Impurity self-energy in the strongly-correlated Bose systems

G. Panochko,1 V. Pastukhov,∗,2 and I. Vakarchuk2

1College of Natural Sciences, Ivan Franko National University of Lviv,
107 Tarnavski Str. Lviv, Ukraine
2Department for Theoretical Physics, Ivan Franko National University of Lviv,
12 Drahomanov Street, Lviv-5, 79005, Ukraine
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We proposed the non-perturbative scheme for calculation of the impurity spectrum in the Bose system at zero temperature. The method is based on the path-integral formulation and describes an impurity as a zero-density ideal Fermi gas interacting with Bose system for which the action is written in terms of density fluctuations. On the example of the 3He atom immersed in the liquid helium-4 a good consistency with experimental data and results of Monte Carlo simulations is shown.

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I. INTRODUCTION

The concept of Bose polaron, i.e., a single impurity particle immersed in the bosonic medium was originally introduced by Landau and Pomeranchuk [1] in the context of the 3He atom moving in the superfluid helium. In work [1] the general structure of low-energy impurity spectrum was established and shown to be dependent on two parameters, namely, a binding energy and the atom effective mass. The latter is known [2] to be uniquely related to the depletion of the superfluid component in the Bose system due to interaction with impurity. Similarly to the original polaron problem the interaction-induced localization is also a characteristic of the impurity in homogeneous bosonic environment [3,4]. Recent renewal of an interest to the Bose polaron problem is associated with growing opportunities of experimental techniques [5,6]. Particularly in Ref. [7] (see also [8]) the strongly-coupled impurity of 40K in the 87Rb Bose condensate was achieved. Besides their profound effect on the future study of mobile impurities in a bosonic medium and strongly interacting Bose systems these experimental results together with Monte Carlo simulations [9,10] can serve as a test for numerous theoretical predictions [11], namely, variational [12–15] diagrammatic [16–20] and recently published renormalization group [21,22] and Hartree-Fock-Bogoliubov [23] approaches.

In the present paper by means of the self-consistent Green’s function approach we have considered the impurity states in liquid 4He.

II. MODEL AND METHOD DESCRIPTION

Instead of studying the properties of a single impurity atom immersed in the non-ideal Bose system we consider a model of very dilute spin-polarized ideal Fermi gas interacting with the Bose condensed medium. This trick provides a possibility to use the advantages of the field-theoretical approaches in order to solve this problem. Adopting imaginary time path-integral formulation we write down the action of our system, which principally contains three terms

\[ S = S_0 + S_B + S_{\text{int}}. \]  

(2.1)

The first one

\[ S_0 = \sum_p \left( i\nu_p - \varepsilon_f(p) + \mu \right) \psi_p^* \psi_p, \]  

(2.2)

describes Fermi gas with dispersion \( \varepsilon_f(p) = \hbar^2 p^2 / 2m_f \) and chemical potential \( \mu \). Here \( \psi_p^*, \psi_p \) are complex Grassmann fields, four-vector \( P = (\nu_p, p) \) where \( \nu_p \) is the fermionic Matsubara frequency. The second term in Eq. (2.1) is the action of the interacting Bose particles. In order to simplify further consideration we adopt Popov’s density-phase formulation [24] with integrated out phase fields (see Ref. [25] for details). The appropriate action written in terms of density fluctuations \( \rho_K \) reads

\[ S_B = -\frac{1}{2} \sum_K D_0(K) \rho_K \rho_{-K} \]  

(2.3)

\[ -\frac{1}{3! \sqrt{\beta V}} \sum_{K_1+K_2+K_3 = 0} D_0(K_1, K_2, K_3) \rho_{K_1} \rho_{K_2} \rho_{K_3} \]

where \( K = (\omega_k, k) \) (note that \( k = 0 \) is omitted in every summation over the wave-vector), \( \omega_k \) is the bosonic Matsubara frequency. We also introduced bare vertex functions

\[ D_0(K) = \frac{m \omega_k^2}{\hbar^2 k^2} + \frac{\hbar^2 k^2}{4m \rho} + \nu(k), \]  

(2.4)

\[ D_0(K_1, K_2, K_3) = \frac{\hbar^2 k_1 k_2}{4m \rho^2} \left( 1 - \frac{\omega_k \omega_{k_2}}{\varepsilon_{k_1} \varepsilon_{k_2}} \right) + \text{perm.} \]  

(2.5)

Microscopic parameters characterizing Bose subsystem \( m, \rho \) and \( \nu(k) \) are the mass of particles, an equilibrium

*e-mail: volodyapastukhov@gmail.com
density and the Fourier transform of the two-body interaction, respectively. For further convenience notation \( \varepsilon_k = \hbar^2 k^2 / 2m \) is introduced. We impose periodic boundary conditions with volume \( V \) in a coordinate space and \( \beta = 1/T \) denotes the inverse temperature of the system. The Gaussian term in Eq. (2.3) represents the action of non-interacting Bogoliubov quasiparticles and the second term takes into account the simplest collisional processes of these excitations.

Finally the last term of action (2.1) that describes interaction between fermions and Bose particles is

\[
S_{int} = -\rho \tilde{\nu}(0) \sum_p \psi_p^\dagger \psi_p - \frac{1}{\sqrt{\beta V}} \sum_{k,P} \tilde{\nu}(k) \rho_k \psi_p^\dagger \psi_{p-K} \tag{2.6}
\]

where \( \tilde{\nu}(k) \) is the Fourier transform of Bose-Fermi two-body interaction and the first term can be absorbed by shifting of the chemical potential \( \tilde{\mu} = \mu - \rho \tilde{\nu}(0) \). Exploring the behavior of an impurity spectrum in the Bose condensate we have to consider fermionic single-particle Green’s function [26]

\[
G(P) = \langle \psi_p^\dagger \psi_p \rangle = \{ i\nu_p - \varepsilon_f(p) + \tilde{\mu} - \Sigma(P) \}^{-1}, \tag{2.7}
\]

(here \( \langle \ldots \rangle \) denotes statistical averaging with action (2.1)) where the exact self-energy \( \Sigma(P) \) is given by a single skeleton diagram depicted in Fig. 1. This is formally equivalent to

![Fig. 1: Diagrammatic representation of the self-energy \( \Sigma(P) \). The exact one-particle Green’s function is denoted by bold solid line with arrow. For the exact bosonic density-density correlator the dashed line is used. Dots stand for zero-order (light) and exact (black) vertices, respectively.](image)

act equation that determines the impurity Green’s function. The perturbation theory is build for boson-fermion vertex \( \Gamma(P, P - K) \) which also functionally depends on \( G(P) \) and \( \langle \rho_{KP} \rangle \). As a result, such a consideration leads to the system of coupled non-linear integral equations which should be solved self-consistently. Then, after analytical continuation in the upper complex half-plane \( \Sigma(P)_{\nu \rightarrow \nu+i0} = \Sigma_R(\nu, p) + i\Sigma_I(\nu, p) \) one obtains the energy \( \varepsilon_f^\dagger(p) = \varepsilon_f(p) + \Sigma_R(\varepsilon_f(p), p) - \Sigma_R(0, 0) \) of the impurity with momentum \( p \). Here we have taken into account the disappearance of radius of the Fermi sphere in the extremely dilute (one-particle) limit, i.e., \( \tilde{\mu} - \Sigma_R(0, 0) \propto 1/V^{2/3} \). The imaginary part \( \Sigma_I(\nu, p) \) of the self-energy determines the damping of impurity spectrum due to collisions with Bose particles. It is not difficult to obtain a diagrammatic representation for \( \Sigma_I(\nu, p) \) by applying of the unitarity conditions [27] for the diagram in Fig. 1. The resulting equation can be written in terms of spectral weights of impurity and phonons as well as the exact vertex \( \Gamma(P, P - K) \) for which we can use the exact estimation \( \Gamma(P, P) = \tilde{\nu}(0) + \partial \Sigma(P) / \partial \rho \) (the derivation is similar to that of Ref. [28]). From the general arguments it is clear that the creation of Bogoliubov excitations in the dilute Bose gas at very low temperatures is only possible when the impurity is moving through the superfluid with velocity \( \hbar p/m_f \) that is larger than the velocity \( c \) of sound propagation. In the liquid helium-4, however, due to presence of a roton minimum in the excitation spectrum this momentum threshold is restricted to a much smaller value [29].

### III. Self-Energy Calculations

The calculation scheme discussed previously is very hard for the practical realization, therefore some approximation procedure should be applied. We will assume that the information about the exact density-density correlation function of Bose system is known and treat only the fermionic self-energy perturbatively. In this way by choosing the appropriate form of \( \langle \rho_{KP} \rangle \) we are in position to predict the behavior of impurity immersed both in the strongly-correlated Bose system like liquid \( ^4 \)He as well as in the weakly-interacting Bose condensates of alkali atoms.

#### A. First-order results

On the one-loop level the self-energy calculation is relatively simple. Neglecting vertex corrections, i.e. \( \Gamma(P, P - K) = \tilde{\nu}(k) \), substituting simple ansatz for the exact Green’s function \( G(P) = [i\nu_p - \varepsilon_f^\dagger(p)]^{-1} \) and making use of the Feynman approximation for the density-density correlation function \( \langle \rho_{KP} \rangle = 2\rho \varepsilon_f / [\omega_k^2 + E_k^2] \) (here \( E_k = \varepsilon_k \alpha_k \), where \( 1/\alpha_k = S_k \) is the static structure factor of the Bose subsystem) we obtain in the low-temperature limit

\[
\Sigma^{(1)}(P) = -\frac{1}{V} \sum_k \rho \frac{\varepsilon_f^2(k)}{\alpha_k} \frac{1}{E_k + \varepsilon_f^\dagger(k + p) - i\nu_p}. \tag{3.8}
\]

We adopt the minimal substitution scheme with \( \varepsilon_f^\dagger(p) = \hbar^2 p^2 / 2m_f \), where the effective mass \( m_f \) should be calculated self-consistently. Such a choice of the impurity Green’s function simplifies further consideration providing that all observables depend on one parameter \( m_f \). It is also believed that this substitution is well-grounded when the major contribution to the integral in Eq. (3.8) is coming from the phonon region, i.e., when \( \tilde{\nu}(k) \) is the rapidly decreasing function of wave-vector. On the other hand, by choosing the skeleton graph expansion even in the simplest effective mass approximation we avoid the unphysical situation with appearance of the finite magnitude damping \( [15] \) for the motionless particle. Note, that we also neglect the renormalization of the quasiparticle residue \( Z^{-1}(p) = 1 - \partial \Sigma_{\varepsilon_f^\dagger(p)} / \partial \varepsilon_f^\dagger(p) \). The presence of \( Z(p) \) in our ansatz for the impurity
Green’s function (where there is no imaginary part in the self-energy) immediately brakes the particle number conservation law and enormously shifts the integral characteristics of the impurity atom, like energy.

B. Second-order results

The second-order diagrams for the self-energy are depicted in Fig. 2. They all stem from the boson-fermion vertex renormalization. We recall that in our field-theoretic skeleton graph expansion we have not to take into account the diagrams with the self-energy insertions. It is also understood that for the full self-consistency of the results one needs to solve the integral equation for \( G(P, P - K) \) in the appropriate approximation and then substitute it in the formula for the self-energy. In the language of Feynman’s diagrams it particularly means that all light dots which represent zero-order vertices with two fermionic and one bosonic lines should be painted in black, i.e., replaced by the exact one. But this program is very difficult for the practical realization. Moreover, in this case we would also have to substitute the exact three-legged bosonic vertex \( D(K, Q, S) \) in the impurity self-energy. The only information known about this vertex is the infrared asymptote \( D(0, 0, 0) = \frac{\partial}{\partial \rho} m e^2 \) and the ultraviolet behavior where it coincides with \( (2.5) \), which is not enough for the proper evaluation of \( \Sigma^{(2)}(P) \). Therefore, in these second-order calculations we continue to use our approximation scheme, where the Green’s function \( G(P) \) is determined by the effective mass only, and the impurity-bosonic vertex is treated perturbatively. The explicit result of these straightforward but nevertheless cumbersome calculations of \( \Sigma^{(2)}(P) \) at zero temperature is given in appendix.

IV. NUMERICAL CALCULATIONS AND DISCUSSION

In this work we considered the impurity states in the liquid \(^4\)He. This is historically the first example of a strongly-correlated Bose liquid for which the information about the structure of excitations is well-measured. The most natural and experimentally relevant choice of the impurity atom is \(^3\)He (or even \(^6\)He). Of course in the adopted approximations the results of numerical calculations depend on the form of the boson-impurity potential \( \hat{\nu}(k) \) only. In the adiabatic approximation the two-body interaction of \(^4\)He-\(^3\)He is the same as \(^4\)He-\(^3\)He, therefore we can easily express \( \hat{\nu}(k) \) via the static structure factor of the superfluid helium. In that way our calculations will not be restricted to the isotopes of helium, but with some assumptions the obtained formulae can be also used for the atoms of rare earth elements. Thus, varying the mass \( m_f \) we can study within our calculational method the observable properties of diverse types of impurity atoms immersed in the liquid \(^4\)He.

The simplest approximation for \( \hat{\nu}(k) \) is obtained through the comparison of Bogoliubov’s and Feynman’s spectra

\[
\hat{\nu}(k) = \xi_k(1/S_k^2 - 1)/2\rho.
\]  (4.9)

Such a procedure of determination of the two-body potential allows [32] to describe the properties of liquid helium-4 in the whole temperature region including second-order phase transition point. Now by calculating \( \Sigma_R(\varepsilon_f^\gamma(p), p) - \Sigma_R(0, 0) \) at small values of the wave-vector one derives the effective mass Fig. 3, which was computed numerically at equilibrium density \( \rho = 0.02185 \text{ Å}^{-3} \) of \(^4\)He. Then these curves were used for calculations of the impurity atom binding energy \( \mu = \rho \hat{\nu}(0) + \Sigma_R(0, 0) \). The latter is presented of the Fig. 4. The obtained within the first-order perturbation theory effective mass of \(^4\)He atom \( m_f^\gamma(1)/m_f = 1.41 \) can be compared to the result 1.58 of [33], where very similar self-consistent calculation scheme was used. Our second-order prediction for the effective mass of \(^3\)He \( m_f^\gamma(3/4)/m_f = 2.13 \) is in agreement with experimental values 2.18 [34], 2.15 [35], results of another theoretical studies 2.09 [36], diffusion 2.20(5) [37] and variational 2.06–2.07 [38] Monte Carlo calculations.
immersed in the Bose system. We applied our approach which is based on skeleton-graph expansion to the problem of impurity states in the liquid helium-4. In particular, the effective mass as well as binding energy of an impurity atom with helium-like interparticle potential are calculated. The obtained value for the hydrodynamic mass of the $^3$He atom immersed in a Bose liquid coincides well both with experiments and results of Monte Carlo simulations. Finally, our calculations can be easily extended onto the low-dimensional systems.

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VI. APPENDIX

In this section we present the explicit form of the second-order impurity self-energy. Actually, the result of calculations of two diagrams depicted in Fig. 2 is given. After simple integration over the Matsubara frequencies with the use of a residue theorem we obtain

$$
\Sigma^{(2)}(P) = \frac{1}{V^2} \sum_{k,s} \xi(k) \xi(s) \xi(|k+s|) \frac{1}{(E_s + \varepsilon_p^*(s - p) - i\nu_p) (E_{k+s} + \varepsilon_p^*(k + p) - i\nu_p)} \\
- \frac{1}{V^2} \sum_{k,s} \xi(k)^2 \xi^2(s) \xi(|k+s|) \frac{1}{(E_{k+s} + \varepsilon_p^*(k + s + p) - i\nu_p) (E_k + \varepsilon_p^*(k) - i\nu_p) (E_k + \varepsilon_p^*(k + p) - i\nu_p)} \\
+ \frac{1}{V^2} \sum_{k,s} \xi(k) \xi(s) \xi(|k+s|) \frac{D_+(k,s)}{E_{k+s} + \varepsilon_p^*(k + s + p) - i\nu_p} \\
\times \frac{1}{E_{k+s} + \varepsilon_p^*(k + s + p) - i\nu_p} \\
+ \frac{1}{V^2} \sum_{k,s} \xi(k) \xi(s) \xi(|k+s|) \frac{D_-(k,s)}{E_{k+s} + \varepsilon_p^*(k + s + p) - i\nu_p} \\
\times \frac{1}{E_{k+s} + \varepsilon_p^*(k + s + p) - i\nu_p},
$$

(6.10)

where the symmetric functions $D_\pm(k,s)$ read

$$
D_\pm(k,s) = \frac{\hbar^2}{2m} \left[ k(k + s)(\alpha_k - 1)(\alpha_{|k+s|} \pm 1) + s(s + k)(\alpha_s - 1)(\alpha_{|k+s|} \pm 1) \pm ks(\alpha_k - 1)(\alpha_s - 1) \right].
$$

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