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Quantum dynamics of ultracold Bose polarons

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We analyze the dynamics of Bose polarons in the vicinity of a Feshbach resonance between the impurity and host atoms. We compute the radio-frequency absorption spectra for the case when the initial state of the impurity is non-interacting and the final state is strongly interacting with the host atoms. We compare results of different theoretical approaches including a single excitation expansion, a self-consistent T-matrix method, and a time-dependent coherent state approach. Our analysis reveals sharp spectral features arising from metastable states with several Bogoliubov excitations bound to the impurity atom. This surprising result of the interplay of many-body and few-body Efimov type bound state physics can only be obtained by going beyond the commonly used Fröhlich model and including quasiparticle scattering processes. Close to the resonance we find that strong fluctuations lead to a broad, incoherent absorption spectrum where no quasi-particle peak can be assigned.

Understanding the role of few-body correlations in many-body systems is a challenging problem that arises in many areas of physics. Few particle systems can be studied using powerful techniques of scattering theory such as Faddeev equations, hyperspherical formalism, or effective field theory [1–5]. These approaches have been successfully applied to investigate collisions of hadrons [6, 7] and Efimov resonances in ultracold atoms [8, 9]. On the other hand the common approach to interacting many-body systems is to use the mean-field approximation, which reduces a many-body problem to an effective single particle Hamiltonian with self-consistently determined fields. While this approach provides a good description of many fundamental states, including magnetic, superconducting, and superfluid phases [10], in many cases it is important to go beyond the mean-field paradigm and include correlations at a few particle level. Recent notable examples include 4e pairing in high-Tc superconductors [11], spin nematic states [12], chains and clusters of molecules in ultracold atoms [13–16], and the QCD phase diagram in high-energy physics [17, 18]. A particularly important class of problems where few-body correlations play a crucial role is the formation of quasiparticles and polarons. The key feature of both is the dramatic change in the particle dynamics due to the interaction with collective excitations of the many-body system. Famous examples include lattice polarons in semiconductors [19, 20], magnetic polarons in strongly correlated systems [21–23], and ^{3}He atoms in superfluid ^{4}He [24].

Recent experiments with ultracold atoms opened a new chapter in the study of polaronic physics [25–56, 61]. These systems have tunable interactions between impurity and host atoms [57] and powerful experimental techniques for characterizing many-body states include spectroscopy [27, 30–32], Ramsey interferometry [36], time of flight experiments [37], and in-situ measurements with single atom resolution [35, 58].

In this paper we explore the dynamics of Bose polarons in the specific setting of radio-frequency (RF) spectroscopy of impurity atoms immersed in a Bose-Einstein condensate (BEC). The most striking finding of our study is the breakdown of the polaron quasiparticle picture close to the resonance (see Fig. 1). This is the result of the interplay between few- and many-body correlations which also manifest themselves as the appearance of sharp spectral lines arising from states of several Bogoliubov quasiparticles bound to the impurity atom. Both effects can be contrasted to earlier theoretical studies that predicted a smooth crossover from an attractive polaron to a molecular state [54, 59, 60, 62–65]. This interplay can not be studied in the commonly used Fröhlich model [19] because the latter does not include two particle scattering processes that results in the Feshbach resonance.

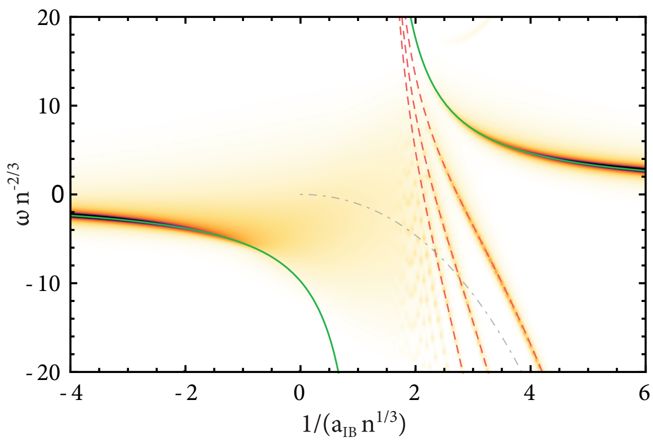

Figure 1. Absorption spectra $A(\omega)$ of a single impurity immersed in a BEC as a function of the inverse interaction strength $1/(n^{1/3}a_{\rm IB})$. The polaron (4) and bound state (7) energies are shown as solid and dashed lines. For $1/(n^{1/3}a_{\rm IB}) \gg 1$ the energy of the first bound state approaches the dimer binding energy (dash-dotted line). The spectrum is shown for a momentum cutoff $\Lambda n^{-1/3} = 20$, Bose scattering length $a_{BB}n^{1/3} = 0.05$, and mass-balanced system $m_I = m_B$.

Model. – We consider an impurity of mass m_I interacting with a weakly interacting BEC of atoms of mass m_B in the vicinity of an inter-species Feshbach resonance. Within the Bogoliubov approximation the system is described by the

Hamiltonian [70]

$$\hat{H} = g_\Lambda n + \frac{\hat{\mathbf{P}}^2}{2m_I} + \sum_{\mathbf{k}} \omega_{\mathbf{k}} \hat{b}^\dagger_{\mathbf{k}} \hat{b}_{\mathbf{k}} + \frac{g_\Lambda \sqrt{n}}{L^{d/2}} \sum_{\mathbf{k}} W_{\mathbf{k}} e^{i\mathbf{k}\hat{\mathbf{R}}} \left(\hat{b}^\dagger_{\mathbf{k}} + \hat{b}_{-\mathbf{k}}\right) + \frac{g_\Lambda}{L^d} \sum_{\mathbf{k}\mathbf{k}'} V^{(1)}_{\mathbf{k}\mathbf{k}'} e^{i(k-k')\hat{\mathbf{R}}} \hat{b}^\dagger_{\mathbf{k}} \hat{b}_{\mathbf{k}'} + \frac{g_\Lambda}{L^d} \sum_{\mathbf{k}\mathbf{k}'} V^{(2)}_{\mathbf{k}\mathbf{k}'} e^{i(k+k')\hat{\mathbf{R}}} \left(\hat{b}^\dagger_{\mathbf{k}} \hat{b}^\dagger_{\mathbf{k}'} + \hat{b}_{-\mathbf{k}} \hat{b}_{-\mathbf{k}'}\right). \quad (1)$$

Here the operators $b^\dagger_{\mathbf{k}}$ create Bogoliubov quasiparticles ('phonons') with momentum $\mathbf{k}$ and dispersion $\omega_{\mathbf{k}}$. The bare inter-species interaction is given by g_Λ. Furthermore $W_{\mathbf{k}} = \sqrt{\varepsilon_{\mathbf{k}}/\omega_{\mathbf{k}}}$, $V^{(1)}_{\mathbf{k}\mathbf{k}'} \pm V^{(2)}_{\mathbf{k}\mathbf{k}'} = (W_{\mathbf{k}} W_{\mathbf{k}'})^{\pm 1}$, and $\varepsilon_{\mathbf{k}} = k^2/2m_B$ is the boson's dispersion relation; n is the condensate density, and L^d the system's volume.

The last two lines in Eq. (1) describe the interaction of the impurity at position $\hat{\mathbf{R}}$ and momentum $\hat{\mathbf{P}}$ with the host bosons. In the Fröhlich model only the interaction term linear in the bosonic operators is present and it describes the creation of excitations directly from the BEC. However, a microscopic derivation reveals that in cold atomic systems also the additional quadratic terms, included in Eq. (1), are present which lead to rich physics beyond the Fröhlich paradigm [59].

The extended Hamiltonian (1) allows for a proper regularization of the contact interaction between the impurity and bosons. From the solution of the two-body scattering problem of Eq. (1) follows the relation of g_Λ to the impurity-boson scattering length a_{IB} by the Lippmann-Schwinger equation

$$g_\Lambda^{-1} = \frac{\mu_{\text{red}}}{2\pi} a_{IB}^{-1} - \frac{1}{L^d} \sum_{\mathbf{k}}^{\Lambda} \frac{2\mu_{\text{red}}}{\mathbf{k}^2}. \quad (2)$$

Here $\mu_{\text{red}} = m_I m_B/(m_I + m_B)$ is the reduced mass and $\Lambda \sim 1/r_0$ denotes an ultraviolet (UV) cutoff scale related to a finite range r_0 of the interaction potential. In the limit $\Lambda \to \infty$ contact interactions are recovered.

We describe the impurity-bath system in the frame co-moving with the polaronic quasiparticle [68]. This is achieved using a canonical transformation $\hat{\mathcal{H}} = \hat{S}^{-1} \hat{H} \hat{S}$ with $\hat{S} = e^{i\hat{\mathbf{R}}\hat{\mathbf{P}}_B}$ where $\hat{\mathbf{P}}_B = \sum_{\mathbf{k}} \mathbf{k} \hat{b}^\dagger_{\mathbf{k}} \hat{b}_{\mathbf{k}}$ is the total momentum operator of the bosons. After the transformation sectors with different total system momentum $\mathbf{P}$ are decoupled in the Hamiltonian $\hat{\mathcal{H}}$. The bosons now interact with each other since the impurity kinetic energy transforms according to $\hat{\mathbf{P}}^2/2M \to (\hat{\mathbf{P}} - \hat{\mathbf{P}}_B)^2/2M$ [56, 69], for details see [70].

Quantum quench dynamics. – In this work we predict the excitation spectrum of Eq. (1). In experiments the spectrum can be explored using 'inverse' RF spectroscopy where the impurity is driven from a state non-interacting with the BEC to an interacting one. Within linear response the absorption spectrum is given by $A(\omega) = 2\,\text{Re} \int_0^\infty dt e^{i\omega t} S(t)$, where $S(t) = \langle \Psi(0)| e^{-i\hat{H}t} |\Psi(0)\rangle$ is a time-dependent overlap. Here $|\Psi(0)\rangle$ denotes the initial state of the system and the overlap $S(t)$ describes the dynamics of the system after a quench of the interactions between impurity and the bath. In real-time the overlap $S(t)$ can be measured using Ramsey interferometry [71, 72].

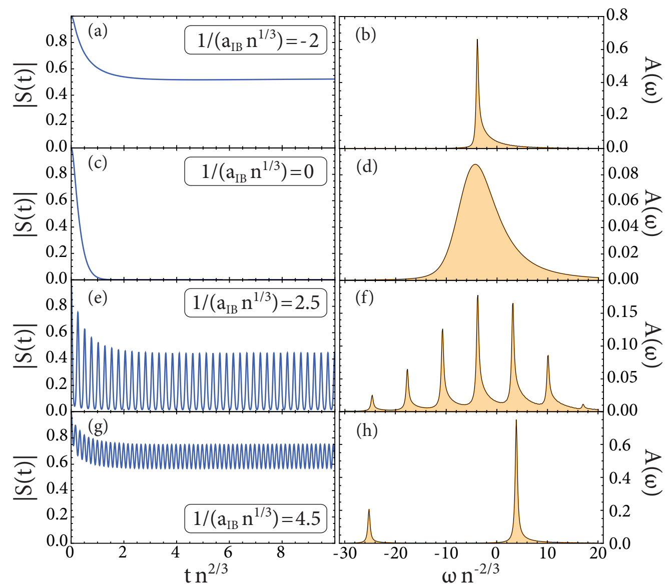

Figure 2. Ramsey contrast $|S(t)|$ and impurity absorption spectra $A(\omega)$ for fixed scattering lengths $1/(n^{1/3}a_{\text{IB}})$. For negative scattering length, panel (a,b), the spectrum reveals the attractive polaron. At unitarity, panel (c,d), the spectrum shows a broad spectral feature and no quasi particle peak can be assigned. For positive scattering lengths, panel (e-f), a series of bound states emerges. Away from the resonance, panel (g-h), their binding energy increases while at positive frequencies a long-lived repulsive polaron becomes the dominant excitation. As for Fig. 1 we broadened the spectrum to make sharp features visible.

In order to predict the real-time evolution as well as the excitation spectrum of the system, we invoke the time-dependent variational principle [73]. The approach relies on a projection of the many-body wave function onto a submanifold of the full Hilbert space spanned by a set of trial wave-functions.

Specifically, we employ a variational state in the form of a product of coherent states [69]

$$|\Psi_{\text{coh}}(t)\rangle = e^{-i\phi(t)} e^{\sum_{\mathbf{k}} \beta_{\mathbf{k}}(t) b^\dagger_{\mathbf{k}} - h.c.} |0\rangle \quad (3)$$

where $\beta_{\mathbf{k}}(t)$ are the coherent amplitudes, $\phi(t)$ is a global phase which ensures energy conservation, and $|0\rangle$ denotes the vacuum of Bogoliubov quasiparticles. The ansatz (3) provides an exact solution when describing the sudden immersion of an impurity of infinite mass into a gas of non-interacting bosons. As such the choice of the wave function is based on an exact limit of the model which is valid for arbitrary interaction strengths between the impurity and Bose gas.

We first calculate the polaron energy from the variation of $\langle \Psi_{\text{coh}}| \hat{\mathcal{H}} |\Psi_{\text{coh}}\rangle$ which for $\mathbf{P} = 0$ yields [70]

$$E_{\text{pol}} = \frac{2\pi}{\mu_{\text{red}}} \frac{n}{a_{IB}^{-1} - a_0^{-1}}. \quad (4)$$

Here $a_0^{-1} = \frac{2\pi}{\mu_{\text{red}}} \sum_{\mathbf{k}} \left(2\mu_{\text{red}}/\mathbf{k}^2 - W_{\mathbf{k}}^2/(\omega_{\mathbf{k}} + \mathbf{k}^2/2m_I)\right)$ defines the shift of the scattering resonance due to the many-body environment. Eq. (4) accounts for the regularization of the short-range interaction as given by Eq. (2) and contains only experimentally accessible parameters.

For the dynamics we treat the parameters $\beta_{\mathbf{k}}(t)$ and $\phi(t)$ as time dependent quantities. The equation of motions $\frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{\beta}} - \frac{\partial \mathcal{L}}{\partial \beta} = 0$ are obtained from the Lagrangian $\mathcal{L} = \langle \Psi_{\text{coh}} | i\partial_t - \hat{\mathcal{H}} | \Psi_{\text{coh}} \rangle$,

$$
\begin{aligned}
i\dot{\beta}_k &= g_\Lambda \sqrt{n} W_{\mathbf{k}} + \left(\omega_{\mathbf{k}} + \frac{\mathbf{k}^2}{2m_I} - \frac{\mathbf{k}\left(\mathbf{P} - \mathbf{P}_B\left[\beta_{\mathbf{k}}\right]\right)}{m_I} \right) \beta_{\mathbf{k}} \\
&\quad + \frac{g_\Lambda}{2} \left[W_{\mathbf{k}} \sum_{\mathbf{k}'} W_{\mathbf{k}'} \left(\beta_{\mathbf{k}'} + \beta^*_{\mathbf{k}'}\right) + W^{-1}_{\mathbf{k}} \sum_{\mathbf{k}'} W^{-1}_{\mathbf{k}'} \left(\beta_{\mathbf{k}'} - \beta^*_{\mathbf{k}'}\right) \right] \\
\dot{\phi}(t) &= g_\Lambda n + \frac{1}{2} g_\Lambda \sqrt{n} \sum_{\mathbf{k}} W_{\mathbf{k}} \left(\beta_{\mathbf{k}} + \beta^*_{\mathbf{k}}\right) + \frac{\mathbf{P}^2 - \mathbf{P}^2_B\left[\beta_{\mathbf{k}}\right]}{2m_I}.
\end{aligned} \tag{5}
$$

Here $\mathbf{P}_B\left[\beta_{\mathbf{k}}\right] = \sum_{\mathbf{k}} \mathbf{k} \left|\beta_{\mathbf{k}}\right|^2$ is the total phonon momentum and g_Λ is defined by Eq. (2) ensuring a time-evolution which is fully regularized and free of any divergencies.

Dynamical overlap and absorption spectra.– In the class of coherent states, Eq. (3), the dynamical overlap becomes $S(t) = \langle 0 | \Psi_{\text{coh}}(t) \rangle = \exp\left[-i\phi(t) - \frac{1}{2}\sum_{\mathbf{k}} |\beta_{\mathbf{k}}(t)|^2\right]$. From its Fourier transform we obtain the RF absorption spectrum, shown in the right panels in Fig. 1, as function of $1/(n^{1/3} a_{\text{IB}})$.

The spectrum exhibits two main excitation branches which follow the energy, Eq. (4): the attractive polaron for $a_{IB} < 0$ and the repulsive polaron for $a_{IB} > 0$. The attractive polaron is formed when the impurity is dressed by bosonic excitations due to the weak attractive interactions with the bath. The corresponding spectral signature, shown in Fig. 2(b), is a sharp quasiparticle peak at negative frequencies given by Eq. (4). The emergence of the polaron is also reflected in the long-time dynamics of the dynamical overlap $|S(t)|$ approaching the quasiparticle weight Z in Fig. 2(a).

As the Feshbach resonance at $1/(n^{1/3} a_{\text{IB}}) = 0$ is approached the attractive polaron peak looses spectral weight, $Z \to 0$, to the scattering continuum at higher frequencies. Close to unitarity, no particular eigenstate of $\hat{\mathcal{H}}$ yields a distinct contribution to the dynamical overlap $S(t)$, and many overlaps between the eigenstates of the many-body Hamiltonian and the non-interacting state of the system are of the same order. Hence the spectrum becomes broad and no coherent quasiparticle excitation is possible any longer. In consequence, perturbative approaches based on expansions around the non-interacting state become particularly unreliable in this strong coupling regime.

For positive scattering length, $1/(n^{1/3} a_{\text{IB}}) > 0$, the effective interaction between the impurity and the bosons is repulsive and leads to the formation of the repulsive polaron. This state manifests itself as a quasiparticle peak at positive frequency and correspondingly $|S(t)|$ saturates at a finite value at long times, see Fig. 2(g,h). As can be seen in Fig. 1, the energy of the repulsive polaron increases as the shifted resonance at $a_{IB} = a_0$ is approached, and it follows the saddle point prediction Eq. (4). Similar to the attractive polaron, close to the resonance, the repulsive polaron quickly looses quasiparticle weight.

However, the spectral weight is transferred not only to incoherent excitations but also to coherent spectral features which appear below the repulsive polaron branch. In Fig. 1 and Fig. 2(f) those features are visible as a series of equidistant peaks. Such excitations are absent in the Fröhlich model since they are a consequence of strong pairing correlations originating from the quadratic interaction terms in Eq. (1). As unitarity is approached, the spacing between these bound state peaks decreases until they eventually cannot be resolved. Such a crossover in the spectral profile from discrete bound states to a broad distribution is reminiscent of superpolarons in Rydberg molecular systems [66, 67].

Many-body bound states. – The emergence of the series of bound states on the repulsive side of the resonance ($1/a_{\text{IB}} > 0$) is a novel feature of impurities immersed in atomic BECs. Each peak corresponds to a single, two, or more Bogoliubov quasiparticles bound to the repulsive polaron.

The structure of the bound state spectrum can be understood analytically. We consider a wave-function which accounts for a single Bogoliubov excitation above the polaron state $\left|\Psi_{\text{pol}}\right\rangle$ [56, 70], which is a coherent state Eq. (3) with the coefficients $\beta_{\mathbf{k}}$ defined by the stationary solution of Eq. (5)

$$
\left|\Psi'(t)\right\rangle = \sum_{\mathbf{k}} \gamma_{\mathbf{k}}(t) \hat{b}^\dagger_{\mathbf{k}} \left|\Psi_{\text{pol}}\right\rangle. \tag{6}
$$

This ansatz can be regarded as a molecular wave-function fully accounting for two-body bound state physics on top of the repulsive polaron state $\left|\Psi_{\text{pol}}\right\rangle$. A calculation shows that the equations of motion of this state have an eigenmode $\gamma_{\mathbf{k}}(t) \sim e^{-i\nu_B t}$ with eigenfrequency ν_B determined by the solution of the equation [70]

$$
\frac{\mu_{\text{red}}}{2\pi a_{IB}} - \sum_{\mathbf{k}} \left[\frac{\left(W^2_{\mathbf{k}} + W^{-2}_{\mathbf{k}}\right)/2}{\nu_B - E_{\text{pol}} - \Omega_{\mathbf{k}}} + \frac{2\mu_{\text{red}}}{\mathbf{k}^2} \right] = 0 \tag{7}
$$

where $\Omega_{\mathbf{k}} = \omega_{\mathbf{k}} + \mathbf{k}^2/2m_I$. In Fig. 1 we show the energy ν_B as red dashed lines. Those occur in integer multiples of ν_B since the bound state can be occupied by several phonons at the same times, an effect taken into account by the exponentiated creation operators in Eq. (3).

For a further understanding of these states we consider the limit of the BEC density going to zero, ie. $n \to 0$, $\left|\Psi_{\text{pol}}\right\rangle \to |0\rangle$, $W_{\mathbf{k}} \to 1$ and $\Omega_{\mathbf{k}} \to \mathbf{k}^2/2\mu_{\text{red}}$. This limit defines the two-body problem where, for zero-range interactions, the bound state energy becomes $\epsilon_B = -\hbar^2/\mu_{\text{red}} a^2_{IB}$ [59], which is fully recovered by Eq. (7). For any finite density of non-interacting bosons, and assuming an infinitely heavy impurity, this bound state can be occupied by arbitrarily many bosons, and each bound atom contributes an energy ϵ_B. In an interacting Bose gas, the infinitely massive impurity scatters with Bogoliubov quasiparticles instead of bare bosons. As a consequence the binding energy ϵ_B is modified. Since in the Bogoliubov model quasiparticles do not interact with each other, they can still occupy the bound state multiple times which leads to the series of spectral lines visible in Fig. 2(c).

The emergence of the many-body bound states revealed in our approach is related to the Efimov effect [8, 9, 74]. Indeed, an exact solution of the corresponding three-body problem reveals that, as the infinite mass condition is relaxed, recoil leads to the splitting of three-, four-, etc. body bound states into an infinite series of bound states situated in a regime exponentially close to the Feshbach resonance [75, 76]. Within our approach this splitting is absent since the effective interactions between phonons vanishes for the class of coherent states Eq. (3). In consequence, in the limit of vanishing density, we effectively recover the Efimov physics of an infinitely mass-imbalanced system, as discussed by Efimov in his seminal work [75, 77].

Comparison to other approaches.– As can be seen from the previous analysis, a simple ansatz such as Eq. (6) can already account for aspects of complex many-body physics. Indeed, the ansatz (6) is related to a variational wave function which is based on an expansion in terms of single particle excitations, first introduced for fermionic systems [78], and later generalized to bosons [52, 56, 59, 60].

Here we present an extension of this equilibrium approach to real-time dynamics by studying the time-dependent variational wave-function

$$|\Psi_{1\text{ex}}(t)\rangle = \alpha_0(t)\,|0\rangle + \sum_{\mathbf{k}} \alpha_{\mathbf{k}}(t)\hat{b}^\dagger_{\mathbf{k}}\,|0\rangle \tag{8}$$

This wave-function accounts for a single phonon excitation on top of the unperturbed BEC state. We calculate the excitation spectrum of the system from the dynamical overlap $S(t) = \alpha_0(t)$ obtained from the equation of motions. This ansatz is connected to the coherent state approach as an expansion in low occupation numbers, which justifies the validity of Eq. (8) in the limit of low densities. While in the weak coupling regime the ansatz (8) reproduces the predictions of the coherent state approach, it fails to describe the intricate many-body physics in regimes where multiple boson excitations become relevant (for a detailed comparison see [70]).

The difference between the approach (3) and the single-excitation expansion (8) can be highlighted when the time evolution of the number of phonon excitations $N_{\text{ph}} = \langle \sum_{\mathbf{k}} \hat{b}^\dagger_{\mathbf{k}} \hat{b}_{\mathbf{k}} \rangle$ is compared. In Fig. 3 we show $N_{\text{ph}}(t)$ for attractive and repulsive interactions. On the attractive side both approaches predict a saturation of the phonon number in the long time limit, see Fig. 3(a). In the single-excitation expansion (dashed lines), the number of excitations is restricted to one. This limitation becomes apparent when comparing to the coherent state approach (solid lines). We find that already for moderate attractive coupling strengths the phonon number exceeds one. Hence, due to the restriction of Eq. (8) to single excitations, both approaches agree only for short times.

On the repulsive side the coherent state approach predicts oscillations of N_{ph} in the long time limit, see Fig. 3(b). These

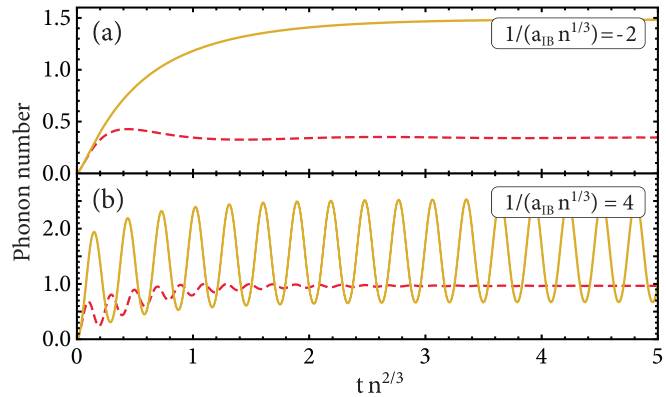

Figure 3. Time evolution of the phonons number N_{ph} for (a) attractive $1/(n^{1/3}a_{\text{IB}}) = -2$ and (b) repulsive $1/(n^{1/3}a_{\text{IB}}) = 4$ interactions, obtained by the coherent state approach (3) and the single-excitation expansion (8) (yellow solid and red dashed lines, respectively).

oscillations appear due to the competition between the many-body polaron branch and the few-body bound states. In contrast, in the single-excitation expansion these oscillations decay gradually, and in the long time limit the number of excitations saturates at one, reflecting the formation of a single molecular state.

Note, a self-consistent T-matrix approach [59] also accounts for an infinite number of bosonic excitations. There it has been found that the inclusion of multiple boson excitations has a profound influence on the spectrum. However, as for the ansatz (8) multiphonon bound states have not been observed in this earlier work. Yet we emphasize that for short times dynamics or moderate interaction strengths, expansions in terms of a few particle excitations remain a viable approach. They correctly describe the weakly attractive and repulsive polaron branches as well as the one-boson bound state present in the spectrum sufficiently far away from the Feshbach resonance.

Summary and Outlook.– We analyzed the dynamics and absorption spectra of an impurity immersed in a BEC. We demonstrated both the disappearance of the sharp quasiparticle spectral feature at strong coupling and the presence of a novel type of excitations in which several Bogoliubov quasiparticles are bound to the impurity. Our analysis highlights the importance of quasiparticle scattering processes that are not present in the commonly used Fröhlich model. They result in strong short distance correlations that give rise to multiparticle bound states and play a crucial role in suppressing the quasiparticle spectral weight close to the Feshbach resonance. Our work opens new directions for studying non-perturbative phenomena in Bose polarons at strong coupling. We expect that new insight into such systems can be gained by extending our analysis to Gaussian variational wave-function [55] and Renormalization Group approach [49]. Our method can also be extended to problems beyond linear response such as Rabi oscillations of strongly driven impurities [31, 79].

Note added. After submission of the manuscript, the first observation of Bose polarons has been reported [80, 81]. In these works absorption spectra were measured using the same 'inverse' RF protocol as put forward here. We added an additional section to the supplementary material where we compare our theory to the experimental data.

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