Two-body effective potential between impurities in ideal BEC

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We exactly calculate the full temperature dependence of the Casimir-like forces appearing between two static impurities loaded in the ideal Bose gas below the Bose-Einstein condensation transition point. Assuming the short-ranged character of the boson-impurity interaction we show how to calculate properties of Bose system with arbitrary number of impurities immersed.

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\section{I. INTRODUCTION}

The presence of impurities in Bose-Einstein condensate (BEC) predetermines a number of experimentally observable phenomena, namely, formation of a single-impurity dressed quasiparticles which are referred to Bose polarons at low temperatures in one- \cite{1} and three-dimensional \cite{2,3} systems and at finite temperatures near the BEC transition point \cite{4}; creation of the Rydberg polaron \cite{5} in Sr condensate. A single ion immersed in BEC may be also used to probe \cite{6} the local atomic density distribution of host atoms. The theoretical investigations of properties of such an objects at finite temperatures are mostly focused on the exploration of the Bose polaron behavior near the superfluid phase-transition point \cite{7,9}, and on the investigation of impurity dynamics \cite{10,11}. Polaron can be also used for the low-temperature thermometry in BECs \cite{12}.

In real experimental conditions, however, the number of impurities is macroscopic nevertheless concentrations are typically small. Therefore, even when impurities are initially non-interacting (spin-polarised fermions, for instance), being immersed in the Bose environment they mutually interact via the effective boson-mediated potential. In general, this effective potential is the many-body one but when the concentration of impurities is small (i.e., average distance between exterior particles is large) it can be freely modelled by the pairwise interactions. Depending on a strength of the boson-impurity coupling the two-impurity system undergoes crossover behavior from two separate Bose polarons interacting via weak Yukawa-like potential \cite{13} through the bipolaron state \cite{14,15} at intermediate couplings to the Efimov trimer \cite{13,16,17} at strong boson-impurity attractions. It is interesting that the binding energy of trimers at unitary is suppressed \cite{18,19} by presence of a Bose condensate.

The medium-induced Casimir-like forces are of great importance in the condensed-matter physics \cite{20}. Being responsible for our understanding of numerous phenomena in many-body systems they have the most profound effect in low dimensions, particularly in 1D \cite{21,22,23}. In this context the simplest system for the visualization of the Casimir forces is two particles interacting with a free scalar field. This is a model of 1D crystal in the harmonic approximation, where the scattering of phonons on impurities leads to the induced long-range interaction between them. A behavior of the effective potential essentially differs for impurities with finite and infinite masses \cite{24}, namely, $\Phi_{\text{eff}}(R_{12}) \propto 1/R_{12}^3$ and $\Phi_{\text{eff}}(R_{12}) \propto 1/R_{12}$, respectively, and becomes exponential at finite temperatures \cite{25}. The appearance of interaction of the Casimir type can be also demonstrated in mixtures of quantum gases \cite{26}, where the effective attraction between ‘heavy’ bosons of $^{133}\text{Cs}$ mediated by degenerated Fermi gas of $^6\text{Li}$ atoms was observed. Theoretically this problem was studied in Ref. \cite{27} both for 2D and 3D cases.

The aim of present article is to explore the finite-temperature Casimir effect associated with the immersion of impurities in 3D ideal Bose gas. In general, a problem of induced forces in Bose systems is not well-studied, especially at finite temperatures. Few exceptions are the following: the perturbative consideration of the effective interaction between static impurities in the spin-orbit-coupled BEC \cite{28}, the detailed discussion of the Landau effective potential for two Bose polarons at absolute zero \cite{29}, and systems confined in 1D (or quasi-1D) geometries, which are now lively discussed and where the peculiarities of the induced interaction in the dilute limit are dictated by the characteristic scale, namely, the coherence length. For distances between impurities less than this scale the Casimir force behaviors exponentially \cite{30}, while decaying power-law-like at large inter-particle spacing \cite{31} with the boundary-conditions-dependent exponent \cite{32}. At that time, the finite-temperature fluctuations not only brake the quasi-long-range order in 1D bosonic systems but also change to exponential \cite{33} the large-distance behavior of the Casimir force.
II. FORMULATION

A. Statement of the problem

We consider a very simple model of a few static (infinite-mass) impurities immersed in ideal BEC. Although below we mainly focus on the one- and two-particle limits, the general calculation scheme is also applicable for an arbitrary number of impurities. Therefore the Hamiltonian of the system

\[ H = \sum_{\mathbf{k}, \mathbf{q}} (\varepsilon + \Phi(\mathbf{r}) ) \psi_{\mathbf{k}}^\dagger \psi_{\mathbf{q}}, \]  

(2.1)
is written down for this latter case, where \( \varepsilon = \frac{p^2}{2m} \) is the one-boson kinetic energy operator, and

\[ \Phi(\mathbf{r}) = \sum_{1 \leq j \leq N} g \delta(\mathbf{r} - \mathbf{R}_j), \]  

(2.2)
is the potential energy due to interaction with \( N \) impurities placed in positions \( \mathbf{R}_j \). Operators \( \psi_{\mathbf{k}}^\dagger \) (\( \psi_{\mathbf{k}} \)) are standard creation (annihilation) bosonic operators of particle with momentum \( \mathbf{k} \), and in (2.1) we used the plane-wave representation defined for large volume \( V \) with periodic boundary conditions imposed. The strength of boson-impurity interaction is controlled by bare coupling constant \( g \), which because of \( \delta \)-type interaction should be renormalized in final formulae \( \frac{1}{a} = \frac{m}{2\pi^2\hbar^2} - \frac{1}{V} \sum_{\mathbf{k}} \frac{1}{\epsilon_k} \) via \( s \)-wave scattering length \( a \).

The thermodynamics of Bose gas loaded in external potential (2.2) can be obtained in usual way. First, we have to solve the single-particle quantum mechanical problem

\[ \{ \varepsilon + \Phi(\mathbf{r}) \} |n \rangle = \mathcal{E}_n |n \rangle, \]  

(2.3)
and then straightforwardly apply the grand-canonical formalism with grand potential given by

\[ \Omega = T \sum_{\mathbf{k}} \ln \left[ 1 - e^{(\mu - \mathcal{E}_k)/T} \right], \]  

(2.4)
where \( \mu \) is the chemical potential that controls the number of bosons. Taking into account the invariance of trace we can equivalently rewrite \( \Omega \) in the plane-wave basis from now on we do not write down in \( \Phi(\mathbf{r}) \) the explicit dependence on \( \mathbf{r} \)

\[ \Omega = T \sum_{\mathbf{k}} \ln \left[ 1 - e^{(\mu - \mathcal{E}_k)/T} \right] |\mathbf{k} \rangle, \]  

(2.5)
or in a form more convenient for practical use

\[ \Omega = T \int d\omega D(\omega) \ln \left[ 1 - e^{(\mu - \omega)/T} \right], \]  

(2.6)
where the density of states \( D(\omega) \) is conventionally written through the one-particle Green’s function \( G_\omega \)

\[ D(\omega) = -\frac{1}{\pi} \sum_{\mathbf{k}} \text{Im} \langle \mathbf{k}|G_{\omega + i0}|\mathbf{k} \rangle, \quad G_\omega = \frac{1}{\omega - \varepsilon - \Phi} \]  

(2.7)
and integration is carried out in the semi axis where \( \omega - \mu > 0 \). So, the further consideration is fully devoted to calculations of the above-presented density of states. Furthermore, in the following we restrict ourselves to the thermodynamic limit, where both volume \( V \) and number of bosons \( N \) rapidly grow, while keeping density \( n = N/V \) of the system fixed. Demanding an additivity of the thermodynamic potential we assume that impurity does not change properties of Bose gas drastically, which particularly means that only scattering states will be accounted. The appearance of bound states at some region of parameters change will immediately lead to the collapse of bosons (in that case the macroscopic number of particles will be localized in a finite volume).

All peculiarities of the density of states can be figured out by computing the \( T \)-matrix

\[ T_\omega = \Phi + \Phi G^{(0)}_\omega T_\omega, \]  

(2.8)
which allows to represent Green’s function in terms of its zero-order counterpart \( G^{(0)}_\omega \)

\[ G_\omega = G^{(0)}_\omega + G^{(0)}_\omega T_\omega G^{(0)}_\omega, \quad G^{(0)}_\omega = \frac{1}{\omega - \mu}. \]  

(2.9)

Working with BECs and assuming the scattering nature of the ground state in a Bose gas with impurities, the zero-momentum term in formula for \( D(\omega) \) should be treated with a great care. First, it is more instructive to rewrite it as follows

\[ \langle 0|G_{\omega + i0}|0 \rangle = \frac{1}{\omega + i0} - \langle 0|T^{(0)}_0|0 \rangle, \]  

(2.10)
where the reduced \( T \)-matrix \( T^{(0)}_0 = \Phi + \Phi G^{(0)}_\omega Q_0 \).

Substitution in Eq. (2.5) leads us to the conclusion that the chemical potential of bosons with microscopic number of impurities reads

\[ \mu = \langle 0|T^{(0)}_0|0 \rangle. \]  

(2.11)

Note that \( \mu \) is of order \( 1/V \) when only few particles are immersed in a system below the critical temperature, and Eq. (2.10) guarantees only a leading-order asymptotics in \( 1/V \). Multiplied by number of bosons \( N \), the result (2.10) represent the impurities binding energy at \( T = 0 \). So, the problem is reduced to the calculations of the \( T \)-matrix of bosonic atom moving in the external potential produced by the static particles. In the two-impurity limit these calculations can be carried out to the very end

\[ V(\mathbf{k}|T^{(0)}_0|\mathbf{k}) = 2t_\omega \frac{1 + \Delta_{12}(R_{12}) \cos(kR_{12})}{1 - \Delta_{12}^2(R_{12})}, \]  

(2.12)
where \( R_{12} = R_1 - R_2 \) is the difference between positions of static particles and we made use of notations

\[ t_\omega^{-1} = \frac{m}{2\pi \hbar^2 a} - \frac{1}{V} \sum_{k \neq 0} \left( \frac{1}{\omega - \varepsilon_k} + \frac{1}{\varepsilon_k} \right). \]  

(2.13)
The evaluation of the above integrals in three spacial dimensions causes any problems and can be found in Appendix. With Eq. (2.11) in hands, which actually gives the density of states, we are free to calculate thermodynamics of the considered system.

The ground-state energy of our system can be also calculated in the plane-wave basis by applying the conventional many-body perturbation techniques directly to Hamiltonian (2.1). With the assumption that presence of impurities does not destroy uniformity of the Bose condensate and the lowest one-particle energy level again corresponds to wave-vector \( k = 0 \), the Hamiltonian reads

\[
H = N\langle0|\Phi|0\rangle + \sum_{k,q \neq 0}\langle k\Phi|q\rangle\psi_k^+\psi_q + \sqrt{N}\sum_{k \neq 0}\left(\langle k|\Phi|0\rangle\psi_k^+ + \langle 0|\Phi|k\rangle\psi_k\right),
\]

where both \( \psi_k^+ \), \( \psi_0 \) are replaced by a c-number \( \sqrt{N} \). Calculated to all orders of perturbation theory, the ground-state energy

\[
E_0 = N\langle0|\Phi|0\rangle + N\sum_{k \neq 0}\langle k|\Phi|k\rangle\frac{1}{-\varepsilon_k} + N\sum_{k,q \neq 0}\langle k|\Phi|q\rangle\frac{1}{-\varepsilon_q} + \ldots
\]

\[= N\langle0|T_0^0|0\rangle,
\]

collapses exactly to the diagonal element of the reduced \( T \)-matrix and reproduces (2.10).

An internal energy of the system at non-zero temperatures is derived by applying a standard relations to the grand potential, or by the quasi-particle-picture arguments

\[
E = N_0\langle0|T_0^0|0\rangle + \int d\omega \frac{\omega D^0(\omega)}{e^{(\omega - \mu)/T} - 1},
\]

where \( N_0 \) is the temperature-dependent number of particles in BEC and superscript near \( D(\omega) \) denotes that term with \( k = 0 \) is omitted in the density of states. This equation allows to obtain (see Appendix) the exact energy that Bose gas gains when two impurities are immersed in it at finite temperatures.

**B. Bound states**

In order to elucidate the limits of applicability of the above formal calculations we must analyze the one-boson bound-state problem. This can be directly done by searching for the \( T \)-matrix (2.11) poles at negative \( \omega \). For a single impurity, they are given by zeros of \( t_{\omega}^{-1} \), which lead to the fictitious pole with a simple mathematical expression \( \epsilon_1 = -\frac{\hbar^2}{2m a^2} \), valid for all positive \( a \). The appropriate one-boson Hamiltonian and the ground-state function read

\[
H = -\frac{\hbar^2}{2m}\nabla^2 + \frac{2\pi \hbar^2 \alpha}{m}\delta(r_1)\frac{\partial}{\partial r_1}, \quad \langle r|0\rangle_{N=1} \propto e^{-r_1/a}\langle r_1\rangle_{N=1}
\]

with shorthand notation \( r_1 = r - R_1 \) for relative boson-impurity position. The above potential energy is the well-known Huang-Yang pseudo-potential, which explicitly represents the Bethe-Peierls boundary condition. In the two-impurity case, the situation with the bound states is more interesting. Now poles, \( \epsilon_2 \), corresponding to bound states are given by two equations [13]

\[
1 - a\sqrt{2m|\epsilon_2|}/\hbar + \frac{a}{R_{12}}e^{-\epsilon_2}\sqrt{2m|\epsilon_2|}/\hbar = 0.
\]

For completeness, we also provide the bound-state wave functions [28], the appropriated Hamiltonian in this case is just a two-centered generalization of (2.17)

\[
\langle r|0\rangle_{N=2} \propto e^{-r_1\sqrt{2m|\epsilon_2|}/\hbar}e^{-r_2\sqrt{2m|\epsilon_2|}/\hbar}.
\]

A graphical representation of solutions for dimensionless quantity \( |\tilde{\epsilon}_2| = |\epsilon_2|/\left(\frac{\hbar^2}{2m R_{12}^2}\right) \) is plotted in Fig. 1 from
number of impurities that is typically produced in experiments and this number is significantly more than two. From the previous analysis is easy to figure out that for arbitrary number \( N \) of static particles the \( N \) wave functions that correspond to bound states are simply given by linear combinations of exponential functions of type \( e^{-r_j \sqrt{2m|\varepsilon_n|}/\hbar} \). In general, these \( N \) energies are complicated functions of relative distances \( R_{jj'} \) between impurities, but when \( a < 0 \) and all \( R_{jj'} \gg |a| \) they disappear. So, whole our previous discussion is plausible for systems with small concentration of uniformly-distributed impurities. The second question raises issue of the experimental visibility of bound states. At finite temperatures the Bose gas collapse dynamics is complicated and require separate investigation, but if we assume that system is initially prepared at very low temperatures without boson-impurity interaction and then this interaction is suddenly switched on, probability of the bound-state realization given by modulus squared of the wave-function overlap

\[
Z = \left| \langle \text{vac} | \psi_{n=0}^N \frac{(\psi_{k=0}^+)^N}{\sqrt{N!}} | \text{vac} \rangle \right|^2 \propto \left( \frac{a^3}{V} \right)^N , \tag{2.20}
\]
is very small. Therefore there is a belief that system remains in the uniform (scattering) BEC state for some time even for set of parameters when true ground state is the collapsed BEC. The obtained power-law behavior of overlap (2.20) which tends to zero very quickly with increasing number of surrounding particles is usually referred to the orthogonality catastrophe. In a case of fermionic bath this phenomenon is observed only in one-dimensional space. For the bosonic environments formed by non-interacting particles, however, such a behavior seems to be generic and independent of spacial dimensionality.

### III. RESULTS

Full information about the temperature dependence of energy of two impurities can be deduced by subtracting the internal energy of ideal Bose gas from Eq. (2.16) (see Appendix). The resulting energy \( \Delta E_2(R_{12}) \) associated with impurities is a complicated function of relative distance \( R_{12} \) but when the latter goes to infinity energy \( \Delta E_2(\infty) \) tends to constant, which is twice the binding energy of a single impurity

\[
\Delta E_1 = \frac{2\pi \hbar^2 a}{m} \left[ n + \int_0^\infty \frac{dk}{(2\pi)^2} \frac{k^2}{e^{k^2/\hbar} - 1} \right] (ak^2) \tag{3.21}
\]

Typical temperature behavior of \( \Delta E_1 \) is presented in Fig. 2, where \( T_0 \) is the BEC temperature and \( E_{MF} = 2\pi \hbar^2 |a| n/m \) is a modulus of the mean-field energy. We also built in Fig. 3 the one-particle energy at several fixed temperatures as a function of dimensionless coupling constant \( an^{1/3} \). The leading-order temperature correction scales like \( (an^{1/3})^2(T/T_0)^{5/2} \) when interaction is weak and \( (T/T_0)^{3/2} \) at unitarity \( |a| n^{1/3} \gg 1 \). The explicit formula for the two-impurity energy \( \Delta E_2(R_{12}) \) is more cumbersome therefore not written here. We can now define the effective potential energy between two impurities induced by the interaction with Bose particles as a difference of energies with fixed \( R_{12} \) and infinite (one-impurity limit) distances between static particles

\[
\Phi_{eff}(R_{12}) = \Delta E_2(R_{12}) - \Delta E_2(\infty). \tag{3.22}
\]

Potential (3.22) in BEC phase has two types of terms and their origin is readily seen from the general formula for energy (2.16) (see also Appendix). The first term is the temperature-independent one with a very simple
mathematical expression

\[
\Phi_{\text{eff}}(R_{12})|_{T \to 0} = \frac{2\pi \hbar^2 a}{m} n \times 2 \left[ \frac{1}{1 + a/R_{12}} - 1 \right],
\]

while the second term contains all thermal effects but can be calculated only numerically. Figure 4 displays the total impact of these two terms. Particularly, we have built the effective potential for only two temperatures, namely, \( T = 0 \) and \( T = T_0 \), because for all other temperatures the curves describing \( \Phi_{\text{eff}}(R_{12}) \) lie between those two. The presented in Fig. 4 graphs of function \( \Phi_{\text{eff}}(R_{12}) \) at various interaction strengths clearly demonstrate the tendency of the Casimir forces mediated by free bosons to increase the potential well with increasing of temperature.

IV. CONCLUSIONS

In summary, we have calculated in details the temperature-dependent energies associated with the immersion of one and two static impurities into ideal three-dimensional Bose-Einstein condensate. The simple and efficient method used here, allows the exact treatment of the problem and could serve a good starting point for possible extensions on case (i) of mobile impurities and (ii) interacting Bose environments. In the present article, however, the main emphasis was made on the Casimir effect that results in the boson-mediated effective impurity-impurity interaction and to a problem of the stability of the system against collapse. The latter question is very important from the point of view of preparation of such a mixture, because in contrast to non-interacting fermions, the ideal Bose gas is a substance with zero compressibility below the critical temperature. In this work we have shown that for small concentrations of uniformly-distributed impurities the system remains stable at least when the short-range boson-impurity interaction has an attractive character.

V. APPENDIX

For completeness we give explicit analytic formulae for the two-body boson-impurity \( T \)-matrix \( t_\omega \) and dimensionless function \( \Delta_\omega(R_{12}) \) introduced in main text

\[
t_\omega+i\theta = \frac{2\pi \hbar^2 a}{m} \frac{1}{1 - ak_{\omega+i\theta}},
\]

\[
\Delta_{\omega+i\theta}(R_{12}) = -\frac{a}{R_{12}} \frac{e^{-R_{12}k_{\omega+i\theta}}}{1 - ak_{\omega+i\theta}},
\]

where \( k_{\omega+i\theta} = \sqrt{2m|\omega|^2/h^2} \left( \theta(-\omega)[1-i\theta(\omega)] \right) \) with \( \theta(x) \) being the Heaviside step function.

Equation (2.16) contains two types of non-vanishing terms in the thermodynamic limit, namely, the ideal Bose gas contribution which is of order \( V \) and the terms of order unity corresponding to the impurities

\[
E = N_0 \langle 0|T_0^0|0 \rangle + \int_\mu d\omega \frac{\omega}{e^{(\omega - \mu)/T} - 1} \times -\frac{1}{\pi} \sum_{k \neq 0} \text{Im} \left\{ \frac{1}{\omega + i\theta - \epsilon_k} + \frac{\langle k|T_{\omega+i\theta}^0|k \rangle}{(\omega + i\theta - \epsilon_k)^2} \right\}.
\]

Shifting the integration limits, recalling that the chemical potential \( \mu = \langle 0|T_0^0|0 \rangle \propto 1/V \) in the BEC phase and
picking up terms of order unity we obtain the energy associated with impurities

$$\Delta E_N = N\langle 0 | T_0^0 | 0 \rangle + \int_0^\infty d\omega \frac{\omega}{e^{\omega/T} - 1} \times \frac{-1}{\pi} \sum_{k \neq 0} \text{Im} \left\{ \frac{\langle k | T_{\omega + i0}^0 | k \rangle - \langle 0 | T_0^0 | 0 \rangle}{(\omega + i0 - \varepsilon_k)^2} \right\}. \quad (5.24)$$

Integration over the wave-vector in Eq. (5.24) is simple in a case of two static particles

$$\frac{-1}{\pi} \sum_{k \neq 0} \text{Im} \left\{ \frac{\langle k | T_{\omega + i0}^0 | k \rangle - \langle 0 | T_0^0 | 0 \rangle}{(\omega + i0 - \varepsilon_k)^2} \right\} = - \left( \frac{m}{\pi \hbar^2} \right) \text{Im} \frac{1}{k_{\omega + i0}} \times \left\{ t_{\omega + i0} \left( 1 + \Delta_{\omega + i0}(R_{12}) e^{-R_{12} k_{\omega + i0}} \right) - t_0 \right\}.$$ 

Substitution in Eq. (5.24) gives the energy $\Delta E_2(R_{12})$ as a function of temperature and relative distance $R_{12}$ between particles. Putting $R_{12} \to \infty$ we recover the doubled binding energy of a single impurity $\Delta E_1(\infty) = 2\Delta E_1$, with $\Delta E_1$ presented in main text.

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