherence and MFF and the experimental data is reached as shown in Figures 3(a) and 3(b). In particular, for this regime, MFF decoherence is small in comparison with the other experimental decoherence effects, however it provides a quantitatively agreement with the experimental contrast, whereas at unitarity is practically negligible.

In Figures 3(c) and 3(d) we show the results at the unitary
tem. In fact, by expanding out the wave-function Eq. (9) one obtains the ansatz Eq. (9) which encodes all correlations of the system. Thus, in the proposed function is heavily based on the initial form of the trial function. Particularly, in Fig. 4 one observes that the polaron is expected to enter the equilibrium regime for times $t \gg t_{d}$ (black dashed line) agree with each other and it follows that

$$S_{\text{2body}}(t) \approx 1 - (1 - i) \frac{16}{9\pi^{3/2}} \left( \frac{t}{t_{n}} \right)^{3/2}.$$  

(24)

The time scale $t_{n}^{3/2}$ is linked with the universal two-body scattering physics, where the impurity interacts with highly energetic bosons of the condensate. Note that the same universal scaling is recovered for impurities immersed in a Fermi sea [44] with a characteristic time scale set by the Fermi time ($\hbar/E_{F}$). In order to bridge the two-body with the many-body physics where the polaron starts its formation, we attempt to find a functional form of the contrast for arbitrary times. Taking advantage of the functional form of Eq. (24), we propose the following expression for arbitrary time

$$S(t) = \exp \left[ S_{\text{2body}}(t) - 1 \right],$$  

(25)

which recovers exactly Eq. (24) for short-times and spans all over one-body, two-body and all high $n-$body correlations for larger times, thus signaling the transition from few-body to the many-body correlated regime (around $t \sim 5\mu s$). The agreement between Eq. (25) depicted by the cyan curve in Fig. 3(c) and the full numerical calculations obtained with the variational ansatz (green curve) is quite remarkable. Interestingly, in Fig. 4 one observes that the polaron is expected to enter the equilibrium regime for times $t \gg 5\mu s$ with a polaron energy near to $E_{P_{\text{eq}}} \approx -E_{\chi}$ at equilibrium. In addition, the proposed function is heavily based on the initial form of the ansatz Eq. (9) which encodes all correlations of the system. In fact, by expanding out the wave-function Eq. (9) one has

$$|\psi(t)| = \exp \left( -i\phi(t) \sum_{k} [\beta_{k}(t) \hat{b}_{k}^{\dagger} - \beta_{k}^{*}(t) \hat{b}_{k}] \right) |0\rangle = \sum_{n=0}^{\infty} \left( -i\phi(t) \sum_{k} \beta_{k}(t) \hat{b}_{k}^{\dagger} - \beta_{k}^{*}(t) \hat{b}_{k} \right) |0\rangle \approx -\phi(t) \sum_{k} \beta_{k}(t) \hat{b}_{k}^{\dagger} |0\rangle,$$

(26)

and taking into account only the first terms of the series, one obtains

$$|\psi(t)| \approx \left( 1 - i\phi(t) \sum_{k} \beta_{k}(t) \hat{b}_{k}^{\dagger} \right) |0\rangle,$$

(26)

which resembles the Chevy ansatz [45] where only a single excitation on top of the unperturbed condensate is included. Eq. (26) is accurate in the weakly interacting regime. Hence, perturbation theory and the variational approach again consistently agree in this regime.

Finally we would like to stress that in the neighborhood of the unitarity regime and for very long time (essentially the polaron state at equilibrium), the variational approach might provide quantitatively results as in this regime the Bogoliubov approximation breaks down. However, for our current work the time scales are way far from equilibrium at unitarity and hence good qualitatively results in the short-time dynamics holds.

**IX. CONCLUSIONS**

In this work we have employed a time-dependent variational approach to investigate the out-of-equilibrium dynamics of impurities interacting with a Bose-Einstein condensate. The main results are two-fold. First, the method is benchmarked against time-dependent perturbative approaches such as MEA, valid in the weakly interacting regime. Second, the method is compared with state-of-the-art experimental data. Besides impurity-bath decoherence, agreement between theory and experiment relies on the inclusion of decoherence effects in the theoretical approaches due to trap inhomogeneity, losses and fluctuations of magnetic field inherently incorporated in the experiment. Close to the unitarity regime, we also bridged in a consistent and quantitatively way the few-body physics characterized by the universal two-body scattering process to the many-body process where polarons starts its formation. Note that, apart from the initial experimental preparation of the system, the contrast might be altered due to the comparable Efimov states energy that are also relevant for polaron physics in bosonic systems [46]. Also, how the polaron formation happens once the resonance is crossed is an open question since a new time scale related with the two-body bound state physics should play an important role. Real-time formation of quasiparticles emerging from impurity-bath
decoherence might be important not only for gases, but also to other exotic many-body environments such as ultra-dilute quantum liquids or recently investigated long ranged polarons such as Rydberg, dipolar and ionic polarons. [14, 47–50].

Acknowledgments

We gratefully acknowledge to Kristian K. Nielsen for discussions at earlier stage of this work. We also thank to Magnus G. Skou, Nils Byg Jørgensen and Jan Arlt for insightful discussions and providing the experimental data. The authors also acknowledge to Luis Santos, Fabian Grusdt, Artem Volosniev and Giacomo Bighin for reading the manuscript and for the critical feedback. Special Acknowledgments to Roberta Giusteri for critical comments on the manuscript. This research was funded by the DFG Excellence Cluster QuantumFrontiers.

APPENDIX A: CONTRAST FOR AN INHOMOGENEOUS TRAP

The density of the condensate can be written in a very simple form as the interaction energy scales with respect to the kinetic energy one, hence the density of the condensate within the Thomas-Fermi (TF) approximation can be written as

\[ n_{\text{TF}}(r) = \begin{cases} \frac{\mu_{\text{TF}} - V(r)}{T_B}, & \mu_{\text{TF}} \geq V(r) \\ 0, & \text{Otherwise} \end{cases} \]

with \( \mu_{\text{TF}} \) the chemical potential in TF regime. In experiments the trapping potential is modeled by \( V(r) = \frac{1}{2} m_B \sum_{i=1}^{3} \sigma_i x_i^2 = \frac{1}{2} m_B \pi^2 \sum_{i=1}^{3} \pi_i^2 \) where the geometric frequency is defined as \( \omega_i = (\omega x_i / \omega) \) and \( \pi_i = x_i / \omega \).

Upon the condition \( \mu_{\text{TF}} = V(r) \), one finds the size of the condensate confined in this potential, namely the Thomas-Fermi radius \( R = \sqrt{\frac{2 \mu_{\text{TF}}}{m_{\text{p}} \omega}} \) and the chemical potential depending on the number of particles of the condensate. Thus, from the normalization condition \( N_B = \int d^3r n_{\text{TF}}(r) \) one obtains

\[ \mu_{\text{TF}} = \frac{\hbar^2}{2} \left[ 15 N_B \frac{a_{\text{B}}}{a_{\text{ho}}} \right]^{2/5}. \]

The contrast for an inhomogeneous distribution can be written as

\[ S(t) = \frac{1}{N_B} \int d^3r n_{\text{TF}}(r) S(r, t) \]

\[ = \frac{1}{N_B} \int d^3r \left[ \frac{\mu_{\text{TF}} - V(r)}{T_B} \right] S(r, t). \quad (27) \]

The contrast \( S(r, t) \) depends on time and density in each point of space. In other words, the spatial dependence of the contrast is implicitly encoded in the density, thus we substitute the homogeneous density \( n \rightarrow n_{\text{TF}}(r) \) using the local density approximation.

[1] L. Landau and S. Pekar, J. Exp. Theor. Phys. 18, 419 (1948).
[2] R. P. Feynman, Phys. Rev. 97, 660 (1955).
[3] J. Devreese and F. Peters, Polaronics and Excitons in Polar Semiconductors and Ionic Crystals (Plenum Press, New York, 1984).
[4] M. R. Mahani, A. Mirsakiyeva, and A. Delin, J. Phys. Chem. C 121, 10317 (2017), URL http://dx.doi.org/10.1021/jpcsc. 7b02368.
[5] M. E. Gershenson, V. Podzorov, and A. F. Morpurgo, Rev. Mod. Phys. 78, 973 (2006), URL https://link.aps.org/doi/10. 1103/RevModPhys.78.973.
[6] S. Watanabe, K. Ando, K. Kang, S. Mooser, Y. Vaynzof, H. Kurebayashi, E. Saitoh, and H. Siringhaus, Nat. Phys. 10, 308 (2014).
[7] P. A. Lee, N. Nagaosa, and X.-G. Wen, Rev. Mod. Phys. 78, 17 (2006), URL https://link.aps.org/doi/10.1103/RevModPhys.78.17.
[8] G. Baym and C. Pethick, Landau Fermi-Liquid Theory: Concepts and Applications (Wiley-VCH-New York., 1991).
[9] I. Bloch, J. Dalibard, and W. Zwerger, Rev. Mod. Phys. 80, 885 (2008), URL https://link.aps.org/doi/10.1103/RevModPhys.80.885.
[10] C. Chin, R. Grimm, P. Julienne, and E. Tiesinga, Rev. Mod. Phys. 82, 1225 (2010), URL https://link.aps.org/doi/10.1103/ RevModPhys.82.1225.
[11] N. B. Jørgensen, L. Wacker, K. T. Skalmstang, M. M. Parish, J. Levinsen, R. S. Christensen, G. M. Bruun, and J. J. Arlt, Phys. Rev. Lett. 117, 055302 (2016), URL https://link.aps.org/doi/10. 1103/PhysRevLett.117.055302.
[12] M.-G. Hu, M. J. Van de Graaff, D. Kedar, J. P. Corson, E. A. Cornell, and D. S. Jin, Phys. Rev. Lett. 117, 055301 (2016), URL https://link.aps.org/doi/10.1103/PhysRevLett.117.055301.
[13] Z. Z. Yan, Y. Ni, C. Robens, and M. W. Zwierlein, Science 368, 190 (2020), ISSN 0036-8075, https://science.sciencemag.org/content/368/6487/190.full.pdf, URL https://science.sciencemag.org/content/368/6487/190.
[14] F. Camargo, R. Schmidt, J. D. Whalen, R. Ding, G. Woehl, S. Yoshida, J. Burgdörfer, F. B. Dunning, H. R. Sadeghpour, E. Demler, et al., Phys. Rev. Lett. 120, 083401 (2018), URL https://link.aps.org/doi/10.1103/PhysRevLett.120.083401.
[15] L. A. Peña Ardila, N. B. Jørgensen, T. Pohl, S. Giorgini, G. M. Bruun, and J. J. Arlt, Phys. Rev. A 99, 063607 (2019), URL https://link.aps.org/doi/10.1103/PhysRevA.99.063607.
[16] A. Schirotzek, C.-H. Wu, A. Sommer, and M. W. Zwierlein, Phys. Rev. Lett. 102, 230402 (2009), URL https://link.aps.org/ doi/10.1103/PhysRevLett.102.230402.
[17] V. Ngaumruekornj, J. Levinsen, and M. M. Parish, EPL (Europhysics Letters) 98, 30005 (2012), URL https://doi.org/10. 1209/0295-5075/98/30005.
[18] M. Koschorreck, D. Pertot, E. Vogt, B. Fröhlich, M. Feld, and M. Köhl, Nature 485, 619 (2012).
[19] C. Kohstall, M. Zaccanti, M. Jag, A. Trenkwalder, P. Massignan, G. M. Bruun, F. Schreck, and R. Grimm, Nature 485, 615 (2012).
[20] M. Cetina, M. Jag, R. S. Lous, I. Fritsche, J. T. Walraven,
[21] F. Scazza, G. Valtolina, P. Massignan, A. Recati, A. Amico, A. Burchianti, C. Fort, M. Inguscio, M. Zaccanti, and G. Roati, Phys. Rev. Lett. 118, 083602 (2017), URL https://link.aps.org/doi/10.1103/PhysRevLett.118.083602.

[22] M. Sidler, P. Back, O. Cotlet, A. Srivastava, T. Fink, M. Kroner, E. Demler, and A. Imamoglu, Nature 485, 615 (2012).

[23] R. S. Christensen, J. Levinsen, and G. M. Bruun, Phys. Rev. Lett. 115, 160401 (2015), URL https://link.aps.org/doi/10.1103/PhysRevLett.115.160401.

[24] M. Mehboudi, A. Lampo, C. Charalambous, L. A. Correa, M. A. García-March, and M. Lewenstein, Phys. Rev. Lett. 122, 030403 (2019), URL https://link.aps.org/doi/10.1103/PhysRevLett.122.030403.

[25] F. Grusdt, N. Y. Yao, and E. A. Demler, Phys. Rev. B 100, 075126 (2019), URL https://link.aps.org/doi/10.1103/PhysRevB.100.075126.

[26] F. Grusdt, K. Seetharam, Y. Shchadilova, and E. Demler, Phys. Rev. A 97, 033612 (2018), URL https://link.aps.org/doi/10.1103/PhysRevA.97.033612.

[27] Q. Bouton, J. Nettersheim, D. Adam, F. Schmidt, D. Mayer, T. Lausch, E. Tiemann, and A. Widera, Phys. Rev. X 10, 011018 (2020), URL https://link.aps.org/doi/10.1103/PhysRevX.10.011018.

[28] F. Grusdt, K. Seetharam, Y. Shchadilova, and E. Demler, Phys. Rev. A 97, 033612 (2018), URL https://link.aps.org/doi/10.1103/PhysRevA.97.033612.

[29] A. G. V olosniev, H.-W. Hammer, and N. T. Zinner, Phys. Rev. A 92, 023623 (2015), URL https://link.aps.org/doi/10.1103/PhysRevA.92.023623.

[30] Y. E. Shchadilova, R. Schmidt, F. Grusdt, and E. Demler, Phys. Rev. Lett. 117, 113002 (2016), URL https://link.aps.org/doi/10.1103/PhysRevLett.117.113002.

[31] A. Lampo, C. Charalambous, M. A. García-March, and M. Lewenstein, Phys. Rev. A 98, 063630 (2018), URL https://link.aps.org/doi/10.1103/PhysRevA.98.063630.

[32] T. Lausch, A. Widera, and M. Fleischhauer, Phys. Rev. A 97, 023621 (2018), URL https://link.aps.org/doi/10.1103/PhysRevA.97.023621.

[33] K. K. Nielsen, L. A. P. Ardila, G. M. Bruun, and T. Pohl, New Journal of Physics (2019), URL http://iopscience.iop.org/10.1088/1367-2630/ab0a81.

[34] W. E. Liu, J. Levinsen, and M. M. Parish, Phys. Rev. Lett. 122, 205301 (2019), URL https://link.aps.org/doi/10.1103/PhysRevLett.122.205301.