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Trapped Ideal Bose Gas with a Few Heavy Impurities

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Abstract: In this article, we formulate a general scheme for the calculation of the thermodynamic properties of an ideal Bose gas with one or two immersed static impurities, when the bosonic particles are trapped in a harmonic potential with either a quasi-1D or quasi-2D configuration. The binding energy of a single impurity and the medium-induced Casimir-like forces between the two impurities are numerically calculated for a wide range of temperatures and boson–impurity interaction strengths.

Keywords: induced forces; trapped Bose gas; Bose polaron

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1. Introduction

The recent activity in the research field of induced forces between particles immersed in bosonic media is mostly stimulated by a rapid development of Bose polaron studies in 3D [1–29], in 1D [30–36] and in 2D [37–39] over the past decade. Particularly important to the problem of induced forces between immersed atoms in a bosonic medium is the Bose bipolaron [40–46]; the problem of two (typically mutually non-interacting) impurities in a dilute Bose gas. In realistic systems, the boson–boson interaction does not allow the exact solution of the problem even in the limit of a single impurity, and only the universal tail of the induced potential at a large separation between immersed particles is accessible [47–53]. An exception is media formed by non-interacting particles, where all details of the (in general $\mathcal{N}$-body) effective interaction can be obtained for point-like impurities. For free fermions, the latter leads to the famous Ruderman–Kittel–Kasuya–Yosida potential. Its bosonic analogue together with the three-body inter-impurity potential were recently studied [54] below the Bose–Einstein condensation (BEC) transition temperature in three dimensions. Thanks to the simplicity of the bosonic ground state in the non-interacting limit, the mean-field predictions [55–59] for the energy of this system with an arbitrary number of point-like impurities coincide with the exact results. The present paper generalizes these exact findings on the trapped ideal Bose gases with quasi-one-dimensional (quasi-1D) and quasi-two-dimensional (quasi-2D) geometries. There are two known facts about such low-dimensional systems: first, the BEC exists only in the ground state, and secondly, the low-energy boson–impurity scattering amplitudes vanish in 1D and 2D. These all lead to a very peculiar behaviour; bosons do not experience the presence of exterior static particles at absolute zero, and the effect of impurities is only visible in the finite temperature thermodynamics of the system.

2. Formulation

We consider a system of a macroscopic number N of non-interacting bosons of mass m with a few $\mathcal{N}$ static (infinite-mass) impurities. The 3D system is assumed to be under external harmonic confinement in one or two directions, and for simplicity, the boson–impurity interaction is taken to be the zero-range s-wave Huang-Yang pseudo-potential $\Phi(\mathbf{r}) = g\delta(\mathbf{r})\frac{\partial}{\partial r}r$. Here, $g = 2\pi\hbar^2 a/m$ with a is the s-wave scattering length. Because there are no interactions between bosons, the ground state of the system can be the non-thermodynamic one. This happens when the boson bind to the $\mathcal{N}$ impurities. Then, their wave-function is independent of the length in the quasi-1D and the area in the quasi-2D cases of non-confined directions. Before we can proceed with the thermodynamic limit, where the number of bosons and the volume of non-confined directions approach infinity in such as manner that the number density is constant, it is very important to reveal all bound states of a boson in the external 'field' of the impurities.

2.1. One-Body Problem

We consider the problem of a single trapped boson interacting with a few infinite-mass impurity particles. The appropriate Hamiltonian is specified as follows

$$h = -\frac{\hbar^2}{2m}\nabla_r^2 + V(\mathbf{r}) + \sum_{1\le\alpha\le\mathcal{N}} \Phi(\mathbf{r}-\mathbf{R}_\alpha), \quad (1)$$

where $V(\mathbf{r}) = \frac{m\omega^2}{2}z^2$ for quasi-2D, and $V(\mathbf{r}) = \frac{m\omega^2}{2}(y^2+z^2)$ for quasi-1D geometries, with ω being the frequency of the harmonic trapping. The set $\{\mathbf{R}_\alpha\}$ represents the three-dimensional positions of impurities. An amazing fact about Hamiltonian (1) with pseudo-potential $\Phi(\mathbf{r})$ is that it is exactly solvable for an arbitrary number of impurities. Furthermore, the proposed approach can be applied for any external potential $V(\mathbf{r})$ (for instance, the linear one [60]) with known eigenvalues ε_q, where q is the set of quantum numbers and appropriately normalized wave-functions $\phi_q(\mathbf{r})$, i.e.,

$$-\frac{\hbar^2}{2m}\nabla_r^2\phi_q(\mathbf{r}) + V(\mathbf{r})\phi_q(\mathbf{r}) = \varepsilon_q\phi_q(\mathbf{r}), \quad (2)$$

In those directions where the trapping potential is absent, we apply periodic boundary conditions with large length-scale L. Here, we are only interested in the bound states of a boson in the presence of $\mathcal{N}$ impurities, so let us define the auxiliary function

$$F_\nu(\mathbf{r},\mathbf{r}') = \sum_q \frac{\phi_q(\mathbf{r})\phi_q^*(\mathbf{r}')}{\varepsilon_q - \nu}, \quad (3)$$

which is the Green function of the differential operator $-\frac{\hbar^2}{2m}\nabla_r^2 + V(\mathbf{r}) - \nu$. The general solution of the bound-states problem can be readily constructed for an arbitrary number $\mathcal{N}$ of impurities

$$\Psi_{\mathcal{N}}(\mathbf{r}) = \sum_{1\le\alpha\le\mathcal{N}} A_\alpha F_{\epsilon_{\mathcal{N}}}(\mathbf{r},\mathbf{R}_\alpha), \quad (4)$$

where the $\{\mathbf{R}_\alpha\}$-dependent constants $\{A_\alpha\}$ are subject to the boundary conditions and determined by a system of linear homogeneous equations

$$\left\{1 + g\frac{\partial}{\partial r} rF_{\epsilon_{\mathcal{N}}}(\mathbf{r}+\mathbf{R}_\alpha,\mathbf{R}_\alpha)\right\}_{\mathbf{r}=0} A_\alpha + \sum_{\beta\ne\alpha} F_{\epsilon_{\mathcal{N}}}(\mathbf{R}_\alpha,\mathbf{R}_\beta)A_\beta = 0. \quad (5)$$

Note that the wave-function (4) is square-integrable even in free space. The non-trivial solutions of this system of coupled equations correspond to the zeros of its determinant. In general, these calculations must be performed numerically, but for $\mathcal{N} = 1$ we have

$$1 + g\left\{\frac{\partial}{\partial r} rF_{\epsilon_1}(\mathbf{r}+\mathbf{R}_1,\mathbf{R}_1)\right\}_{\mathbf{r}=0} = 0, \quad (6)$$

while for $\mathcal{N} = 2$ we have

$$\left[\frac{1}{g} + \left\{\frac{\partial}{\partial r} r F_{\epsilon_2}(\mathbf{r}+\mathbf{R}_1, \mathbf{R}_1)\right\}_{\mathbf{r}=0}\right]\left[\frac{1}{g} + \left\{\frac{\partial}{\partial r} r F_{\epsilon_2}(\mathbf{r}+\mathbf{R}_2, \mathbf{R}_2)\right\}_{\mathbf{r}=0}\right] - [F_{\epsilon_2}(\mathbf{R}_1, \mathbf{R}_2)]^2 = 0, \tag{7}$$

where we used the fact that $F_{\epsilon_2}(\mathbf{r}, \mathbf{r}')$ is a symmetric function of its arguments for real energies ϵ_2. We see that ϵ_1 and ϵ_2, because of the partially broken continuous translation symmetry, depend on $\mathbf{R}_1$ and $\mathbf{R}_1, \mathbf{R}_2$, respectively. Recall that without trapping, potential ϵ_1 is independent of position $\mathbf{R}_1$ of impurity, while ϵ_2 is a function of distance $|\mathbf{R}_1 - \mathbf{R}_2|$.

2.2. Many-Body Consideration

The considered system allows for all the bosons to be in the same bound state. The total energy of the system in these collapsed BEC states is simply given by $N\epsilon_{\mathcal{N}}$. In the following, however, we mainly focus on configurations of impurities, where there are no bound states in the single-boson spectrum and the ground state of the $N + \mathcal{N}$ particle system is very similar to the one without impurities. Aiming at the finite-temperature description of the Bose gas with immersed impurities, we apply the path-integral formulation with the Euclidean action

$$S = \sum_{q,n}\{i\nu_n - \varepsilon_q + \mu\}\psi^*_{q,n}\psi_{q,n} - \sum_{q,q',n} g_{qq'}\psi^*_{q,n}\psi_{q',n} \tag{8}$$

written down on a one-body basis $\phi_q(\mathbf{r})$. In (8), ε_q denotes the shifted one-particle energies such that $\varepsilon_{q=0} = 0$ in the lowest state $q = 0$; ν_n and μ stand for the Matsubara frequencies ($\nu_n = 2\pi nT$, where $n = 0, \pm 1, \pm 2, \ldots$ and T is the temperature of the system) and the bosonic chemical potential, respectively. The latter fixes the density of the Bose gas. The couplings

$$g_{qq'} = \int d\mathbf{r}\phi^*_q(\mathbf{r}) \sum_{1\le\alpha\le\mathcal{N}} \Phi(\mathbf{r} - \mathbf{R}_\alpha)\phi_{q'}(\mathbf{r}), \tag{9}$$

represent the matrix elements of the boson–impurities interaction. One way [61] of dealing with (8) is to introduce auxiliary fields that split, by means of the Hubbard–Stratonovich transformation, the last term of the action and then integrate out the bosonic fields $\psi_{q,n}$. The remaining effective action of the auxiliary fields is Gaussian, so the integrations can be performed analytically. Here, however, we provide a somewhat different approach by calculating the thermal average $\langle\psi_{q,n}\psi^*_{q',n}\rangle$ explicitly. With this correlator in hand, we can obtain an equation that relates the chemical potential to the equilibrium number of bosons

$$N = \lim_{\tau\to+0} T\sum_{q,n} e^{i\nu_n\tau}\langle\psi_{q,n}\psi^*_{q,n}\rangle, \tag{10}$$

and taking into account the 'equation of motion' generated by (8), $-\langle\psi^*_{q',n}\delta S/\delta\psi^*_{q,n}\rangle = \delta_{qq'}$

$$\{\varepsilon_q - \mu - i\nu_n\}\langle\psi_{q,n}\psi^*_{q',n}\rangle + \sum_{q''} g_{qq''}\langle\psi_{q'',n}\psi^*_{q',n}\rangle = \delta_{qq'}, \tag{11}$$

the internal energy of the system with $\mathcal{N}$ impurities reads

$$E_{\mathcal{N}} = \mu N + \lim_{\tau\to+0} T\sum_{q,n} e^{i\nu_n\tau} i\nu_n\langle\psi_{q,n}\psi^*_{q,n}\rangle. \tag{12}$$

Being interested only in the diagonal element of correlator $\langle\psi_{q,n}\psi^*_{q',n}\rangle$, we can adopt the Dyson-like form

$$\langle\psi_{q,n}\psi^*_{q,n}\rangle^{-1} = \varepsilon_q - \mu - i\nu_n + \mathcal{T}_{qq,n}, \tag{13}$$

found in Ref. [62]. Here, $\mathcal{T}_{qq,n}$ plays the role of the self energy, which is equal to the diagonal matrix element of the reduced t-matrix determined by the following equation

$$\mathcal{T}_{qq',n} = g_{qq'} - \sum_{q''\neq q} \frac{g_{qq''}\mathcal{T}_{q''q',n}}{\varepsilon_{q''} - \mu - i\nu_n}. \tag{14}$$

Similarly to the translationally invariant system of bosons and impurities [54], the structure of the solution can be guessed by iterating Equation (14). By making use of the notation $\mathcal{T}_{qq',n} = \sum_{\alpha,\beta} \phi^*_q(\mathbf{R}_\alpha)T_{\alpha\beta}\phi_{q'}(\mathbf{R}_\beta)$ and plugging it in Equation (14), we obtain the linear equation for the matrix $T_{\alpha\beta}$

$$\left[\frac{1}{g} + \left\{\frac{\partial}{\partial r} r F_{\mu+i\nu_n}(\mathbf{r}+\mathbf{R}_\alpha, \mathbf{R}_\alpha)\right\}_{\mathbf{r}=0}\right] T_{\alpha\beta} + \sum_{\gamma\neq\alpha} F_{\mu+i\nu_n}(\mathbf{R}_\alpha, \mathbf{R}_\gamma)T_{\gamma\beta} = \delta_{\alpha\beta}. \tag{15}$$

This finishes the formal part of our calculations in the many-body limit at temperatures above the Bose–Einstein condensation (BEC) point.

There is no BEC at finite temperatures for the considered system in quasi-1D or quasi-2D. Here, we do not assume any special thermodynamic limit, where the frequency of the trapping potential approaches zero together with $N \to \infty$. It is only assumed that $N/L^2 = \text{const}$ in quasi-2D and $N/L = \text{const}$ in quasi-1D. Note that the adopted calculation scheme can be adjusted for any other external potentials, which can support the BEC transition of the system at finite temperatures. In the BEC phase, which in our case is rather interesting from the methodological point of view, one has to modify the above consideration. Keeping in mind the restrictions on the configurations of impurities that do not provide the boson–impurity bound states, we have to single out the Bose condensate contributions to the action (8) $\psi_{q,n} = \sqrt{N_0/T}\delta_{q,0}\delta_{n,0} + \psi_{q,n}(1-\delta_{q,0})$ (and same for $\psi^*_{q,n}$)

$$\begin{aligned} S = {} & \frac{N_0}{T}(\mu - g_{00}) + \sum_{q\neq 0,n} \{i\nu_n - \varepsilon_q + \mu\}\psi^*_{q,n}\psi_{q,n} \\ & -\sqrt{\frac{N_0}{T}} \sum_{q\neq 0} \left\{g_{q0}\psi^*_{q,0} + \text{c.c.}\right\} - \sum_{q,q'\neq 0,n} g_{qq'}\psi^*_{q,n}\psi_{q',n} \end{aligned} \tag{16}$$

where N_0 represents the number of bosons in BEC. Indeed, the total number of particles (10) now implies

$$N = N_0 + \lim_{\tau\to+0} T \sum_{q\neq 0,n} e^{i\nu_n\tau}\langle\psi_{q,n}\psi^*_{q,n}\rangle, \tag{17}$$

Similar to the way Equation (11) was obtained, we can write down for $q, q' \neq 0$

$$\{\varepsilon_q - \mu - i\nu_n\}\langle\psi_{q,n}\psi^*_{q',n}\rangle + \sqrt{\frac{N_0}{T}}\delta_{n,0}g_{q0}\langle\psi^*_{q',0}\rangle + \sum_{q''\neq 0} g_{qq''}\langle\psi_{q'',n}\psi^*_{q',n}\rangle = \delta_{qq'}, \tag{18}$$

where the non-zero average $\langle\psi^*_{q,0}\rangle$ appears due to presence of impurities. Physically, the quantity $\langle\psi^*_{q,0}\rangle$ accounts for the deformation of the lowest-energy single-boson wave function in the external potential of point-like impurities. The average $\langle\psi^*_{q,0}\rangle$ of the static part of the bosonic fields can be calculated by using Equation (18), or equivalently derived from $-\langle\delta S/\delta\psi_{q,0}\rangle = 0$

$$\{\varepsilon_q - \mu\}\langle\psi^*_{q,0}\rangle + \sqrt{\frac{N_0}{T}}g_{0q} + \sum_{q'\neq 0}\langle\psi^*_{q',0}\rangle g_{q'q} = 0. \tag{19}$$

It is straightforward to find the solution of the above equation $\langle \psi^*_{q,0} \rangle = -\sqrt{N_0/T}\mathcal{T}_{0q,0}/(\varepsilon_q - \mu)$, and by minimizing the grand potential with respect to N_0 we have

$$\mu - g_{00} - \frac{1}{2}\sqrt{\frac{T}{N_0}} \sum_{q \neq 0} \left\{ g_{q0} \langle \psi^*_{q,0} \rangle + \text{c.c.} \right\} = 0. \tag{20}$$

Combining with the average $\langle \psi^*_{q,0} \rangle$, one obtains an equation for the chemical potential below the BEC transition temperature

$$\mu = g_{00} - \sum_{q \neq 0} \frac{\mathcal{T}_{0q,0} g_{q0}}{\varepsilon_q - \mu} = \mathcal{T}_{00,0}. \tag{21}$$

Note that $\mu = \mathcal{T}_{00,0}$ can be obtained from the condition of having a pole in correlator (13) at zero Matsubara frequency and $q \to 0$. For our discussion, ($N \gg \mathcal{N}$) the chemical potential can be ommited in $\mathcal{T}_{00,0}$. Remarkably, the formula for the internal energy of the system in the BEC phase is very similar to Equation (12), except that the zero mode in the sum over q has been omitted.

3. Results

It is natural to start the discussion of our results with the bound states of a single boson in the presence of impurities. The energies of these bound states determine the thermodynamic stability of the many-body system. A detailed analysis of the single-boson bound states both in quasi-1D and quasi-2D geometries were previously performed in Refs. [63,64], while here we mostly focus on the case with two impurities. The numerical solutions to Equation (7) in the quasi-1D and quasi-2D cases are presented in Figures 1 and 2, respectively.

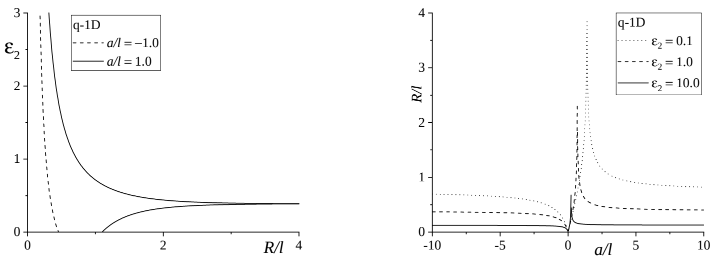

Figure 1. Left panel: Contour graph of the bound states ($\varepsilon_2 = |\epsilon_2|/\hbar\omega$) energy of a single boson with two static impurities in quasi-1D geometry as a function of impurity separation R and s-wave scattering length (in units of the oscillator length $l = \sqrt{\hbar/m\omega}$). Right panel: bound state energies as a function of separation R at $a/l = 1.0$ (solid lines) and $a/l = -1.0$ (dashed line).

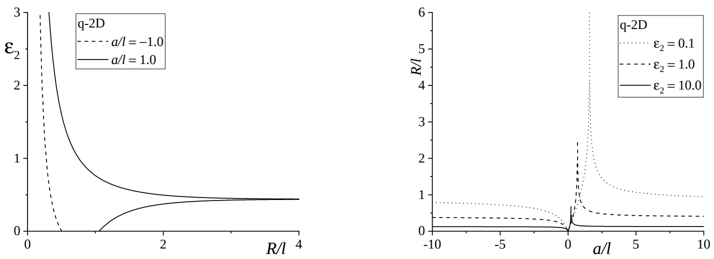

Figure 2. Same as in Figure 1 but for the quasi-2D case.

In order to understand the form of the bound-state energy surface, we plotted the lines of equal ϵ_2 and R-dependence of ϵ_2 at a fixed scattering length. Note that in both quasi-1D and quasi-2D, both impurities are located at the minimum of the harmonic potentials (i.e., on the x-axis in quasi-1D geometry and in the xy-plane in quasi-2D case) because otherwise the bound states and energies are exponentially small compared to $\hbar\omega$. It is readily seen in Figures 1 and 2 that the qualitative picture is the same for the two geometries. There are at most two bound states for $a > 0$ and at most one for $a < 0$. If we increase the number of impurities to $\mathcal{N}$, there will be at most $\mathcal{N}$ branches of bound states for $a > 0$ and maximally $\mathcal{N} - 1$ branches of bound states for negative as. This distribution of branches is completely analogous [54] to the translation invariant three-dimensional case. For both quasi-1D and quasi-2D, the small-R behaviours of the binding energy of the $a > 0$ and $a < 0$ branches are universal, Efimov-like, and approach $\varepsilon_2 = -\frac{\hbar^2 W^2(1)}{2mR^2}$, with $W(1) = 0.5671\ldots$ and a/l of order unity.

In quasi-1D and quasi-2D cases at zero temperature, if all bosons are not in the bound state they are insensitive to the presence of static impurities. This happens because the 1D and 2D t-matrices vanish for a boson, colliding with an impurity at zero collision energy, and only thermally stimulated bosons that scatter from impurities affect the energy of the system at finite temperatures. Another way to provide a non-zero population of excited states (and consequently, non-zero corrections to energy associated with the immersion of impurities) is to turn on the interaction between bosons [51].

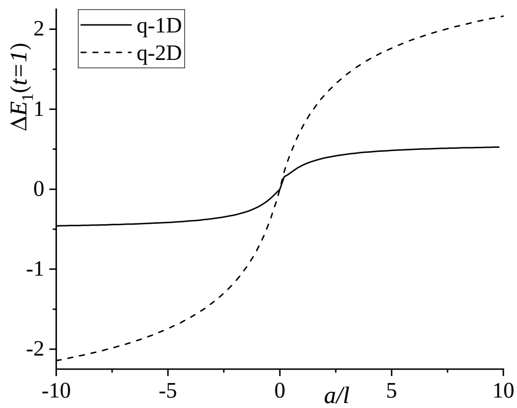

Figure 3. A single impurity contribution (in units of $\hbar\omega$) to the internal energy of quasi-1D and quasi-2D Bose gases at finite temperature $t = T/\hbar\omega = 1$.

In Figure 3 we plotted a typical dependence of the correction to the internal energy, i.e., $E_1 - E_1|_{a=0}$, of an ideal Bose gas caused by a single impurity as a function of the s-wave scattering length a in quasi-1D and quasi-2D geometries at temperature $t = T/\hbar\omega = 1$ and at fixed densities of quasi-1D and quasi-2D Bose gases of $n_{1D}l = 1$ and $n_{2D}l^2 = 1$, respectively. It should be noted that in the case of an ideal Bose gas, the only physical region is $a < 0$, where there is no bound states formation. However, if we assume any weak repulsion between bosons with the coupling g_b, the collapse of the system will be prevented. Indeed, the decrease of energy by $N\epsilon_1$ due to the bound state formation of N bosons will be accompanied by its enormous increase by $\propto N^2 g_b/(al^2)$ in quasi-1D and $\propto N^2 g_b/(a^2 l)$ in quasi-2D, due to boson–boson interaction. Our calculations, therefore, can be extended to impurities immersed in Bose gas with any weak repulsion that does not considerably change the properties of Bose gas itself, but prevents the collapse on impurities. Although, the general behaviour of the curves is qualitatively the same, the spatial dimensionality affects the magnitude of the correction.

We have also analyzed the temperature dependence of the one-impurity correction to the thermodynamics of an ideal Bose gas at the fixed scattering length of $a = \pm l$ in quasi-1D and quasi-2D in Figures 4 and 5, respectively.

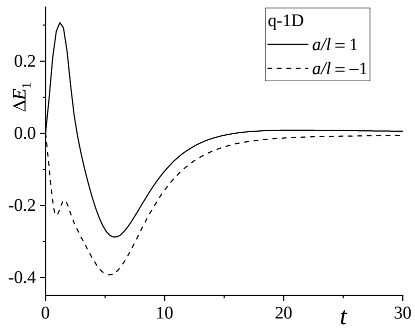

Figure 4. Temperature-dependence of the effect of a single impurity contribution on the internal energy (in units of $\hbar\omega$) of a quasi-1D ideal Bose gas.

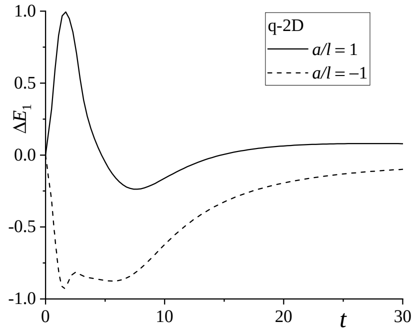

Figure 5. Same as in Figure 4, but for quasi-2D geometry.

Two important conclusions of these calculations are that the one-impurity correction depends non-monotonically on the temperature, and the character of the curves is different for attractive ($a < 0$) and repulsive ($a < 0$) boson–impurity interactions. We believe that the non-monoticity is due to the presence of the trapping potential because such a behaviour was not observed [54] in the 3D case, at least in the BEC region.

For the determination of the effective induced two-body potential between infinitely heavy particles, we calculate the internal energy Equation (12) of the bosonic system with two immersed impurities, set at a separation R one from another, and subtract the double correction to the internal energy of the system caused by a single impurity. In other words, we subtract the two-impurity energy with $R \to \infty$

$$\Phi_{\text{eff}}(R) = E_2 - E_2|_{R\to\infty}. \tag{22}$$

The results of the numerical calculations of $\Phi_{\text{eff}}(R)$ for the quasi-1D and quasi-2D cases are presented in Figures 6 and 7, respectively. Data are shown for two values of the scattering length and three temperatures. The physical region for an ideal Bose gas is again restricted to $a < 0$ and large R. However, any weak inter-boson repulsion extends this region to arbitrary Rs and signs of a. Let us make two comments about the behaviour of $\Phi_{\text{eff}}(R)$. First, it is seen that in both quasi-1D and quasi-2D, the character of the curves is quantitatively similar for the same set of parameters, and visible discrepancies only appear in the high-temperature region, as shown by comparing the y axes of the insets in Figures 6 and 7. In order to visualize this pattern, we plotted $\Phi_{\text{eff}}(R = 0.1l)$ in Figure 8 at various temperatures. Secondly, as a function of temperature, the effective two-body potential changes its sign from repulsive at low temperatures to attractive in the high-temperature region.

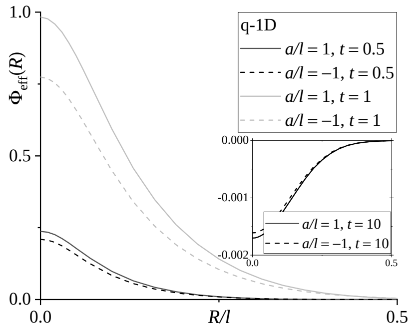

Figure 6. The effective medium-induced two-body potential (in units of $\hbar\omega$) as function of separation R between two static impurities immersed in a quasi-1D ideal Bose gas. Curves are shown for $a/l = \pm 1$ and $t = T/\hbar\omega = 0.5$, 1, and 10.

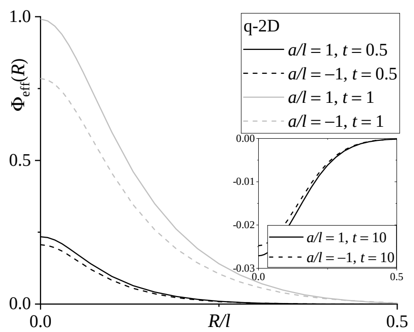

Figure 7. Same as in Figure 6, but for the quasi-2D geometry.

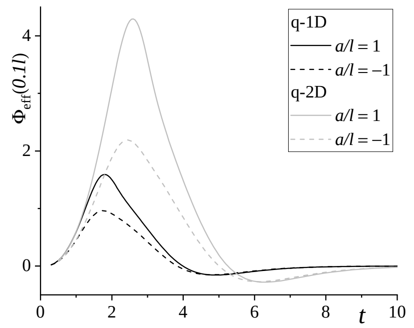

Figure 8. Temperature dependence of the effective impurity–impurity potential at $R = 0.1l$.

The obtained curves suggest the emergence of the thermally stimulated two-body bound state of impurities with finite (but large) masses, but to find the solution to this problem, one needs to go beyond the approximation of static impurities.

4. Summary

In conclusion, we have presented a detailed analysis of the effect of one and two static impurities on the properties of the harmonically trapped ideal quasi-1D and quasi-2D Bose gases. Within the assumption of a short-range boson–impurity interaction, the formulated scheme allows us to calculate the thermodynamics of the system in any external potential and with an arbitrary number of impurities. In particular, we have elucidated the dependence of the energy of a single impurity immersed in the quasi-low-dimensional trapped Bose gas on the temperature and interaction strength. The calculations of the medium-induced effective potential between two impurities in the system of free bosons revealed an interesting behaviour: repulsion at low temperatures that changes to attraction in the high-temperature limit. As a byproduct of this study, we have identified the bound states of a single particle interacting through the Huang-Yang pseudopotential with two static impurities separated by arbitrary distances in quasi-1D and quasi-2D geometries. Our results should also be valid in the case of a non-zero interaction between bosons, but when the system is extremely dilute [65].

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