

**Phonon-mediated Casimir interaction between finite-mass impurities**

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The Casimir effect, a two-body interaction via vacuum fluctuations, is a fundamental property of quantum systems. In solid state physics it emerges as a long-range interaction between two impurity atoms via virtual phonons. In the classical limit for the impurity atoms in  $D$  dimensions the interaction is known to follow the universal power law  $U(r) \sim r^{-D}$ . However, for finite masses of the impurity atoms on a lattice, it was predicted to be  $U(r) \sim r^{-2D-1}$  at large distances. We examine how one power law can change into another with an increase of the impurity mass and in the presence of an external potential. We provide the exact solution for the system in one dimension. At large distances indeed  $U(r) \sim r^{-3}$  for finite impurity masses, while for the infinite impurity masses or in an external potential it crosses over to  $U(r) \sim r^{-1}$ . At short distances the Casimir interaction is not universal and depends on the impurity mass and the external potential.

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In his pioneering work [1], Casimir showed that a change of the zero-point energy due to a perturbation of the electromagnetic fluctuations by two neutral metallic plates leads to observable forces between these plates. In fact, this is only one example of the broad class of phenomena, which are based on the concept of the perturbation of long-range fluctuations, e.g., Goldstone modes in the media with broken symmetry. Nowadays, this effect, named after Casimir, can be encountered in various fields of physics, chemistry, and biology [2–8]. For instance, in high-energy physics the existence of the Casimir effect sets natural constraints on the Yukawa forces, appearing due to the exchange of light elementary particles, and/or extra-dimensional physics [9]. In cosmology the Casimir effect helps to interpret the cosmological constant for a scalar field [10–12]. In chemistry, in particular, it is used to explain the interactions of molecules [13,14]. In biology, the Casimir interaction is, for instance, found to be responsible for the organization of the bilayer structure of cell membranes [15].

In condensed matter physics the effect of the Casimir interaction is extensively discussed with respect to the interaction of conducting surfaces [16], graphene and conducting plates [17], mesoscopic particles in a critical fluid through critical fluctuations [18], and ultracold atomic gases [19–23].

In the latter case it is possible to study the Casimir interaction in ultraclean bosonic or fermionic gases on tunable lattices with tunable spatial dimensionality and interaction strength. In this context, one-dimensional (1D) setups attract the most attention since the fluctuations are the strongest in 1D.

Precisely this situation was considered in Refs. [19–21]. The authors studied the interaction between two static impurities due to the perturbation of phonon spectra in a Luttinger liquid. Since the mechanism is similar to the one proposed by Casimir, we hereafter denote it as the Casimir interaction. The examination of the energy of zero-point motion of the Luttinger liquid in the presence of two impurities yielded the Casimir interaction  $U(r) \sim -1/r$ . This dependence can

be easily understood considering the zero-point energy of phonons in a potential well formed by two static impurities. The direct calculation leads to the following expression for the Casimir interaction [24,25],

$$U(r) = -\frac{c\pi}{24r} \quad (1)$$

(here and below we use  $\hbar = 1$ ).

At the same time, for two dynamical impurities which can move inside the medium, Schecter and Kamenev [26] proposed an essentially different  $r$  dependence,  $U(r) = -mc^2 \frac{\Gamma_1 \Gamma_2}{32\pi} \frac{\xi^3}{r^3}$ , where  $m$  is the mass of particles in the fluid,  $c$  is the sound velocity,  $\xi = 1/mc$ , and the dimensionless parameters  $\Gamma_{1,2}$  are impurity-phonon scattering amplitudes. How the power law for dynamic impurities transforms to another for the static impurities is an open question.

To address this question, we investigate two impurities interacting with Goldstone phonons. To avoid possible ultraviolet divergences we map the model on a harmonic crystal lattice with two impurity neutral atoms. It is arguably the simplest model in which one can tune impurities continuously from dynamic to static and keep track of the evolution of the Casimir interaction.

In this model the Casimir interaction emerges naturally between two impurity atoms as soon as their mass is different from the masses of the lattice atoms or an external potential is applied. Then we consider the corresponding continuous model of two atoms interacting via virtual phonons.

We find that the Casimir interaction has different asymptotics in these two cases. In the former one, for any finite mass of the impurity atoms, the Casimir interaction tends to the  $1/r^3$  law at large distances, in agreement with Ref. [26]. At the same time, in the limit of infinite impurity mass the long-range asymptotic tends to  $1/r$ , in agreement with Refs. [19–21]. In the case of an external potential the asymptotics is always  $1/r$ .

Our Rapid Communication is organized as follows. First, we consider two neutral impurity atoms embedded in a har-

monic crystal lattice. Using the exact diagonalization method we show that the power law at short distances strongly deviates from  $1/r^3$  and the characteristic distance of the crossover to  $1/r^3$  law depends on the masses of the impurity atoms. Then we provide the exact solution for the model and formulate the continuum model. In the second part we formulate and exactly solve the model of two impurity atoms in an external harmonic potential. We show that the model has  $1/r$  asymptotic behavior. Finally, we provide a discussion of the obtained results and conclusion.

*The model.* We analyze an ideal harmonic cubic lattice described by  $H_0 = \sum_i \frac{p_i^2}{2m} + \frac{m\omega_0^2}{2} \sum_{\langle i,j \rangle} (u_i - u_j)^2$ , with two embedded impurity atoms, which have mass or an external potential different from the mass/potential of the atoms of the lattice. Here,  $p_i$  and  $u_i$  are the momentum and coordinate operators,  $m$  is the mass of the atoms of the cubic lattice, and  $m\omega_0^2$  is the interaction potential.

The Bogoliubov transformation brings  $H_0$  to the Hamiltonian of noninteracting phonons,

$$H_0 = \sum_{\mathbf{k}} \omega_{\mathbf{k}} \left( b_{\mathbf{k}}^\dagger b_{\mathbf{k}} + \frac{1}{2} \right), \quad (2)$$

with the phonon spectrum  $\omega_{\mathbf{k}} = \omega_0 \sqrt{Z(1 - \gamma_{\mathbf{k}})}$ . Here,  $\gamma_{\mathbf{k}} = \frac{1}{Z} \sum_{\Delta} e^{i\mathbf{k}\Delta}$  with the summation over the nearest neighbors and  $Z$  the number of the nearest neighbors. In the one-dimensional case it reduces to  $\omega_{\mathbf{k}} = 2\omega_0 |\sin(ka/2)|$ , where  $a$  is the lattice constant. In the low-energy limit  $\omega_{\mathbf{k}} = c|k|$  with the phonon velocity  $c = \omega_0 a$ . Further, for simplicity, we put  $a = 1$ .

*Two impurity atoms having different masses.* First, we consider two impurity atoms with masses  $M$  located at the sites  $a$  and  $b$ . The resulting Hamiltonian of the system is  $H = H_0 + V$  with the perturbation term of the kinetic energy,

$$V = -\frac{g}{2m} (p_a^2 + p_b^2), \quad (3)$$

where the effective coupling constant  $g = (1 - m/M)$ .

*Exact diagonalization.* The Hamiltonian with two embedded impurity masses  $M$  cannot be reduced to the Hamiltonian of free phonons. However, one can find the Casimir interaction, i.e., the dependence of the total energy of zero-point motion  $E = \frac{1}{2} \sum_{\mathbf{k}} \omega_{\mathbf{k}}$  of all atoms of the lattice on the distance between the impurity atoms.

The result of the exact diagonalization method for a 200-atom chain for various masses of impurity atoms is shown in Fig. 1. Surprisingly, the Casimir energy  $U(r)$  between dynamic, finite-mass impurities does not follow  $U(r) \sim 1/r^3$ . Rather, the interaction is nonuniversal and depends on the mass of the impurity atoms (Fig. 1). One can note that the normalized Casimir interaction for masses larger than  $m$  is in the range  $1/r^3 < E < 1/r$  for  $r > 1$ , and for light impurities ( $M < m$ ) it is  $E < 1/r^3$ . For impurity masses close to  $m$ , the Casimir interaction tends to the  $1/r^3$  law and in the limit  $M \rightarrow \infty$  (static impurities) one observes the  $1/r$  law.

*Perturbation theory.* To find the reason for this drastic deviation of the  $r$  dependence of the Casimir interaction from the  $1/r^3$  law, we employ the perturbation theory. For the

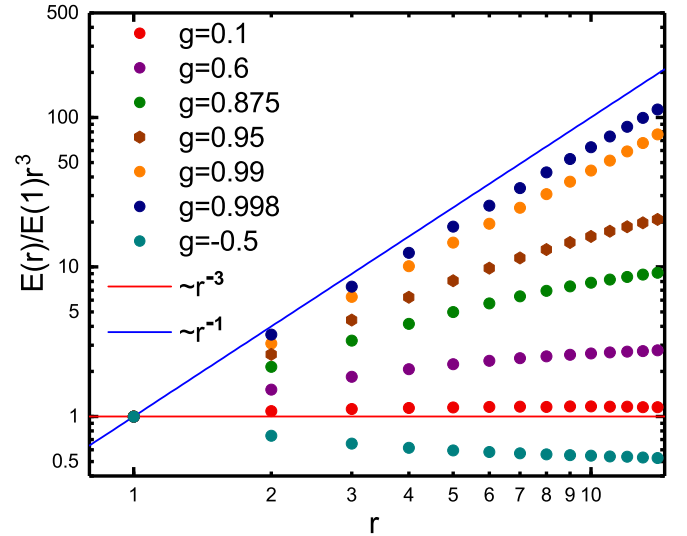


FIG. 1. Normalized Casimir interaction  $U_{\text{eff}}(r)$  calculated for a chain of 200 atoms with two impurity atoms with various masses [27]: Red dots,  $g = 0.1$  ( $M/m = 1.1$ ); purple,  $g = 0.6$  ( $M/m = 2.5$ ); green,  $g = 0.875$  ( $M/m = 8$ ); brown,  $g = 0.95$  ( $M/m = 20$ ); orange,  $g = 0.99$  ( $M/m = 100$ ); blue,  $g = 0.998$  ( $M/m = 500$ ); turquoise,  $g = -0.5$  ( $M/m = 0.5$ ). The red line shows the  $1/r^3$  law, the blue line shows  $1/r$ .

calculation we express Eq. (3) in the phonon operators,

$$V = \sum_{\mathbf{q}, \mathbf{q}'} \left( V_{\mathbf{q}, \mathbf{q}'}^{(1)} b_{\mathbf{q}}^\dagger b_{\mathbf{q}'} + V_{\mathbf{q}, \mathbf{q}'}^{(2)} \frac{b_{\mathbf{q}} b_{\mathbf{q}'}}{2} + \text{H.c.} \right). \quad (4)$$

Here, the vertices are

$$V_{\mathbf{q}, \mathbf{q}'}^{(1)} = -V_{\mathbf{q}, \mathbf{q}'}^{(0)} \cos \frac{(\mathbf{q} - \mathbf{q}')\mathbf{r}}{2},$$

$$V_{\mathbf{q}, \mathbf{q}'}^{(2)} = V_{\mathbf{q}, \mathbf{q}'}^{(0)} \cos \frac{(\mathbf{q} + \mathbf{q}')\mathbf{r}}{2},$$

with  $\mathbf{r} = \mathbf{r}_a - \mathbf{r}_b$  and  $V_{\mathbf{q}, \mathbf{q}'}^{(0)} = g \sqrt{\omega_{\mathbf{q}}} \sqrt{\omega_{\mathbf{q}'}}$ , where  $\omega_{\mathbf{q}}, \omega_{\mathbf{q}'}$  are the free-phonon spectra given above. We choose  $\mathbf{r}_a + \mathbf{r}_b = \mathbf{0}$  for simplicity.

The first-order term of the perturbation theory is  $r$  independent and therefore does not contribute to the Casimir interaction. The lowest contributing order is the second order of the perturbation theory,

$$U_{\text{eff}}^{(2)}(r) = -2T \sum_n \frac{|V_{\mathbf{k}, \mathbf{k}+\mathbf{q}}^{(2)}|^2 \omega_{\mathbf{k}} \omega_{\mathbf{k}+\mathbf{q}}}{(\omega_n^2 + \omega_{\mathbf{k}}^2)(\omega_n^2 + \omega_{\mathbf{k}+\mathbf{q}}^2)}. \quad (5)$$

Here,  $\omega_n = 2\pi T n$  is the Matsubara frequency.

At large distances  $r \gg 1$  the leading contribution comes from the small momenta. At zero temperature the integration Eq. (5) can be performed analytically for the linearized spectrum  $\omega_{\mathbf{k}} = ck$  with the use of the substitution  $T \sum_n \rightarrow \int d\omega_n/2\pi$ . The result is the  $1/r^3$  law,

$$U_{\text{eff}}^{(2)}(r) = -\frac{g^2 \omega_0}{32\pi} \frac{1}{r^3}. \quad (6)$$

This dependence agrees with that previously found in Ref. [26], but disagrees with the results of the exact diagonalization.

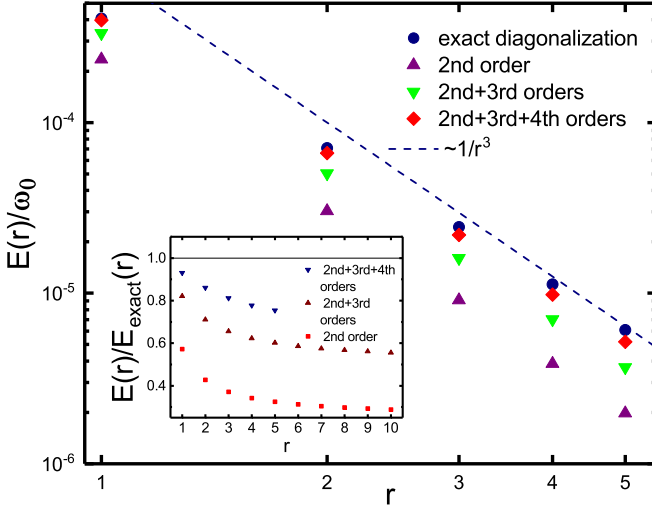


FIG. 2. Casimir interaction in the perturbation theory: Gray dots, second order; brown dots, diagrams up to the third order; red dots, up to the fourth order; blue dots, energies obtained by the exact diagonalization. Inset: Contribution of different orders of the perturbation theory to the total result.

*Higher order of perturbation theory.* To understand the origin of the deviation from  $1/r^3$  law, we explore higher-order phonon processes, which correspond to the multiple scattering of phonons on the impurities. The result of the perturbation theory up to four-phonon processes for  $g = 0.5$  is presented in Fig. 2. Here, we keep only  $r$ -dependent terms. One immediately notes that the third and fourth orders of the perturbation theory significantly renormalize the Casimir interaction. Plotting the sum of all terms up to the fourth order, one can see a good match with the results of the exact diagonalization.

One can find exactly the thermodynamic potential in this model. It is given by diagrams shown in Fig. 3. The obtained thermodynamic potential  $\Phi(r)$  contains an  $r$ -independent term, which is related to the perturbation of the zero-point motion by uncorrelated impurity atoms ( $r \rightarrow \infty$ ). Defining  $U_{\text{eff}}(r) = \Phi(r) - \Phi(\infty)$  we arrive at the following expression,

$$U_{\text{eff}}(r) = \frac{1}{2}T \sum_n \ln \left[ 1 - \left( \frac{gG(\omega_n, r)}{1 - gG_0(\omega_n)} \right)^2 \right], \quad (7)$$

where  $G(\omega_n, r)$  are the phononic Green's functions in the coordinate space. Here, we define the phononic field so that  $k$  dependence is transferred from the vertex to the Green's

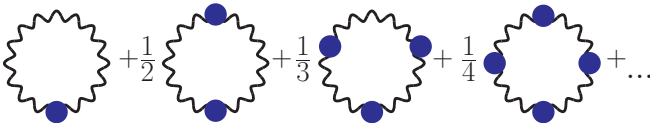


FIG. 3. The diagrammatic representation of the thermodynamic potential.

function (for details, see the Supplemental Material [28]),

$$\begin{aligned} G(\omega_n, r) &= \int_{-\pi}^{\pi} \frac{dk}{2\pi} \cos(kr) \frac{\omega_k^2}{\omega_n^2 + \omega_k^2} \\ &= -\frac{\omega_0}{c} f\left(\frac{|\omega_n|}{2\omega_0}, r\right), \end{aligned} \quad (8)$$

with

$$f(x, r) = \frac{x}{\sqrt{1+x^2}} (x + \sqrt{1+x^2})^{-2r},$$

and

$$G_0(\omega_n) = 2 \int_0^{\pi} \frac{dk}{2\pi} \frac{\omega_k^2}{\omega_n^2 + \omega_k^2} = 1 - \frac{\omega_0}{c} f\left(\frac{|\omega_n|}{2\omega_0}, 0\right). \quad (9)$$

One can note that the Green's function for  $r \gg 1$  decays exponentially,  $\sim e^{-2r\omega_n/\omega_0}$ . It means that the main contribution to the Casimir interaction comes from the low-energy acoustic phonons.

*Continuum limit.* The low-energy Hamiltonian can be obtained from Eqs. (2) and (4) by linearization of the spectrum for small momenta  $\omega_k = c|k|$ . The corresponding Hamiltonian is

$$\begin{aligned} H &= \sum_k c|k| b_k^\dagger b_k + gc \sum_{k,k'} \sqrt{|k||k'|} \\ &\times \cos\left[\frac{(k+k')r}{2}\right] \left( b_k^\dagger b_{k'} + \frac{b_k b_{k'} + b_k^\dagger b_{k'}^\dagger}{2} \right). \end{aligned} \quad (10)$$

This expression is similar to that used in Ref. [26]. To calculate the thermodynamic potential in the continuum limit we use the results of the previous section, changing the limits of the integration from the Brillouin zone to infinity. Note that the integral in Eq. (9) becomes divergent and has to be renormalized. For this we use the mapping to the lattice model of the previous section (this procedure is discussed in Ref. [29]). In this approach, at  $T = 0$  the Casimir energy reads

$$U_{\text{eff}}(r) = \int_0^\infty \frac{d\omega_n}{2\pi} \ln \left[ 1 - \left( \frac{\frac{g\omega_n}{2c} e^{-\frac{\omega r}{c}}}{1 - g + \frac{g\omega_n}{2c}} \right)^2 \right]. \quad (11)$$

To trace the dependence of the Casimir interaction on the coupling constant  $g < 1$  and distance  $r$  at  $T = 0$  we introduce the logarithmic derivative  $\nu = -\frac{d \ln[E(r)]}{d \ln(r)}$ . For power-law functions  $1/r^\nu$  it gives the power  $\nu$ . The results are summarized in Fig. 4. The interval  $0 < g \leq 1$  describes the impurity masses  $m < M \leq \infty$ . The line  $g = 0$  is the singular line where  $U_{\text{eff}} = 0$ , and the interval  $-\infty < g < 0$  corresponds to  $M < m$ . One can see from the figure that although for small distances the Casimir interaction cannot be described by the functions  $1/r^\nu$ , at large distances the dependence tends to  $1/r^3$ . The characteristic distance of the crossover to the  $1/r^3$  law is  $r_g = \frac{g}{1-g}$  (see Supplemental Material [28]). Finally, in the limit  $g \rightarrow 1$ , the Casimir interaction depends as  $1/r$  from the distance between the impurity atoms and coincides with Eq. (1).

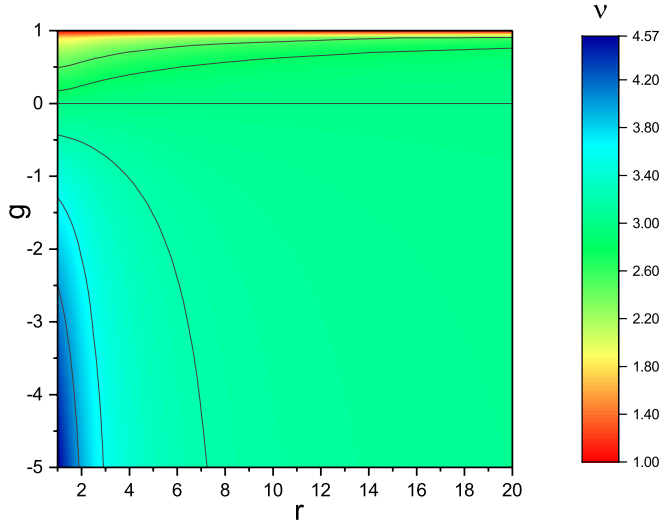


FIG. 4. Logarithmic derivative  $\nu = -\frac{d \ln U_{\text{eff}}(r)}{d \ln r}$  as the function of  $r$  and  $g$  of the Casimir interaction between two impurity atoms having different masses.

*External potential.* Now we consider two atoms in an external harmonic potential which is defined by the following Hamiltonian,

$$V = gm\omega_0^2(u_a^2 + u_b^2), \quad (12)$$

with the interaction constant  $g \geq 0$ . It leads to the new interaction term  $V_{\mathbf{q},\mathbf{q}'}$ ,

$$V_{\mathbf{q},\mathbf{q}'}^{(0)} = -\frac{g\omega_0^2}{\sqrt{\omega_{\mathbf{q}}}\sqrt{\omega_{\mathbf{q}'}}}. \quad (13)$$

The bosonic Green's functions are (see Ref. [28] for the definition)

$$G(\omega_n, r) = \frac{\omega_0}{c} \frac{\omega_0^2}{\omega_n^2} f(|\omega_n|/2\omega_0, r), \quad (14)$$

$$G_0(\omega_n) = \frac{\omega_0}{c} \frac{\omega_0^2}{\omega_n^2} f(|\omega_n|/2\omega_0, 0). \quad (15)$$

The direct calculation exhibits that all orders of the perturbation theory are divergent at the low-energy limit [28], but the summation of the whole series of the diagrams (Fig. 3) leads to cancellation of the singularities and a finite expression for the thermodynamic potential [Eq. (7)]. The phononic Green's functions are given by Eqs. (14) and (15).

The correspondent continuous model is different from Eq. (10) and is given by

$$H = \sum_k c|k|b_k^\dagger b_k + g \sum_{k,k'} \frac{\omega_0^2}{c\sqrt{|kk'|}} \times \cos\left[\frac{(k+k')r}{2}\right] \left(b_k^\dagger b_{k'} + \frac{b_k b_{k'} + b_k^\dagger b_{k'}^\dagger}{2}\right). \quad (16)$$

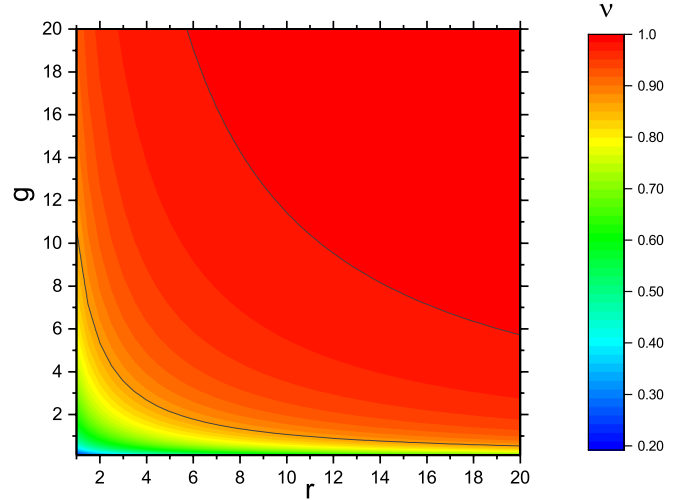


FIG. 5. Logarithmic derivative  $\nu = -\frac{d \ln U_{\text{eff}}(r)}{d \ln r}$  as the function of  $r$  and  $g$  for the Casimir interaction between two masses in an external potential.

The Casimir interaction has the form

$$U_{\text{eff}}(r) = T \sum_{n>0} \ln \left[ 1 - \left( \frac{g \frac{\omega_0^2}{2c\omega_n} e^{-\frac{\omega_n}{c} r}}{1 + \frac{g\omega_0^2}{2c\omega_n}} \right)^2 \right]. \quad (17)$$

A similar expression was obtained in Ref. [20]. To understand the scaling behavior at  $T = 0$  we plot the logarithmic derivative  $\nu$  of the Casimir interaction  $U_{\text{eff}}$  given by Eq. (17) as a function of  $r$  and  $g$  in Fig. 5. For small values  $gr$  the law is not universal, but  $U_{\text{eff}}$  tends to  $1/r$  as soon as  $gr \ll 1$ . The integral Eq. (17) in the limit  $gr \gg 1$  matches the previously found expression for  $M \rightarrow \infty$  [Eq. (1)].

*Discussion and conclusions.* The obtained long-range interaction can be observed experimentally in ultracold atomic gases as was shown in Ref. [20]. Since the competing Casimir-Polder interaction falls off much faster, namely, as  $1/r^6$ , in the experimental setup of Ref. [30] for the impurities at a distance of  $1 \mu\text{m}$ , the phonon-induced Casimir interaction should dominate [31].

Summarizing, we have analyzed the evolution of the phonon-induced Casimir interaction between two impurity atoms. We have given the exact solution of the model and have studied the evolution of the Casimir interaction with a change of the impurity atoms' masses and the effect of an external potential. We have shown that multiboson processes change the scaling of the interaction decay with distance and the mass of the considered object plays an important role. As a consequence, the behavior at small distances differs from the power law at large. At large distances between two dynamic impurities the Casimir interaction is universal and obeys the  $1/r^3$  law. For static impurities it tends to the  $1/r$  law.

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