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Editors' Suggestion

Quantum Behavior of a Heavy Impurity Strongly Coupled to a Bose Gas

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We investigate the problem of an infinitely heavy impurity interacting with a dilute Bose gas at zero temperature. When the impurity-boson interactions are short-ranged, we show that boson-boson interactions induce a quantum blockade effect, where a single boson can effectively block or screen the impurity potential. Since this behavior depends on the quantum granular nature of the Bose gas, it cannot be captured within a standard classical-field description. Using a combination of exact quantum Monte Carlo methods and a truncated basis approach, we show how the quantum correlations between bosons lead to universal few-body bound states and a logarithmically slow dependence of the polaron ground-state energy on the boson-boson scattering length. Moreover, we expose the link between the polaron energy and the spatial structure of the quantum correlations, spanning the infrared to ultraviolet physics.

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The scenario of an infinitely heavy impurity in a quantum medium is a fundamental problem in physics, with relevance ranging from electron gases [1] to open quantum systems [2]. The behavior is well understood in the case of an ideal Fermi medium [3,4] where the problem can be solved exactly. Here, Anderson famously demonstrated that any interaction with the impurity leads to the orthogonality catastrophe in the thermodynamic limit [5]. However, there is currently much debate over the nature of the ground state for a fixed impurity strongly coupled to a dilute Bose gas, which is of immediate importance to ongoing cold-atom experiments [6–12].

The bosonic problem—termed the Bose polaron—appears straightforward at first glance, since there is the possibility of describing the condensed ground state of the Bose gas as a classical field, e.g., in the form of a coherent state [13–17], or governed by an effective Gross-Pitaevskii equation [18–20]. Furthermore, when the Bose gas is noninteracting, the ground state corresponds to all bosons occupying the lowest single-particle state in the system, making it even simpler than the fermionic case [21]. However, this tendency of bosons to cluster also means that, in the absence of boson-boson interactions, the Bose polaron ground-state energy diverges when the impurity-boson interaction is attractive enough to support a bound state [19,22]. Thus, it is an important and nontrivial question how this pathological behavior is cured by boson-boson interactions, and whether the details of the impurity-boson interaction play a key role. This is of particular interest in the case of short-range resonant impurity-boson interactions, where the scattering length $a \to \pm\infty$ and there is the prospect of universal physics, independent of the microscopic details.

In this Letter, we show that in order to describe the ground state of the Bose polaron, it is crucial to go beyond classical-field descriptions and include the quantum "granular" nature of the Bose gas. Specifically, once the boson-boson scattering length a_B is comparable to or larger than the range r_0 of the attractive impurity-boson potential, a single boson from the gas can effectively screen or block the impurity potential, as illustrated in Fig. 1. For a sufficiently attractive impurity-boson potential with $r_0 \to 0$, we find that this quantum blocking effect leads to universal few-body bound states involving the impurity, in agreement with Refs. [23,24]. Using exact quantum Monte Carlo (QMC) methods [25–27], we show that the polaron energy in the many-body limit exhibits a *logarithmic* dependence on a_B in the unitary regime $a \to \pm\infty$. We further illustrate the importance of quantum correlations between bosons by

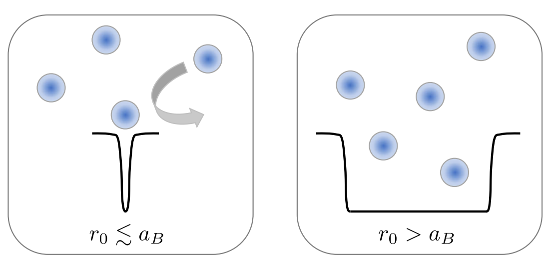

FIG. 1. Bosons (circles) in the presence of an attractive impurity potential. If the range of the potential r_0 is comparable to or smaller than the boson-boson scattering length a_B, then a single boson can block the potential (left). Conversely, if $r_0 > a_B$, as for a Rydberg [9] or ionic [31] impurity, then many bosons can interact with the potential at once (right).

showing that the QMC results for the polaron ground-state energy are well captured by a truncated basis variational approach [28–30] across a range of interactions.

Model.—We consider the following Hamiltonian for a single infinitely heavy impurity in a Bose gas:

$$\hat{H} = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} b_{\mathbf{k}}^{\dagger} b_{\mathbf{k}} + \sum_{\mathbf{k}\mathbf{k}'\mathbf{q}} \frac{V(\mathbf{q})}{2} b_{\mathbf{k}}^{\dagger} b_{\mathbf{k}'}^{\dagger} b_{\mathbf{k}'+\mathbf{q}} b_{\mathbf{k}-\mathbf{q}} + g \sum_{\mathbf{k}\mathbf{k}'} b_{\mathbf{k}}^{\dagger} b_{\mathbf{k}'}. \tag{1}$$

The three terms correspond, respectively, to the kinetic energy of the bosons, the boson-boson interaction, and the boson-impurity interaction, where we have set the system volume and $\hbar$ to one. In this model, a boson of mass m and momentum $\mathbf{k}$ is created by the operator $b_{\mathbf{k}}^{\dagger}$, and we consider bosons with the quadratic dispersion $\epsilon_{\mathbf{k}} = |\mathbf{k}|^2/2m \equiv k^2/2m$. Furthermore, we describe their interaction using the short-range potential $V(\mathbf{q})$, which results in a low-energy boson-boson scattering length $a_B > 0$. The interaction between the impurity and a boson is taken to be short-ranged and of strength g up to a momentum cutoff Λ. The bare parameters g and Λ can be related to the physical impurity-boson scattering length a via $m/2\pi a = 1/g + \sum_{\mathbf{k}}^{\Lambda}(1/\epsilon_{\mathbf{k}})$. In the following, we take the zero-range limit $r_0 \to 0$, which requires $\Lambda \to \infty$. For the QMC calculations, we solve the problem in real space, using a Bethe-Peierls boundary condition for the impurity-boson interactions, and taking the boson-boson potential to be a hard-sphere potential, where the diameter of the sphere coincides with the s-wave scattering length a_B (see Supplemental Material [32]).

Few-body bound states.—We first discuss the few-body physics of an infinitely heavy impurity interacting with N_B identical bosons, where we assume that $a > 0$ such that the impurity potential supports a bound state. For $N_B = 1$, we simply have the impurity-boson bound state with energy $-\epsilon_b = -1/2ma^2$, while $N_B = 2$ corresponds to the minimal number of bosons where boson-boson correlations can emerge. In Fig. 2(a) we display the QMC results for the $N_B = 2$ energy for a range of a_B. We find that a trimer (2-boson) bound state only exists when the scattering length a is above a critical value $a^* \simeq 10a_B$ set by the boson repulsion. Moreover, the trimer energy remains close to $-\epsilon_b$ (i.e., the result for $N_B = 1$) for the plotted range of a_B/a spanning several orders of magnitude, and it only slowly approaches the result for uncorrelated bosons, $-2\epsilon_b$, as we take $a_B/a \to 0$. A similar behavior is observed for $N_B = 3$, since we see that the tetramer (3-boson) bound state also only exists when $a > a^*$, and the tetramer energy lies well above the uncorrelated result, $-3\epsilon_b$. Therefore, we conclude that boson repulsion dominates the few-body behavior.

Indeed, we find that we can reproduce these few-body states when the bosons only block each other at the impurity and are noninteracting otherwise. Such a scenario is achieved with a bosonic Anderson model [23,24], where the impurity-boson interaction features an open and closed channel like in a realistic cold-atom scattering process [41]. Here, the impurity is unavailable for interactions with other bosons once a boson enters the closed-channel state, thus mimicking the quantum blockade effect in Fig. 1. We previously solved the $N_B = 2$ problem exactly analytically for this model and we obtained the critical scattering length $a^* = 3.1426|r_{\text{eff}}|$, where r_{eff} is the (negative) effective range of the impurity-boson interactions [23,24]. Moreover, we found that a^* corresponded to a multibody resonance beyond which all $N_B > 1$ bound states cease to exist. We display the results of this two-channel model in Fig. 2(a) and find good agreement with the QMC data. This demonstrates two points: the few-body energies universally depend on the ratio a^*/a, and the behavior is determined by quantum blocking at the impurity.

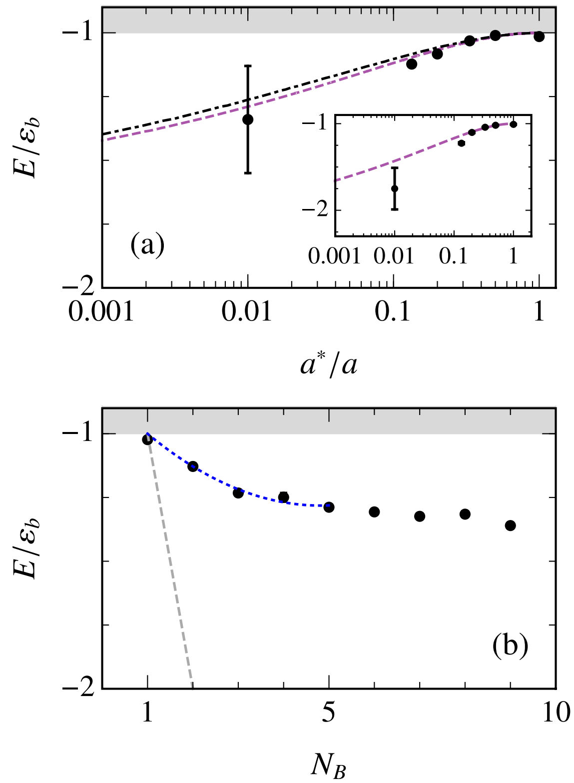

FIG. 2. (a) Trimer energy as a function of inverse scattering length obtained from QMC (black circles), bosons with attractive contact interaction (black dot dashed line), and the Anderson model (purple dashed line). The inset compares the tetramer energy in the QMC with those of the Anderson model. (b) Few-body energy at $a/a_B = 75$ as a function of boson number calculated within the QMC (black circles). We also show the energy of uncorrelated bosons, $E = -N_B\epsilon_b$ (gray dashed line), and that of interacting bosons in an effective potential that accounts for three-body correlations, Eq. (2), with $U = 0.04\epsilon_b = 1.5a_B/ma^3$ (blue dotted line). Data for the Anderson model are taken from Ref. [23].

Such few-body universality also extends to models with *zero-range* boson-boson interactions. In this case, a finite positive a_B requires an underlying attractive potential $V(\mathbf{q})$, which features Efimov physics as well as deeply bound dimers [32]. Thus, the relevant few-body states with effective boson-boson repulsion are actually metastable excited states. Nonetheless, it is possible to solve for the energy of the metastable trimer state [32] and we see that it agrees well with the results of the other models in Fig. 2(a). We also find the critical scattering length to be $a^* = 20.0a_B$, which differs slightly from that estimated from the QMC simulations for a hard-sphere potential, indicating that finite-range effects are relevant in the relationship between a^* and boson repulsion.

Within QMC, we can extend our results to even larger N_B complexes. Fixing $a^*/a < 1$, we observe in Fig. 2(b) that the energy strongly deviates from the uncorrelated result $E = -N_B\varepsilon_b$ (dashed gray line) and appears to saturate to a finite value with increasing N_B. Moreover, this does not match the energy of interacting bosons in a potential, $E = -N_B\varepsilon_b + UN_B(N_B - 1)/2$, for *any* interaction energy U. We expect this behavior to also hold for a nonzero range r_0 as long as we satisfy the blocking condition $r_0 \lesssim a_B$, illustrated in Fig. 1. This condition is equivalent to requiring that the boson interaction energy, $\sim a_B/mr_0^3$, exceeds the depth of the potential, $\sim 1/mr_0^2$, assuming that the potential is close to resonance and using the fact that bosons within the potential interact over a volume set by r_0^3 [42].

We can understand the result of Fig. 2(b) by considering instead $N_B - 1$ bosons moving in the longer-ranged potential originating from the infinitely heavy dimer consisting of the impurity and a boson. In this case, the range of the effective potential is $\sim a$ and the energy of interacting bosons is

$$E = -\varepsilon_b - (N_B - 1)\varepsilon_T + \frac{U}{2}(N_B - 1)(N_B - 2), \quad (2)$$

where ε_T is the trimer binding energy. In Fig. 2(b), where $a \gg a_B$ and $\varepsilon_T \ll \varepsilon_b$, we see that the small-$N_B$ behavior is well captured by Eq. (2) using $U \sim a_B/ma^3$. This illustrates the importance of three-body correlations as well as demonstrating the role of the potential range.

Many-body limit.—We now turn to the behavior of an impurity in a Bose gas of finite density n. In the absence of the impurity and in the limit of vanishing boson-boson interactions, the ground state is a Bose-Einstein condensate (BEC): $|\Phi\rangle = e^{\sqrt{n}(b_\mathbf{0}^\dagger - b_\mathbf{0})}|0\rangle$, where $|0\rangle$ is the vacuum state for bosons. Thus, we can replace operators $b_\mathbf{0}^\dagger$ and $b_\mathbf{0}$ in the Hamiltonian (1) by $\sqrt{n}$. Introducing the impurity and turning on interactions, the polaron ground state can be written in the general form [29],

$$|\Psi\rangle = \left(\alpha_0 + \sum_{\mathbf{k}\neq\mathbf{0}} \alpha_\mathbf{k} b_\mathbf{k}^\dagger + \frac{1}{2}\sum_{\mathbf{k}_1,\mathbf{k}_2\neq\mathbf{0}} \alpha_{\mathbf{k}_1\mathbf{k}_2} b_{\mathbf{k}_1}^\dagger b_{\mathbf{k}_2}^\dagger \ldots\right)|\Phi\rangle, \quad (3)$$

where the complex coefficients α_j are associated with different numbers of bosons excited out of the condensate, and $\alpha_{\mathbf{k}_1\mathbf{k}_2} = \alpha_{\mathbf{k}_2\mathbf{k}_1}$. In principle, one could write the expansion in Eq. (3) in terms of Bogoliubov excitations rather than bare bosonic excitations [28,44]. However, this only modifies the operators at low momenta $k < 4\sqrt{\pi n a_B}$, and this is not expected to affect the leading order behavior of the polaron energy in the extremely dilute limit $n^{1/3}a_B \ll 1$ [29]. It is also likely that the Bogoliubov approximation breaks down in the regime of strong impurity-boson interactions [45,46].

Applying the Hamiltonian (1) to the state (3) and keeping only the leading order boson-boson interaction terms in the limit $n^{1/3}a_B \ll 1$, we obtain the ground-state polaron energy [32]:

$$E = n\left[\frac{m}{2\pi a} + \sum\nolimits_\mathbf{k}\left(\frac{1}{\epsilon_\mathbf{k} + G_\mathbf{k}} - \frac{1}{\epsilon_\mathbf{k}}\right)\right]^{-1}. \quad (4)$$

Crucially, we find that it depends on the repulsive correlations between bosons via the positive function

$$G_\mathbf{k} = g\sqrt{n}\left(\sum_{\mathbf{k}'}\alpha_{\mathbf{k}\mathbf{k}'}/\alpha_\mathbf{k} - \sum_{\mathbf{k}'}\alpha_{\mathbf{k}'}/\alpha_0\right). \quad (5)$$

Note that the case of uncorrelated noninteracting bosons corresponds to $\alpha_{\mathbf{k}\mathbf{k}'} = \alpha_\mathbf{k}\alpha_{\mathbf{k}'}/\alpha_0$, which gives $G_\mathbf{k} = 0$, such that the polaron energy $E = 2\pi na/m$, in agreement with previous work [19,22]. Thus, the presence of correlations is necessary to ensure that the ground-state energy remains finite in the unitarity limit $1/a \to 0$.

This behavior is confirmed in Fig. 3, where we display the polaron ground-state energy obtained using exact QMC methods for two different densities differing by 2 orders of magnitude. For weak impurity-boson attraction $1/n^{1/3}a \ll -1$, we recover the mean-field uncorrelated result $E = 2\pi na/m$, which corresponds to the leading order dependence of Eq. (4) on a. However, as anticipated, the energy becomes sensitive to boson-boson correlations as we increase the interactions toward unitarity. This behavior is not just limited to zero-range impurity-boson interactions since the same result is obtained for a finite-range potential when $r_0 < a_B$ [25]. Note that this behavior goes beyond the few-body results discussed previously since the impurity-boson bound state is either absent (when $a < 0$) or larger than the interparticle spacing ($n^{1/3}a \gtrsim 1$).

To further characterize the correlations, we also calculate the polaron energy using a variational approach [29], where we truncate the number of bosonic excitations in the polaron ground state in Eq. (3) [32]. Here we again use the Anderson model to mimic the blockade effect at the

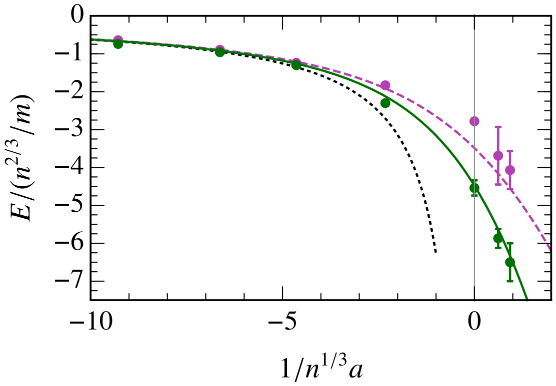

FIG. 3. Ground-state energy of the infinitely heavy Bose polaron as a function of inverse impurity-boson scattering length at fixed $n^{1/3}a^* = 0.215$ (purple dashed line) and $n^{1/3}a^* = 0.00215$ (green solid line). We show the results of the QMC (symbols) together with the results of the truncated basis approach in the Anderson model with up to three excitations (lines). The mean-field result, $E = 2\pi na/m$, is depicted as a dotted line.

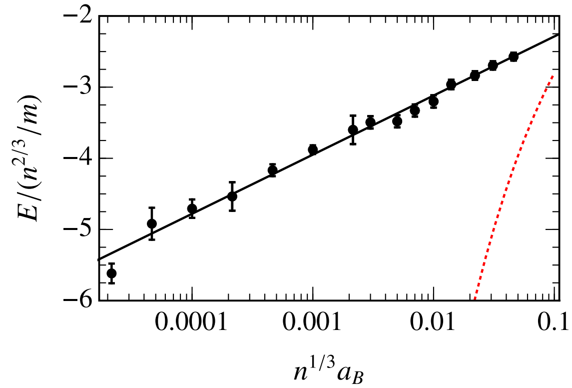

FIG. 4. Bose polaron ground-state energy in the unitarity regime of impurity-boson interactions, $1/a = 0$. The QMC results (symbols) are consistent with a logarithmic dependence of the form $E^{\mathrm{QMC}} \simeq 0.36 \ln(0.019 n^{1/3} a_B) n^{2/3}/m$ (solid line). The dashed red line is the prediction of the coherent state ansatz within the Bogoliubov approximation [13].

impurity, and we use an effective range $r_{\mathrm{eff}} \simeq -3a_B$. This ensures that the value of the three-body parameter a^* that quantifies the boson-boson repulsion matches the one from the QMC simulations. As shown in Fig. 3, we find that the truncated basis approach accurately reproduces the QMC results across a wide range of $n^{1/3}a^*$ (up to 2 orders of magnitude) when we include up to three excitations only. This suggests that the boson-boson repulsion suppresses impurity-induced excitations of the condensate, and that this suppression is universal, i.e., independent of the microscopic origin of a^*. We stress that this is a highly quantum effect that cannot be captured by a classical mean-field description [47].

At unitarity $1/a = 0$, the polaron energy takes the universal form,

$$E = -f(n^{1/3}a_B)n^{2/3}/m, \tag{6}$$

where $f(x)$ is a dimensionless function. When $a_B \to 0$ at fixed density, we know that $E \to -\infty$, while in the zero-density limit $n \to 0$, we must have $E \to 0$ since there are no bound states. Thus, in the limit $n^{1/3}a_B \to 0$, we require $f(x) \to \infty$ slower than $\sim 1/x^2$. Indeed, our QMC results reveal a *logarithmically* slow dependence $f(x) \sim -\ln(x)$, as shown in Fig. 4. This behavior is difficult to fully capture within the truncated basis approach [32] since it requires an increasingly larger number of boson excitations as $n^{1/3}a_B \to 0$. On the other hand, if we use a coherent-state ansatz [13] with an infinite number of excitations but only the approximate mean-field repulsion of the Bogoliubov Hamiltonian, then we have $f(x) = \sqrt{\pi/4x}$, which drastically overestimates the change in energy (see Fig. 4). The classical-field approach in Ref. [20] also predicts a power-law behavior $f(x) \sim 1/x^{1/3}$, but this is only valid when $r_0 \gg a_B$, which is different from the regime considered here [48].

Indeed, the polaron energy is intimately connected to the spatial structure of the boson-boson correlations via the function $G_{\mathbf{k}}$ in Eq. (4), which can be viewed as an effective interaction potential between two excited bosons. In the infrared limit $k \to 0$, where the bosons are at large separation, we should recover the behavior of uncorrelated bosons. Here, we expect that the difference in energy between one and two excited bosons is their mean-field interaction with the condensate, $8\pi a_B n/m$. This large-distance infrared behavior is correctly captured by the coherent state ansatz [13], which, however, fails at shorter length scales since it predicts a constant $G_{\mathbf{k}} = 8\pi a_B n/m$ for all k and a [32]. In reality, we expect the blockade effect to dominate at short distances such that $\alpha_{\mathbf{kk}'} \to 0$, and in this case one can show that $G_{\mathbf{k}} \to -E$ as $k \to \infty$ [32]. This short-distance ultraviolet behavior is captured by a "Chevy-type" ansatz with a single boson excitation [44,50,51], but this ansatz does not describe the large-distance physics since it has $G_{\mathbf{k}} = -E$ at all momenta. However, the momentum dependence of $G_{\mathbf{k}}$ can be well approximated within a truncated basis approach that includes more boson excitations [32], as considered in this work. In particular, our results indicate that quantum blocking at short distances dominates the behavior of the polaron energy while the infrared physics only provides a small correction.

Conclusion.—To conclude, we have shown that the ground state of the Bose polaron exhibits strong quantum correlations between bosons when the impurity-boson potential is short-ranged. This is due to a quantum blockade effect at the position of the impurity, which gives rise to universal few-body bound states and a logarithmically slow dependence of the polaron energy on boson-boson interactions in the unitarity limit $1/a \to 0$. Our results should be directly applicable to cold-atom experiments, where typically $r_0 \sim a_B$ [41], and they should also extend to a heavy but finite impurity mass m_I since Efimov physics is exponentially suppressed as a function of m_I/m [52]. More generally, the Bose polaron scenario could provide a route to probing and engineering quantum correlations in other bosonic systems such as photons in microcavities [53,54].

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