Impurity in three-dimensional unitary Bose gas

O. Hryhorchak, G. Panochko, and V. Pastukhov

1Department for Theoretical Physics, Ivan Franko National University of Lviv, 12 Drahomanov Str., Lviv, Ukraine
2Department of Optoelectronics and Information Technologies, Ivan Franko National University of Lviv, 107 Tarnavskij Str., Lviv, Ukraine

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Based on the simple and efficient method we discuss properties of a single impurity immersed in three-dimensional Bose gas with the interaction between particles tuned to unitary limit. Particularly, we present the first estimations for the low-momentum parameters of the impurity spectrum, namely, the binding energy and the effective mass both for repulsive and attractive Bose polarons in the unitary gas.

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I. INTRODUCTION

The creation of the Bose-Einstein condensed state in ultra-dilute alkalies [1, 2] 25 years ago opened up new horizons for studying collective phenomena in these essentially quantum systems. The next step in the experimental progress was achieved by the possibility of controlling the small amount of particles, which provided the observation of Efimov’s states [3] and more recently the so-called Fermi [4] and Bose polarons [5–8], i.e., a single impurity atom immersed in majority of host fermions and bosons, respectively. Such a success of experimental techniques provided the verification of numerous theoretical predictions of the Bose polaron properties in three dimension, based on variational [9, 10], renormalization-group [11, 12], field-theoretical [13, 14] and Monte Carlo [15–17] methods which allow the description of the quantum effects for weak [18–20] and strong [21] boson-impurity interactions and were applicable at low temperatures and in the vicinity of the Bose-system superfluid transition point [22, 23].

Along with such a wide range of works where polarons are investigated in diluted Bose gases, the properties of impurities in the strongly-interacting systems are well-studied only in a context of liquid $^3$He [24, 25]. But properties of superfluid helium itself and impurity atoms immersed in it are strongly dependent on the details of the two-body $^3$He-$^4$He potential. There is, however, another experimentally realizable $^3$He-$^4$He gas of bosons with short lifetime and strong point-like inter-particle interactions, the so-called unitary Bose gas. The two-body $s$-wave scattering length formally diverges in this system, and thermodynamics is universal [36] in a sense that is fully controlled by one dimensionless parameter, namely, temperature in units of bosonic analog of the Fermi energy. To our knowledge, behavior of exterior particles immersed in unitary Bose gas was not yet explored. The objective of this article is, therefore, partially to fill this gap by utilizing the semi-phenomenological approach of Ref. [37] to the problem of impurity in a three-dimensional unitary Bose gas at absolute zero. Such a mean-field-like treatments [38, 39], regardless of their simplicity, were recently demonstrated [40–43] to be quite efficient for the description, in reasonable agreement with the Monte Carlo simulations [44, 45] of Bose polarons in one dimension. In contrast to one-dimensional systems, where the effects of quantum fluctuations are strongly exhausted [46] a behavior of impurities in higher dimensions is known to be much influenced by the few-body physics. Of course, the mean-field ansatz cannot describe a formation of the boson-impurity dimers, trimers etc. [47], but it gives reliable results for the Bose-polaronic state at any strength of the boson-impurity couplings.

II. MODEL AND METHOD

The considered model consists of a single impurity atom immersed in a bosonic medium at absolute zero. The Bose subsystem that contains $N$ spinless particles is described by the semi-phenomenological model with the Hamiltonian that goes back to the seminal work of Landau [48]

$$H_B = \int d\mathbf{r} \left\{ -\frac{\hbar^2}{2m} \psi^+ \nabla^2 \psi + \mathcal{E}[n(\mathbf{r})] \right\}, \quad (2.1)$$

where the integration is carried out over large volume $V$ with periodic boundary conditions, $m$ is the mass of bosons and $\mathcal{E}[n]$ stands for the normal-ordered energy density of the uniform system at rest. The field operators $\psi^+(\mathbf{r})$, $\psi(\mathbf{r})$ obey standard bosonic commutation relations and $n(\mathbf{r}) = \psi^+(\mathbf{r})\psi(\mathbf{r})$ denotes the operator of a local bosonic density. The part of total Hamiltonian which is fully microscopical and refers to the impurity, reads

$$H_I = -\frac{\hbar^2}{2m_I} \frac{\partial^2}{\partial r_I^2} + \int d\mathbf{r} \Phi(|\mathbf{r}_I - \mathbf{r}|) n(\mathbf{r}), \quad (2.2)$$

where $\mathbf{r}_I$ and $m_I$ denote a position and a mass of an impurity, respectively. The second term in (2.2) is the en-
energy of impurity-Bose-system interaction with the two-body potential \( \Phi(r) \) that will be specified below. Our choice of bosonic Hamiltonian is a very flexible one, because with such a form it exactly reproduces bosons with the point-like interaction and allows the phenomenological generalizations, in the spirit of local density approximation, by varying the energy density \( E[n] \).

The whole zero-temperature analysis below is based on the variation principle for total Hamiltonian \( H_B + H_I \). As a trial wave function we choose the mean-field ansatz (here \( |\text{vac}\rangle \) is the normalized Fock vacuum state)

\[
|\Psi\rangle_N = \frac{(b_0^+)^N}{\sqrt{N!}} |\text{vac}\rangle, \tag{2.3}
\]

with the bosonic creation operator defined as follows

\[
b_0^+ = \frac{1}{\sqrt{N}} \int d\mathbf{r} \phi(\mathbf{r}_I - \mathbf{r})\psi^+(\mathbf{r}), \tag{2.4}
\]

where unknown function \( \phi(\mathbf{r}) \) is the subject for minimization of the energy functional

\[
E = \frac{1}{V} \int d\mathbf{r} N\langle\Psi|H_B + H_I|\Psi\rangle_N, \tag{2.5}
\]

with additional constrain \( \int d\mathbf{r} |\phi(\mathbf{r})|^2 = N \), which accounts for the correct normalization (we chose the one, where \( N\langle\Psi|n(\mathbf{r})|\Psi\rangle_N = |\phi(\mathbf{r}_I - \mathbf{r})|^2 \) is the local density of bosons). It is readily seen that our trial wave function, unlike previous studies [19–54], preserves the continuous translation symmetry of the system. It means, that this ansatz is capable to capture polaronic behavior and cannot provide the description of states with formation of the boson-impurity molecules. It is well-known that the mean field approximation typically misses important aspects of the few-body physics, but can describe the self-localization phenomenon. The latter can be traced back by the enormous increase of the impurity effective mass, but has not been confirmed by the Monte Carlo simulations [10] of Bose polarons. One more important thing about the ansatz is that the average total momentum of the system provided by the wave function \( |\Psi\rangle_N \) is equal to zero identically. But slight modification of \( |\Psi\rangle_N \), namely

\[
|\Psi_\mathbf{p}\rangle_N = e^{i\mathbf{p}\mathbf{r}_I/\hbar} \frac{(b_0^+)^N}{\sqrt{N!}} |\text{vac}\rangle, \tag{2.6}
\]

with \( b_0^+ \) being almost equal to \( b_0^+ \) except for the replacement \( \phi(\mathbf{r}_I - \mathbf{r}) \to \phi_\mathbf{p}(\mathbf{r}_I - \mathbf{r}) \), can describe the impurity moving with finite momentum \( \mathbf{p} \). When the polaron moves through the Bose condensate slowly enough, its spectrum

\[
\varepsilon_I(p) = \varepsilon_I + \frac{p^2}{2m_I^*} + \mathcal{O}(p^4), \tag{2.7}
\]

is characterized by two parameters, namely, the binding energy \( \varepsilon_I \) and the effective mass \( m_I^* \). The latter, as can be shown from general arguments, does not depend on a sign of the boson-impurity coupling and is always larger than bare mass of the impurity atom. Being the first correction to the Bose polaron spectrum at small \( \mathbf{p} \), the effective mass is fully determined [37], in thermodynamic limit, by the density profile of bosons in presence of motionless impurity

\[
\frac{m_I^*}{m_I} = 1 + \frac{m_r}{m_I} \int d\mathbf{r} \frac{[\phi(\mathbf{r})]^2 - |\phi_\infty|^2}{2|\phi_\infty|^2 + |\phi(\mathbf{r})|^2}, \tag{2.8}
\]

where \( \phi_\infty = \phi(\mathbf{r} \to \infty) \). Therefore we only have to obtain function \( \phi(\mathbf{r}) \) for motionless impurity in order to calculate two parameters in the r.h.s. of Eq. \( (2.7) \) of the low-momentum Bose polaron spectrum.

The computation of functional \( (2.5) \) is rather trivial if one notices that \( \psi(\mathbf{r})|\Psi\rangle_N = |\psi(\mathbf{r}_I - \mathbf{r})|\Psi\rangle_{N-1} \). Then an averaging (in \( N \gg 1 \) limit) of \( H_B \) and the second term in \( H_I \) reduces to the replacement of field operators \( \psi^+(\mathbf{r}) \) and \( \psi(\mathbf{r}) \) by \( \delta^+(\mathbf{r}_I - \mathbf{r}) \) and \( \phi(\mathbf{r}_I - \mathbf{r}) \), respectively. The appropriate calculations for the impurity kinetic energy operator yield \( \frac{\hbar^2}{m_I} \int d\mathbf{r} |\frac{\partial}{\partial \mathbf{r}_I} \phi(\mathbf{r}_I - \mathbf{r})|^2 \). Combining everything together, we have

\[
E = \int d\mathbf{r} \left\{ \frac{\hbar^2}{2m_r} |\nabla \phi(\mathbf{r})|^2 + \Phi(\mathbf{r})|\phi(\mathbf{r})|^2 + E'[|\phi(\mathbf{r})|^2]|\phi(\mathbf{r}) = \mu \phi(\mathbf{r}) \right\}, \tag{2.9}
\]

where \( m_r = m_I m/\left(m_I + m\right) \) is the boson-impurity reduced mass. Minimization of the above functional leads to the non-linear Schrödinger equation

\[
-\frac{\hbar^2 \nabla^2}{2m_r} \phi(\mathbf{r}) + \Phi(\mathbf{r})\phi(\mathbf{r}) + E'[|\phi(\mathbf{r})|^2] \phi(\mathbf{r}) = \mu \phi(\mathbf{r}), \tag{2.10}
\]

where prime near \( E[n] \) denotes the derivative with respect to density \( n \), the Lagrange multiplier \( \mu \) accounts for the proper normalization of \( \phi(\mathbf{r}) \) which, in turn, can be chosen as the real-valued function. With the solution of Eq. \( (2.10) \) in hands we can calculate the impurity effective mass \( m_I^* \) as well as the total energy \( E \) of the system ‘impurity+bosons’. Then by subtracting the energy of ‘pure’ bosons \( V E[n] \) (here \( n = N/V \) is the uniform density of Bose particles without an impurity) we obtain the Bose polaron binding energy \( \varepsilon_I \).

### III. RESULTS

Before proceeding with the discussion of our main results concerning a behavior of the impurity in unitary Bose gas, it is instructive to test this approach on the Bose polaron immersed in a dilute gas. The case of repulsive \( \Phi(\mathbf{r}) \) has been already reported [37], therefore, here we mainly focus on the attractive branch.
A. Attractive Bose polaron in dilute gas

In the extremely dilute limit the energy density of bosons is well-described by the mean-field expression \( \mathcal{E}[n] = \frac{2a^2}{m} n^2 \), where \( a \) is the two-boson \( s \)-wave scattering length. In order to model an attractive boson-impurity interaction we have chosen the spherical potential well

\[
\Phi(r) = \begin{cases} 
-\Phi_0, & r \leq R \\
0, & r > R 
\end{cases},
\]  
(3.11)

with finite range \( R \). The depth of potential \( \Phi_0 \) can be easily related \[55\] through the transcendental equation

\[
a_I = R \left\{ 1 - \frac{\tan(k_0 R)}{k_0 R} \right\}, \quad k_0 = \frac{\sqrt{2m\Phi_0}}{\hbar},
\]  
(3.12)

to the boson-impurity \( s \)-wave scattering length \( a_I \) and range \( R \). The numerical solution of Eq. (2.10) (with \( \Phi(r) \) and \( \mathcal{E}[n] \) inserted) was performed for dimensionless boson-boson interaction \( na^3 = 10^{-5} \), equal masses of particles \( m_I = m \) and negative values of \( a_I \). For comparison with Monte Carlo simulations [16], the range of the boson-impurity potential was taken as follows \( R = a/5 \). In fact, equilibrium properties of the impurity is almost unaffected by a precise value of this parameter and results for a smaller \( R \)s only slightly differ but require much more computer time. Note also that choice of \( \Phi(r) \) allows the unitary limit, where formally \( a_I \to -\infty \). The results of numerical calculations for the mean field binding energy and the effective mass of polaron immersed in a dilute Bose gas are presented in Figs. 1, 2. For comparison, we also plotted the results of the second-order perturbation theory and a quantum Monte Carlo. Importantly that our mean field calculations qualitatively agree with Monte Carlo results in the whole range of the boson-impurity coupling including an unitary limit, where the perturbation theory is clearly inapplicable. Another interesting consequence of this study is that, likewise the Monte Carlo results, both the binding energy and the effective mass are finite at unitary limit signaling the absence of the impurity self-localization phenomenon.

B. Impurity in unitary Bose gas

At unitary, the two-boson scattering amplitude diverges in the infrared region, and as a consequence, the many-particle system demonstrates universal behavior. Particularly, at absolute zero the energy density is given by \( \mathcal{E}[n] = \xi^2 \frac{\hbar^2}{m} n^{5/3} \) with \( \xi \) (in case of fermions it is often called the Bertsch parameter) being the true number. A cursory glance on the literature concerning the determination of parameter \( \xi \) for bosons shows that there is no consensus at this point. Various theoretical approaches give quite different values, for instance, 22.22 [56], 5.0 [57] and 4.0 [58]. For the numerical calculations, however, we used experimental result 3.40 [59] and the one obtained in the quantum Monte Carlo simulations 5.32 [60].

![FIG. 1: Impurity binding energy (in units of the mean field chemical potential \( \mu = \frac{\hbar^2 a^2}{m} n \) of bosons) in dilute Bose gas, \( na^3 = 10^{-5} \). A solid line is our mean field result, a dashed line displays the perturbative calculations up to the second order [18][20]. Symbols denote results of the Monte Carlo simulations [16].](image1)

![FIG. 2: The effective mass of the Bose polaron in dilute gas, \( na^3 = 10^{-5} \). Solid and dashed lines display the present mean field calculations and the perturbative result up to the second order [18][20], respectively. Symbol is the quantum Monte Carlo data from [16].](image2)
reason for this is that we could not find a unique stable solution of the non-linear differential equation (2.10) with the spherical-well boson-impurity interaction for positive scattering lengths. For the hard-sphere potential the s-wave scattering length $a_I$ coincides with the radius of hard core and mathematically the role of potential reduces to the change of boundary condition at the origin by the following one $\phi(a_I) = 0$. The results for the binding energy and the effective mass as functions of dimensionless scattering length $a_I^3n$ for the impurity in unitary Bose gas are presented in Figs. 3, 4. We see again that the self-localization does not occur for an impurity immersed in the strongly-interacting Bose gas, particularly, parameters of the low-momentum Bose-polaron spectrum remain finite even in the limit $a_I \to -\infty$. It worth recalling that the hard-sphere potential inadequately describes properties of the model at large positive $a_I$s, therefore, results for the repulsive branch should be applicable only in the weakly-interacting $na_I^2 \ll 1$ regime. A very unexpected conclusion of these calculations is that, in general, a behavior of impurity (see insets in Figs. 3,4) is almost unaffected by the interaction with bosons, especially the effective mass $m_I^*$, which at unitary is less than 10% larger the particle bare mass $m_I$. The mean-field approximation, however, provides only the lower bound for low-energy parameters of the impurity spectrum and results obtained here awaiting for confirmation by more sophisticated approaches.

**IV. SUMMARY**

In conclusion, we have explored, for the first time, properties of a single impurity atom immersed in unitary Bose gas. Particularly, by utilizing original mean-field-like approach, which was shown to describe a behavior of Bose polaron in the dilute Bose gas on the qualitatively correct level, we have calculated the low-momentum parameters of the impurity spectrum, i.e., the binding energy and the effective mass in a wide region of the boson-impurity couplings. Although, the experimental realization of such systems is complicated by the meta-stable nature of a unitary Bose gas prepared in the so-called ‘upper branch’ [61], it will be interesting to test our predictions in Monte Carlo simulations. Another possible application of the presented approach is the problem of impurity in fermionic superfluids at unitary. The only modifications of the presented scheme required for such a calculations are the use of fermionic Bertsch parameter and $m$ should be identified with the doubled mass of Fermi particles.

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