Interaction of impurity atoms in Bose-Einstein condensates

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The interaction of two spatially separated impurity atoms through phonon exchange in a Bose-Einstein condensate is studied within a Bogoliubov approach. The impurity atoms are held by deep and narrow trap potentials and experience level shifts which consist of a mean-field part and vacuum contributions from the Bogoliubov phonons. In addition, there is a conditional energy shift resulting from the exchange of phonons between the impurity atoms, which can be employed for a transfer of quantum information between the atoms.

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I. INTRODUCTION

The ability to engineer the collisional interaction of ultracold individual atoms or ions as well as degenerate ensembles of atoms, such as Bose-Einstein condensates (BECs) [1], has dramatically improved in the last couple of years by the development of quantum-optical tools such as single-atom microtraps [2–4], optical lattices [5–7], atom chips [8], and others. Controlled collisional interactions of individual atoms are of fundamental interest but also have important potential applications in quantum information processing [9]. Recently, the coupling of single-atom quantum dots to Bose-Einstein condensates was studied in [10] and the use of an impurity atom in a one-dimensional optical lattice as an atom transistor was proposed [11]. We study here the mutual interaction between two separated, well localized impurity atoms through the exchange of Bogoliubov phonons in a BEC at zero temperature and its potential application for the transfer of quantum information between the atoms. This is motivated by the analogy to cavity quantum electrodynamics where the off-resonant scattering of resonator photons from two atoms or quantum dots in the strong-coupling regime can be used to implement a universal two-qubit gate [12]. When impurity atoms in a BEC undergo a state-dependent scattering with the condensate atoms, in addition to mean-field level shifts and levels shifts from the interaction with the vaccum fluctuations of the Bogoliubov phonons, also a conditional level shift emerges which results from phonon exchange between the impurities. This conditional shift is calculated and its dependence on trap geometry, impurity separation, and the strength of the interactions within the condensate is studied and applications to quantum information processing are discussed.

In Sec. II, we derive an effective coarse-grained interaction Hamiltonian for the impurity atoms and relate the level shifts to correlation functions of quasiparticle excitations. These will then be calculated within a Bogoliubov approximation for a condensate in a box potential in Sec. III. It is shown that the coupling between the impurity atoms is strongest for a highly asymmetric geometry. For this reason, we consider in Sec. IV a quasi-one-dimensional condensate. A simple analytic expression for the level shift is derived using a Thomas-Fermi approximation.

II. EFFECTIVE INTERACTION OF IMPURITY ATOMS IN A BEC

We consider here a Bose-Einstein condensate at $T=0$ with impurity atoms at fixed locations, $\mathbf{r}_1$ and $\mathbf{r}_2$, which can be realized, e.g., by tightly confining trap potentials as shown in Fig. 1. The traps are separated such that any direct interaction of the atoms can be excluded. The atoms are assumed to have two relevant internal states $|0\rangle$ and $|1\rangle$ and shall undergo *s*-wave scattering interactions with the atoms of the BEC if they are in state $|1\rangle$. If the traps are sufficiently deep, the atoms will stay in the corresponding ground state ϕ_0, whose size is assumed to be small compared to the coherence length of the BEC. In this case, the interaction of the condensate and the impurities can be expressed by the local Hamiltonian

$$\hat{H}_{\mathrm{int}} = \frac{\kappa}{2}\sum_{\alpha,\beta} |\alpha,\beta\rangle\langle\alpha,\beta|[\delta_{\alpha 1}\hat{\psi}^{\dagger}(\mathbf{r}_1)\hat{\psi}(\mathbf{r}_1) + \delta_{\beta 1}\hat{\psi}^{\dagger}(\mathbf{r}_2)\hat{\psi}(\mathbf{r}_2)], \tag{1}$$

where $|\alpha,\beta\rangle$ denotes the αth internal state of the first and the βth internal state of the second impurity atom. The coupling to the condensate is described by the state-dependent coupling constant κ. The condensate wave function is denoted by $\hat{\psi}$.

In order to derive an effective Hamiltonian for the two impurity atoms, it is convenient to first separate the interaction (1) into a mean-field and a fluctuation part,

$$\hat{H}_{\mathrm{int}} = \frac{\kappa}{2}\sum_{j=1,2} |1\rangle_{jj}\langle 1|\langle\hat{\psi}^{\dagger}(\mathbf{r}_j)\hat{\psi}(\mathbf{r}_j)\rangle + \frac{\kappa}{2}\sum_{\alpha,\beta} |\alpha,\beta\rangle\langle\alpha,\beta|[\delta_{\alpha 1}\hat{B}_1(t) + \delta_{\beta 1}\hat{B}_2(t)], \tag{2}$$

where

$$\hat{B}_l(t) = \hat{\psi}^{\dagger}(\mathbf{r}_l)\hat{\psi}(\mathbf{r}_l) - \langle\hat{\psi}^{\dagger}(\mathbf{r}_l)\hat{\psi}(\mathbf{r}_l)\rangle. \tag{3}$$

The terms in the first line of Eq. (2) result in a mean-field level shift of the internal state $|1\rangle$. They are of no interest in the present discussion and will be absorbed in the free Hamiltonian of the impurity atoms.

We proceed by deriving an equation of motion for the statistical operator of the impurities interacting with the BEC

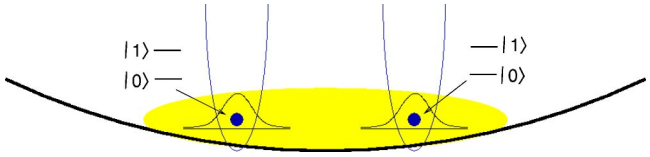

FIG. 1. (Color online) Impurity atoms held by tight confining potentials in a Bose-Einstein condensate. When in internal state $|1\rangle$, the atoms undergo *s*-wave scattering interactions with the condensate.

following the quantum optical approach as it is used, e.g., in cavity QED. Within the lowest-order Born approximation and as outlined in Appendix A, one finds

$$\partial_t \tilde{\varrho}_{10,00} = -\frac{\kappa^2}{4\hbar^2}\int_{t_0}^{t} \mathrm{d}t' \tilde{\varrho}_{10,00}(t')\langle \tilde{B}_1(t)\tilde{B}_1(t')\rangle, \tag{4}$$

$$\partial_t \tilde{\varrho}_{01,00} = -\frac{\kappa^2}{4\hbar^2}\int_{t_0}^{t} \mathrm{d}t' \tilde{\varrho}_{01,00}(t')\langle \tilde{B}_2(t)\tilde{B}_2(t')\rangle, \tag{5}$$

$$\partial_t \tilde{\varrho}_{11,00} = -\frac{\kappa^2}{4\hbar^2}\int_{t_0}^{t} \mathrm{d}t' \tilde{\varrho}_{11,00}(t')\{\langle \tilde{B}_1(t)\tilde{B}_1(t')\rangle + \langle \tilde{B}_1(t)\tilde{B}_2(t')\rangle + (\text{terms with } 1 \leftrightarrow 2)\}, \tag{6}$$

where the tilde denotes quantities in the interaction picture and the matrix elements of the statistical operator are denoted by $\tilde{\varrho}_{\alpha\beta,\gamma\delta}=\langle \alpha\beta,t|\tilde{\varrho}|\gamma\delta,t\rangle$. In the first-order Born approximation, the correlation functions $\langle \tilde{B}_l(t)\tilde{B}_{l'}(t)\rangle$ are to be taken in the absence of the coupling to the impurity atoms. We will show in Appendix B that the first-order Born approximation is here well justified.

The correlations $\langle \tilde{B}_l\tilde{B}_{l'}\rangle$ are calculated using the standard Bogoliubov approach, i.e., by setting

$$\hat{\psi}(\mathbf{r},t) = \psi_0(\mathbf{r}) + \hat{\xi}(\mathbf{r},t) \tag{7}$$

with ψ_0 being the solution of the Gross-Pitaevskii equation and $\hat{\xi}$ a small operator-valued correction and neglecting higher-order terms in $\hat{\xi}$ (see Appendix C). Within the Bogoliubov approach, we disregard terms of the order $O(\hat{\xi}^4)$ in $\langle \tilde{B}_i\tilde{B}_j\rangle$ and find

$$\langle \tilde{B}_l(t)\tilde{B}_{l'}(t')\rangle = {\sum_j}' \mathrm{e}^{-(i/\hbar)E_j(t-t')}S_j(l,l'). \tag{8}$$

The E_j's are the Bogoliubov energies and

$$S_j(l,l') = \psi_0(\mathbf{r}_l)\psi_0(\mathbf{r}_{l'})[u_j(\mathbf{r}_l) - v_j(\mathbf{r}_l)][u_j^*(\mathbf{r}_{l'}) - v_j^*(\mathbf{r}_{l'})]. \tag{9}$$

The functions u_j and v_j are the solutions of the Bogoliubov–de Gennes equations (cf. Appendix C) and the prime at the sum indicates that the ground state is excluded.

A calculation of the correlation functions shows that the Markov approximation often used in a quantum optical context cannot straightforwardly be applied to Eqs. (4)–(6). However, if we are interested only in a coarse-grained time evolution corresponding to frequencies below the lowest excitation frequency, the interaction of the impurity atoms with the condensate simply results in level shifts (cf. Appendix A), i.e.,

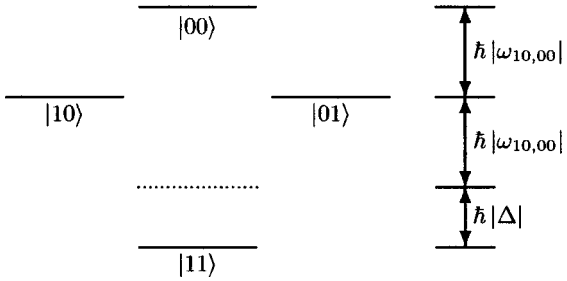

FIG. 2. Energy scheme of the effective Hamiltonian for symmetric arrangement of impurity atoms. Here, a negative sign of Δ was assumed, although positive values are possible.

$$\tilde{\varrho}_{\alpha\beta,\gamma\delta}(t) = \tilde{\varrho}_{\alpha\beta,\gamma\delta}(0)\mathrm{e}^{-i\omega_{\alpha\beta,\gamma\delta}t}. \tag{10}$$

The corresponding frequencies read

$$\omega_{\alpha\beta,\gamma\delta} = \frac{\kappa^2}{4\hbar}{\sum_j}' \frac{1}{E_j}\{S_j(1,1)(\delta_{\gamma 1} - \delta_{\alpha 1}) + S_j(2,2)(\delta_{\delta 1} - \delta_{\beta 1}) + [S_j(1,2) + S_j(2,1)](\delta_{\gamma 1}\delta_{\delta 1} - \delta_{\alpha 1}\delta_{\beta 1})\}. \tag{11}$$

This corresponds to an effective—coarse-grained—Hamiltonian

$$\tilde{H}_{\mathrm{eff}} = |10\rangle\langle 10|\hbar\omega_{10,00} + |01\rangle\langle 01|\hbar\omega_{01,00} + |11\rangle\langle 11|\hbar\omega_{11,00}. \tag{12}$$

The energy scheme of this Hamiltonian is shown in Fig. 2. One recognizes from Eq. (12) for symmetric impurity locations a level shift

$$\delta = \omega_{10,00} = \omega_{01,00} = -\frac{\kappa^2}{4\hbar}{\sum_j}' \frac{1}{E_j}S_j(1,1) < 0 \tag{13}$$

of each impurity atom independent of the presence of the other. This level shift is due to the interaction with vacuum fluctuations of the Bogoliubov quasiparticles (phonons). In addition, there is a conditional level shift due to the exchange of Bogoliubov quasiparticles (phonons) between the two impurities,

$$\Delta = \omega_{11,00} - \omega_{10,00} - \omega_{01,00} = -\frac{\kappa^2}{4\hbar}{\sum_j}' \frac{1}{E_j}\{S_j(1,2) + S_j(2,1)\}. \tag{14}$$

It should be noted that the coarse-graining approximation is consistent with the collective level shift only if

$$\Delta \ll \frac{1}{\hbar}\min_j{}'(E_j), \tag{15}$$

where the prime indicates that the ground state is excluded. In the following, we will explicitly calculate the level shifts for a homogeneous condensate, for an ideal condensate in a

harmonic trap, and a weakly interacting condensate in a trap in the Thomas-Fermi limit.

III. HOMOGENEOUS CONDENSATE

In this section, we calculate the energy shifts δ and Δ for the case of an interacting, homogeneous condensate with periodic boundary conditions of spatial periodicity L_x, L_y, L_z, respectively. The solutions of the Bogoliubov–de Gennes equations are then given by plane waves $u_{\mathbf{k}}=(f_{\mathbf{k}}^{+}+f_{\mathbf{k}}^{-})/2$ and $v_{\mathbf{k}}=(f_{\mathbf{k}}^{+}-f_{\mathbf{k}}^{-})/2$ with

$$f_{\mathbf{k}}^{\pm}(\mathbf{r})=\frac{1}{\sqrt{V}}\left(\sqrt{\frac{E_{\mathbf{k}}}{\varepsilon_{\mathbf{k}}^{0}}}\right)^{\pm 1}e^{i\mathbf{k}\cdot\mathbf{r}}. \tag{16}$$

The wave vectors $\mathbf{k}$ have to be chosen in such a way that they fulfill the periodic boundary conditions. Since the $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$'s have to be orthogonal to the ground state, the case $\mathbf{k}=\mathbf{0}$ is excluded. The Bogoliubov energies are given by

$$E_{\mathbf{k}}=\sqrt{\varepsilon_{\mathbf{k}}^{0}(\varepsilon_{\mathbf{k}}^{0}+2gn_0)} \tag{17}$$

with $\varepsilon_{\mathbf{k}}^{0}=\hbar^2k^2/2m_{\mathrm{B}}$. One can easily calculate the correlation functions,

$$\langle\tilde{B}_l(t)\tilde{B}_{l'}(t')\rangle=\frac{N_0}{V^2}{\sum_{\mathbf{k}}}'\frac{\varepsilon_{\mathbf{k}}^{0}}{E_{\mathbf{k}}}\exp\left(-\frac{i}{\hbar}E_{\mathbf{k}}(t-t')\right)\times\exp[i\mathbf{k}\cdot(\mathbf{r}_l-\mathbf{r}_{l'})]. \tag{18}$$

Here, N_0 denotes the number of atoms in the condensate and $V=L_xL_yL_z$. It should be noted that the sum in Eq. (18) is in general UV-divergent, which is due to the assumption of a pointlike interaction in Eq. (1). In a more accurate description, the small but finite extension z_0 of the ground state of the impurity trap should be taken into account, which would lead to an effective cutoff at $|\mathbf{k}|\sim 1/z_0$. The value of z_0 is, however, of no relevance for the conditional phase shift and is dropped here. With Eq. (18), one finds for the level shifts

$$\delta=-\frac{\kappa^2N_0}{4\hbar V^2}{\sum_{\mathbf{k}}}'\frac{\varepsilon_{\mathbf{k}}^{0}}{E_{\mathbf{k}}^{2}}, \tag{19}$$

$$\Delta=-\frac{\kappa^2N_0}{2\hbar V^2}{\sum_{\mathbf{k}}}'\frac{\varepsilon_{\mathbf{k}}^{0}}{E_{\mathbf{k}}^{2}}\cos(\mathbf{k}\cdot\Delta\mathbf{r}), \tag{20}$$

where $\Delta\mathbf{r}=\mathbf{r}_1-\mathbf{r}_2$. The conditional energy shift Δ is shown in Fig. 3. For very small distances of the impurities, Δ is negative and its absolute value approaches its maximum, i.e., that of 2δ (a finite value of δ is obtained only with a cutoff). For increasing distance, the value of Δ increases monotonously and eventually changes its sign. The monotonous increase would correspond to an attractive force between the impurity atoms if they could move freely. One recognizes that for larger values of the dimensionless interaction parameter $K=2L_z^2/l_{\mathrm{coh}}^2\sim g$, where $l_{\mathrm{coh}}=\hbar/\sqrt{mgn(0)}$ is the coherence length, the energy shift decreases and the spatial dependence becomes less pronounced. This can be explained by the increasing self-energy of the Bogoliubov excitations. Thus the conditional energy shift is appreciable only in finite systems,

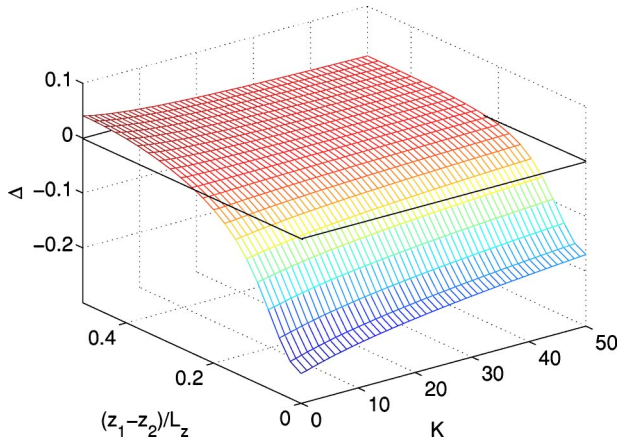

FIG. 3. (Color online) Energy shift in units of $\kappa^2N_0m_{\mathrm{B}}L_z^2/\hbar^3V^2$ for two impurities in a homogeneous condensate with periodic boundary conditions. The interaction of BEC atoms is characterized by the dimensionless parameter $K=gN_02m_{\mathrm{B}}L_z^2/\hbar^2V=2L_z^2/l_{\mathrm{coh}}^2$. The impurities are located on the z axis, $L_x=L_y=0.5L_z$, and a finite size $z_0=0.05L_z$ of the impurity traps was assumed to eliminate the singularity at $z_1=z_2$.

where L_z/l_{coh} is not too large. In the thermodynamic limit, the shift disappears.

It is also very instructive to consider the dependence of the conditional level shift Δ on the aspect ratio of the condensate, i.e., on the ratio L_{rad}/L_z, where $L_{\mathrm{rad}}=L_x=L_y$. This is illustrated in Fig. 4. One recognizes that the absolute value of the energy shift increases as the ratio L_{rad}/L_z decreases. Thus the energy shift is largest for a highly nonsymmetric geometry of the BEC. The strongest effect is thus to be expected in a quasi-one-dimensional condensate of sufficiently small size. For this reason, we will investigate in the following section the energy shift in the case of a BEC in a harmonic trap only for a one-dimensional condensate.

IV. 1D CONDENSATE IN A TRAP

In this section, we consider a quasi-one-dimensional condensate confined in a harmonic trap $V_{\mathrm{ext}}=m_{\mathrm{B}}\omega_{\mathrm{B}}^2z^2/2$. We first

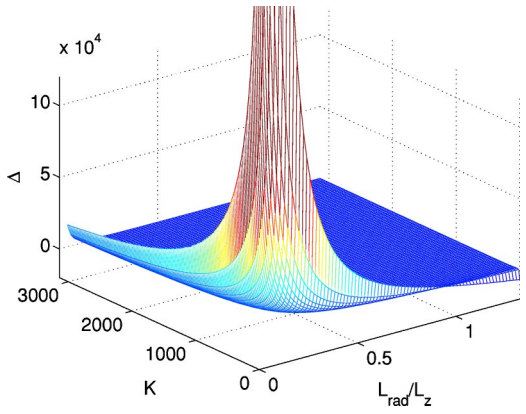

FIG. 4. (Color online) Influence of condensate geometry on energy shift in a box with periodic boundary conditions. Δ is in units of $\kappa^2 2m_{\mathrm{B}}/4\hbar^3$, K is defined as in Fig. 3. The impurities are located on the z axis with a distance of $0.5L_z$. $L_z=12\times10^{-6}$ m, and $L_x=L_y$ has been varied.

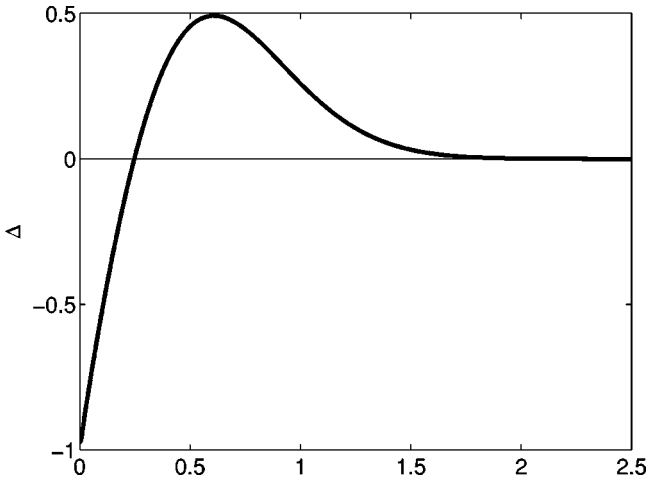

FIG. 5. Energy shift Δ in an ideal 1D condensate as a function of impurity distance. The shift is given in units of $\kappa_{1D}^2 N_0/2\hbar^2\omega_B\pi z_B^2$. Here $\check{z}_1=-\check{z}_2$.

consider the case of an ideal, i.e., noninteracting gas. In this case, the solutions of the Gross-Pitaevskii equation and the Bogoliubov–de Gennes equations are just the solutions of the harmonic oscillator,

$$\psi_0(z) = \sqrt{\frac{N_0}{\sqrt{\pi}z_B}}e^{-z^2/2z_B^2}, \tag{21}$$

$$u_j(z) = \frac{1}{\sqrt{2^j j!\sqrt{\pi}z_B}}e^{-z^2/2z_B^2}H_j\left(\frac{z}{z_B}\right), \tag{22}$$

$$v_j(z) = 0, \tag{23}$$

$$E_j = j\hbar\omega_B. \tag{24}$$

Here, $z_B=\sqrt{\hbar/m\omega_B}$ is the ground-state width of the 1D harmonic trap. By calculating Eq. (9), one finds

$$\Delta = -\frac{\kappa_{1D}^2}{2\hbar}\sum_{\nu=1}^{\infty}\frac{N_0\exp(-\check{z}_1^2-\check{z}_2^2)}{\hbar\omega_B\pi z_B^2\nu 2^\nu\nu!}H_\nu(\check{z}_1)H_\nu(\check{z}_2), \tag{25}$$

where $\check{z}_l=z_l/z_B$. We also have introduced the one-dimensional coupling constant $\kappa_{1D}=\kappa/(2\pi a_\perp^2)$ with the radial confinement $a_\perp^2=\hbar/m_B\omega_\perp$. The conditional level shift is shown in Fig. 5.

It is interesting to note that, different from the case of a condensate in a box, the force between the impurities is not always attractive. One recognizes that this is only the case if the distance is sufficiently small. If the distance is larger than a certain value, in our case $\check{z}_1-\check{z}_2\approx 2\times 0.6$, the force becomes repulsive.

We now consider the case of a weakly interacting 1D gas. In order to solve the Gross-Pitaevskii equation, we make use of the Thomas-Fermi (TF) approximation. Although the results obtained in this way cannot be smoothly connected to the ideal-condensate case, the TF approximation allows us to derive a compact expression for the level shift. The TF condensate wave function is given by

$$\psi_0(z) = \sqrt{\frac{\mu}{g_{1D}}\left(1-\frac{z^2}{R_{TF}^2}\right)}, \tag{26}$$

where the TF radius is given by $R_{TF}=\sqrt{2\mu/m_B\omega_B^2}$. μ denotes the chemical potential, and the one-dimensional interaction parameter g_{1D} is defined analogous to κ_{1D}. To solve the Bogoliubov–de Gennes equations analytically, further approximations are needed as discussed in [13]. We here take over the results for the functions $f_j^\pm$ obtained in [14],

$$f_j^\pm(z) = \sqrt{\frac{2j+1}{2R_{TF}}}\left[\frac{2\mu}{E_j}\left(1-\frac{z^2}{R_{TF}^2}\right)\right]^{\pm 1/2}P_j\left(\frac{z}{R_{TF}}\right) \tag{27}$$

with the energies $E_j=\hbar\omega_B\sqrt{j(j+1)/2}$. The P_j are Legendre polynomials. Using the completeness of the Legendre polynomials, one can explicitly evaluate expression (14). As shown in Appendix D, the sum *including* the $j=0$ term vanishes if the overlap of the impurity wave functions is negligible. Thus the energy shift (14) is determined only by the $j=0$ term, which yields the simple expression

$$\Delta = \frac{\kappa_{1D}^2}{8\hbar R_{TF}g_{1D}}. \tag{28}$$

This result does not depend on the distance of the impurity atoms, which is due to the Thomas-Fermi approximation. The shift is always positive and becomes larger for smaller interactions in the BEC and, as expected from the noninteracting case, for larger 1D confinement. It is instructive to express Δ in terms of the impurity-BEC stattering length a_i and the BEC scattering length a. One finds

$$\Delta = \frac{\omega_\perp}{4}\frac{m_B^2}{m_i^2}\frac{a_i^2}{R_{TF}a}. \tag{29}$$

Here we have $m_i=2m_Bm_S/(m_B+m_S)$. Thus assuming a tight transversal confinement with $\omega_\perp=2\pi\times 10^4$ Hz, a large scattering length between impurities and BEC $a_i=200$ nm, a small scattering within the BEC $a=5$ nm, a small trap with $R_{TF}=20\mu$m, and $m_S\approx m_B$, one finds a conditional frequency shift of $2\pi\times 10^3$ Hz.

As shown in Appendix D, the result of Eq. (28) should be valid as long as the following conditions are fulfilled:

$$\delta r, |z_1-z_2| \gg z_B. \tag{30}$$

Here, δr denotes the distance of one of the impurities to the edge of the condensate. Furthermore, due to the Thomas-Fermi approximation, the interaction strength of the condensate has to fulfill the condition

$$g_{1D} \gg \frac{2\hbar\omega_B R_{TF}}{3N_0}. \tag{31}$$

Hence, we have the restriction

$$\Delta \ll \min\left\{\omega_B, \frac{3N_0\kappa_{1D}^2}{16\hbar^2R_{TF}^2\omega_B}\right\}. \tag{32}$$

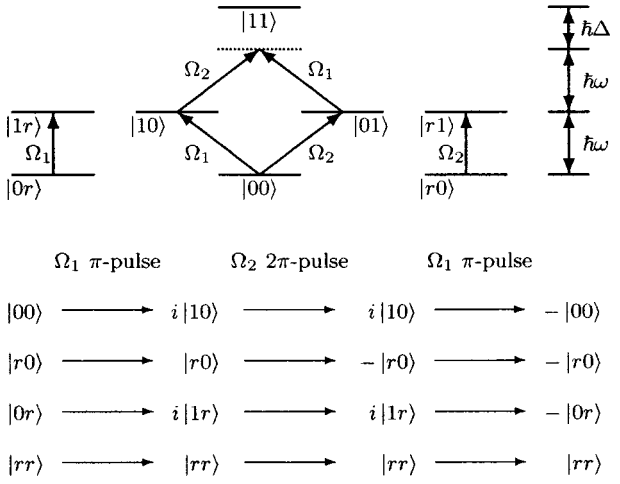

FIG. 6. Implementation of a quantum phase gate: $|0\rangle$ and $|r\rangle$ are the logical states of the qubit, where $|r\rangle$ does not couple to the other states. Ω_j is the Rabi frequency of the transition from $|0\rangle$ to $|1\rangle$ of the jth impurity. The pulse sequence for the implementation of the gate is explained in the text.

V. CONDITIONAL PHASE GATE

The conditional frequency shift of the two-atom state $|1,1\rangle$ due to phonon exchange can be used to implement a universal two-qubit gate, which is an essential building block of any quantum computer [9]. To this end, we extend the two-state model of Eq. (1) to a third state $|r\rangle$, in which there shall be no scattering with condensate atoms. The states $|0\rangle_j$ and $|r\rangle_j$, $j\in\{1,2\}$ of the two atoms encode a qubit each. Since in both internal states there is no scattering interaction with the condensate, the two qubits are decoupled. In order to provide a qubit-qubit interaction, which is required for the quantum gate, we assume that a laser couples $|0\rangle$ and $|1\rangle$. Then a so-called quantum phase gate, up to an overall phase characterized by the truthtable

$$\begin{aligned} |00\rangle &\to -|00\rangle, \\ |r0\rangle &\to -|r0\rangle, \\ |0r\rangle &\to -|0r\rangle, \\ |rr\rangle &\to |rr\rangle, \end{aligned} \tag{33}$$

can be realized by the following sequence of operations (see also Fig. 6).

(i) A π pulse is applied to the first atom, i.e., the laser is controlled in such a way that $\int_0^t \Omega_1(t')dt' = \pi$. This leads to the transitions $|0\rangle \to i|1\rangle$ and $|r\rangle \to |r\rangle$ of the first atom independently of the state of atom 2.

(ii) To the second impurity, a 2π pulse is applied. Since the doubly excited state $|1,1\rangle$ is detuned by the amount Δ, the effect of this pulse on the second atom depends on the state vector of the first atom. If the first atom is in state $|r\rangle_1$, one gets $|0\rangle_2 \to -|0\rangle_2$. If the first atom is, however, in state $|1\rangle$, nothing happens because the transition frequency is shifted by Δ, see Fig. 6.

(iii) Finally, another π pulse is applied to the first impurity atom. The atoms are again in their original state but now with conditional phases as indicated in Fig. 6.

The result of the pulse sequence is equivalent to the truthtable of a phase gate up to an unimportant local operation. To implement this scheme successfully, it is necessary that the characteristic time of the pulses is long compared to the inverse frequency shift Δ^{-1}. Hence the main restriction results from condition (32), i.e., the gate speed is limited by the trap frequency ω_B.

VI. CONCLUSIONS

In the present paper, we have analyzed the interaction of impurity atoms in a Bose-Einstein condensate localized at specific positions by tight confining potentials. It was shown that in addition to the level shift caused by s-wave scattering with the macroscopic condensate field, there are also contributions from the interaction with vacuum fluctuations of the Bogoliubov phonons. The self- and conditonal energy shifts were calculated for a BEC in a box with periodic boundary conditions. It was shown that size and sign of the conditional energy shift depends on the separation of the impurities and is largest for a highly anisotropic condensate geometry and for small interactions within the condensate. With increasing interaction of the condensate atoms, the spatial dependence becomes less and less pronounced. Motivated by these findings, the level shift in a quasi-one-dimensional harmonic trap was calculated. In the Thomas-Fermi limit, a rather simple analytic expression was obtained from a Bogoliubov approach. For small trap sizes, a conditional frequency shift in the range of several kHz seems feasible, which could be of interest for the implementation of a quantum phase gate.

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APPENDIX A: DERIVATION OF THE EQUATION OF MOTION FOR THE STATISTICAL OPERATOR

The total statistical operator of both the condensate and the impurities is denoted by $\hat{\chi}$. Its time evolution is then given by the Liouville–von Neumann equation $i\hbar\partial_t\hat{\chi}(t) = [\hat{H},\hat{\chi}(t)]$, where $\hat{H}=\hat{H}_B+\hat{H}_S+\hat{H}_{int}$ is the Hamiltonian of the whole system, with $\hat{H}_B$ being the Hamiltonian of the condensate, $\hat{H}_S$ that of the impurities and $\hat{H}_{int}$ the interaction. Changing into the interaction picture yields

$$i\hbar\partial_t\tilde{\chi}(t) = [\tilde{H}_{int}(t),\tilde{\chi}(t)]. \tag{A1}$$

Formal integration and resubstitution leads to

$$i\hbar\partial_t\tilde{\chi}(t) = [\tilde{H}_{int}(t),\tilde{\chi}(t_0)] + \frac{1}{i\hbar}\int_{t_0}^{t} dt'[\tilde{H}_{int}(t),[\tilde{H}_{int}(t'),\tilde{\chi}(t')]]. \tag{A2}$$

Here, t_0 is the time when the interaction starts. The statistical operator for the impurity atoms can be obtained by tracing

out the condensate, i.e., $\tilde{\varrho}(t)=\mathrm{Tr}_B[\tilde{\chi}(t)]$. This yields

$$i\hbar\partial_t\tilde{\varrho}(t) = \mathrm{Tr}_B\{[\tilde{H}_{\mathrm{int}}(t),\tilde{\chi}(t_0)]\} + \frac{1}{i\hbar}\int_{t_0}^{t} dt' \mathrm{Tr}_B\{[\tilde{H}_{\mathrm{int}}(t),[\tilde{H}_{\mathrm{int}}(t'),\tilde{\chi}(t')]]\}. \tag{A3}$$

Following the standard approach, we assume that the influence of the impurity atoms on the condensate can be neglected and that the statistical operator of the whole system seperates as

$$\tilde{\chi}(t) = \tilde{\varrho}(t)\otimes\tilde{\varrho}_B(t) + \tilde{\chi}_{\mathrm{corr}}(t) \approx \tilde{\varrho}(t)\otimes\tilde{\varrho}_B(t_0). \tag{A4}$$

Furthermore, since we have incorporated the mean-field contribution to the free Hamiltonian of the impurities, the expectation value of the interaction Hamiltonian vanishes, i.e., $\mathrm{Tr}_B[\tilde{\varrho}_B(t_0)\tilde{H}_{\mathrm{int}}(t)]=0$. With these approximations, we obtain

$$\partial_t\tilde{\varrho}(t) = -\frac{1}{\hbar^2}\int_{t_0}^{t} dt' \mathrm{Tr}_B([\tilde{H}_{\mathrm{int}}(t),[\tilde{H}_{\mathrm{int}}(t'),\tilde{\varrho}(t')\otimes\tilde{\varrho}_B(t_0)]]). \tag{A5}$$

The interaction Hamiltonian in the interaction picture can be expressed as

$$\tilde{H}_{\mathrm{int}}(t) = \sum_{\alpha,\beta}\frac{\kappa}{2}|\alpha\beta,t\rangle\langle\alpha\beta,t|[\delta_{\alpha,1}\tilde{B}_1(t)+\delta_{\beta,1}\tilde{B}_2(t)], \tag{A6}$$

where

$$|\alpha\beta,t\rangle\langle\alpha\beta,t| = e^{(i/\hbar)(\hat{H}_S+\hat{H}_B)t}|\alpha\beta\rangle\langle\alpha\beta|e^{-(i/\hbar)(\hat{H}_S+\hat{H}_B)t}. \tag{A7}$$

Substituting this into Eq. (A5) yields

$$\begin{aligned}\partial_t\tilde{\varrho}_{\alpha\beta,\gamma\delta}(t) = -\frac{\kappa^2}{4\hbar^2}\int_{t_0}^{t} dt' \tilde{\varrho}_{\alpha\beta,\gamma\delta}(t')[&\langle\tilde{B}_1(t)\tilde{B}_1(t')\rangle(\delta_{\alpha,1}-\delta_{\alpha,1}\delta_{\gamma,1}) + \langle\tilde{B}_1(t)\tilde{B}_2(t')\rangle(\delta_{\alpha,1}\delta_{\beta,1}-\delta_{\beta,1}\delta_{\gamma,1}) + \langle\tilde{B}_2(t)\tilde{B}_1(t')\rangle(\delta_{\alpha,1}\delta_{\beta,1}\\ &-\delta_{\alpha,1}\delta_{\delta,1}) + \langle\tilde{B}_2(t)\tilde{B}_2(t')\rangle(\delta_{\beta,1}-\delta_{\beta,1}\delta_{\delta,1}) + \langle\tilde{B}_1(t')\tilde{B}_1(t)\rangle(\delta_{\gamma,1}-\delta_{\alpha,1}\delta_{\gamma,1}) + \langle\tilde{B}_1(t')\tilde{B}_2(t)\rangle(\delta_{\gamma,1}\delta_{\delta,1}-\delta_{\beta,1}\delta_{\gamma,1})\\ &+\langle\tilde{B}_2(t')\tilde{B}_1(t)\rangle(\delta_{\gamma,1}\delta_{\delta,1}-\delta_{\alpha,1}\delta_{\delta,1}) + \langle\tilde{B}_2(t')\tilde{B}_2(t)\rangle(\delta_{\delta,1}-\delta_{\beta,1}\delta_{\delta,1})].\end{aligned} \tag{A8}$$

Because the Markov approximation cannot be applied, we instead first use a Laplace transformation. Setting $t_0=0$, we find

$$\mathcal{L}[\tilde{\varrho}_{\alpha\beta,\gamma\delta}(t)](p) = \frac{\tilde{\varrho}_{\alpha\beta,\gamma\delta}(0)}{p+\frac{1}{4\hbar^2}M_{\alpha\beta,\gamma\delta}(p)} \tag{A9}$$

with

$$\begin{aligned}M_{\alpha\beta,\gamma\delta}(p) = {\sum_j}'\Bigg\{&S_j(1,1)\left(\frac{\kappa_\alpha^2-\kappa_\alpha\kappa_\gamma}{p+\frac{i}{\hbar}E_j}+\frac{\kappa_\gamma^2-\kappa_\alpha\kappa_\gamma}{p-\frac{i}{\hbar}E_j}\right)\\ &+S_j(1,2)\left(\frac{\kappa_\alpha\kappa_\beta-\kappa_\beta\kappa_\gamma}{p+\frac{i}{\hbar}E_j}+\frac{\kappa_\gamma\kappa_\delta-\kappa_\beta\kappa_\gamma}{p-\frac{i}{\hbar}E_j}\right)\\ &+S_j(2,1)\left(\frac{\kappa_\alpha\kappa_\beta-\kappa_\alpha\kappa_\delta}{p+\frac{i}{\hbar}E_j}+\frac{\kappa_\gamma\kappa_\delta-\kappa_\alpha\kappa_\delta}{p-\frac{i}{\hbar}E_j}\right)\\ &+S_j(2,2)\left(\frac{\kappa_\beta^2-\kappa_\beta\kappa_\delta}{p+\frac{i}{\hbar}E_j}+\frac{\kappa_\delta^2-\kappa_\beta\kappa_\delta}{p-\frac{i}{\hbar}E_j}\right)\Bigg\}.\end{aligned} \tag{A10}$$

In general, the Laplace transformation (A9) cannot be inverted analytically. However, if we are interested only in a coarse-grained time evolution, it follows from the properties of the Laplace transformation that only small p are important. If, furthermore, the condition

$$\hbar p \ll \min_j{}'(E_j) \tag{A11}$$

is fullfiled, it is possible to neglect the p dependence of $M_{\alpha\beta,\gamma\delta}$, which amounts to $M_{\alpha\beta,\gamma\delta}(p)\to M_{\alpha\beta,\gamma\delta}(0)$. Hence result (10) follows directly.

It is also clear that this result is only valid for frequencies which are consistent with the coarse-graining assumption, leading to condition (15).

APPENDIX B: BACKACTION OF IMPURITIES ON BEC

In this appendix, we will calcualte the influence of the impurity atoms on the condensate wave function for the case of the ideal, one-dimensional condensate in the harmonic trap. The Hamiltonian of the full problem reads

$$\hat{H} = -\frac{\hbar^2}{2m_B}\frac{d^2}{dz^2}+\frac{1}{2}m_B\omega_B^2z^2-\mu+\hat{H}_1 \tag{B1}$$

with

$$\hat{H}_1 = \frac{\kappa}{2}\delta(z-z_1). \tag{B2}$$

The solutions of the unperturbed Hamiltonian are

$$\psi_j^{(0)}(z) = \frac{1}{\sqrt{2^j j!\sqrt{\pi} z_B}} e^{-z^2/2z_B^2} H_j\left(\frac{z}{z_B}\right) \tag{B3}$$

with the energies $E_j = \hbar\omega_B j$ and $\mu = \hbar\omega_B/2$. Calculating the wave functions in first-order pertubation theory, one gets

$$\psi_0^{(1)}(z) = \frac{\kappa}{2\hbar\omega_B(\sqrt{\pi} z_B)^{3/2}} \exp\left(-\frac{z_1^2}{z_B^2} - \frac{z^2}{2z_B^2}\right) \times \sum_{l=1}^{\infty} \frac{-1}{l 2^l l!} H_l\left(\frac{z_1}{z_B}\right) H_l\left(\frac{z}{z_B}\right). \tag{B4}$$

The sum in this expression is of the order of 1. Since we want to neglect the influence of $\psi_0^{(1)}$, we require

$$1 \gg \frac{|\psi_0^{(1)}|^2}{|\psi_0^{(0)}|^2} \approx \frac{\kappa^2}{4\hbar^2\omega_B^2 \pi z_B^2}. \tag{B5}$$

Because of restriction (15), we have that

$$\hbar\omega_B \gg \hbar\Delta \sim \frac{N_0\kappa^2}{\hbar\omega_B z_B^2 \pi}. \tag{B6}$$

Thus, condition (B5) holds. Because of the interactions the influence of the impurities should be even smaller in the nonideal case. For the homogeneous condensate, one gets analogous results.

APPENDIX C: BOGOLIUBOV THEORY

In this appendix, we briefly summarize the main results of the Bogoliubov approach. We start with the Hamiltonian of the Bose gas in the *s*-wave-scattering approximation,

$$\hat{H}_B = \int d\mathbf{r}\hat{\psi}^\dagger(\mathbf{r})\left(-\frac{\hbar^2}{2m_B}\Delta + V_{ext}(\mathbf{r}) - \mu\right)\hat{\psi}(\mathbf{r}) + \frac{g}{2}\int d\mathbf{r}\hat{\psi}^\dagger(\mathbf{r})\hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r})\hat{\psi}(\mathbf{r}). \tag{C1}$$

The field operator $\hat{\psi}$ of the condensate is then devided into a $\mathbb{C}$-number function ψ_0 which represents the condensed part of the Bose gas and an operator $\hat{\xi}$ of quantum fluctuations: $\hat{\psi}(\mathbf{r}) = \psi_0(\mathbf{r}) + \hat{\xi}(\mathbf{r})$. The wave function of the condensate is given by the Gross-Pitaevskii equation

$$\left(-\frac{\hbar^2}{2m_B}\Delta + V_{ext}(\mathbf{r}) - \mu + g|\psi_0(\mathbf{r})|^2\right)\psi_0(\mathbf{r}) = 0. \tag{C2}$$

By plugging this into the Hamiltonian and neglecting terms of the order $O(\hat{\xi}^3)$ and higher, one gets

$$\hat{H}_B \approx H_B^0 + \int d\mathbf{r}\left\{\hat{\xi}^\dagger(\mathbf{r})\left(-\frac{\hbar^2}{2m_B}\Delta + V_{ext}(\mathbf{r}) - \mu\right)\hat{\xi}(\mathbf{r}) + \frac{g}{2}\left[4|\psi_0(\mathbf{r})|^2\hat{\xi}^\dagger(\mathbf{r})\hat{\xi}(\mathbf{r}) + \psi_0^2(\mathbf{r})\hat{\xi}^\dagger(\mathbf{r})\hat{\xi}^\dagger(\mathbf{r}) + \psi_0^{*2}(\mathbf{r})\hat{\xi}(\mathbf{r})\hat{\xi}(\mathbf{r})\right]\right\}. \tag{C3}$$

The terms linear in $\hat{\xi}$ vanish because of the Gross-Pitaevskii equation. The term H_B^0 does not depend on operators and is without consequence. In order to diagonalize the Hamiltonian, we employ the Bogoliubov ansatz

$$\hat{\xi}(\mathbf{r}) = \sum_\nu{}' u_\nu(\mathbf{r})\hat{b}_\nu - v_\nu^*(\mathbf{r})\hat{b}_\nu^\dagger, \tag{C4}$$

$$\hat{\xi}^\dagger(\mathbf{r}) = \sum_\nu{}' u_\nu^*(\mathbf{r})\hat{b}_\nu^\dagger - v_\nu(\mathbf{r})\hat{b}_\nu. \tag{C5}$$

Here, $\hat{b}_\nu^\dagger$ and $\hat{b}_\nu$ are bosonic creation and annihilation operators of the Bogoliubov quasiparticles. The prime at the sum indicates that the ground state is excluded in the summation. If the wave functions u_ν and v_ν fulfill the Bogoliubov–de Gennes equations (ψ_0 is taken to be real),

$$\left[-\frac{\hbar^2\Delta}{2m_B} + V_{ext}(\mathbf{r}) - \mu\right]u_\nu + g|\psi_0|^2(2u_\nu - v_\nu) = E_\nu u_\nu, \tag{C6}$$

$$\left[-\frac{\hbar^2\Delta}{2m_B} + V_{ext}(\mathbf{r}) - \mu\right]v_\nu + g|\psi_0|^2(2v_\nu - u_\nu) = -E_\nu v_\nu, \tag{C7}$$

with the normalization,

$$\int \{u_\nu(\mathbf{r})u_{\nu'}^*(\mathbf{r}) - v_\nu(\mathbf{r})v_{\nu'}^*(\mathbf{r})\}d\mathbf{r} = \delta_{\nu\nu'} \tag{C8}$$

$$\int \{v_\nu(\mathbf{r})u_{\nu'}(\mathbf{r}) - u_\nu(\mathbf{r})v_{\nu'}(\mathbf{r})\}d\mathbf{r} = 0, \tag{C9}$$

the Hamiltonian takes the very simple form

$$\hat{H}_B = H_B^0 - \sum_\nu{}' E_\nu\int |v_\nu(\mathbf{r})|^2 d\mathbf{r} + \sum_\nu{}' E_\nu\hat{b}_\nu^\dagger\hat{b}_\nu. \tag{C10}$$

With this, the operators $\tilde{\xi}$ in the interaction picture can easily be calculated

$$\tilde{\xi}(\mathbf{r},t) = \sum_\nu{}' u_\nu(\mathbf{r})\hat{b}_\nu e^{-iE_\nu t/\hbar} - v_\nu^*(\mathbf{r})\hat{b}_\nu^\dagger e^{+iE_\nu t/\hbar}. \tag{C11}$$

APPENDIX D: VALIDITY OF EQ. (28)

In order to estimate the range of validity of the expression for the conditional shift in TF approximation, Eq. (28), we start with the sum given in (14), but including the $j=0$ term:

$$\sum_{j=0}^{M}\frac{S_j(1,2)}{E_j} = \sum_{j=0}^{M}\frac{1}{E_j}\psi_0(z_1)f_j^-(z_1)\psi_0(z_2)f_j^-(z_2), \tag{D1}$$

where $f_j^- = u_j - v_j$. By using (27) we find

$$\sum_{j=0}^{M}\frac{S_j(1,2)}{E_j} \sim f_P^M\left(\frac{z}{R_{TF}}, \frac{z'}{R_{TF}}\right), \tag{D2}$$

where we have introduced

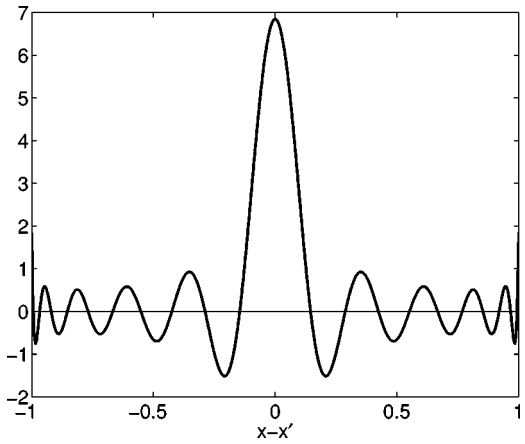

FIG. 7. Picture of f_{P}^{M} for $M=20$.

$$f_{\mathrm{P}}^{M}(x,x') = \sum_{n=0}^{M} \frac{2n+1}{2} P_n(x) P_n(x'). \tag{D3}$$

If $M \to \infty$ the sum approaches the δ-function and f_{P}^{M} gets zero as long as $x \neq x'$. On the other hand the solutions (27) of the Bogoliubov-de Genne equations used here are only valid for [13]

$$\frac{\delta r}{R_{\mathrm{TF}}} \gg \max\left[\frac{\sqrt{M(M+1)}\zeta}{\sqrt{2}}, \sqrt{\frac{\sqrt{2}\zeta}{\sqrt{M(M+1)}}} \right], \tag{D4}$$

where δr is the distance from the edge of the condensate, $\zeta = \hbar\omega_{\mathrm{B}}/2\mu = z_{\mathrm{B}}^2/R_{\mathrm{TF}}^2$.

This implies $M \ll \sqrt{2}\,\delta r/R_{\mathrm{TF}}\zeta$ and with $\delta r \gg R_{\mathrm{TF}}\sqrt{\zeta}$, also following from Eq. (D4) we arrive at $M \ll \sqrt{\frac{2}{\zeta}}$. Thus the limit $M \to \infty$ cannot be taken in (D2). Nevertheless even for a finite but sufficiently large upper limit of summation M the sum is to a good approximation zero as can be seen as follows: In Fig. 7 f_{P}^{20} is shown. One recognizes a pronounced central maximum and vanishingly small oscillations. Hence, Eq. (D2) gets almost zero if the distance of the impurities is much bigger than the width of the central maximum. We thus need to estimate the width of this central peak. With the Stirling formula, one finds asymptotically for large M

$$f_{\mathrm{P}}^{M}(0,0) \approx \frac{M}{\pi}. \tag{D5}$$

Since $\int f_{\mathrm{P}}^{M}(0,s)\mathrm{d}s = 1$, the width of the central peak can be approximated as $\Delta s = \pi/M$. This finally yields the condition

$$\frac{z_1 - z_2}{R_{\mathrm{TF}}} > \Delta s \gg \sqrt{\zeta} = \frac{z_{\mathrm{B}}}{R_{\mathrm{TF}}} \tag{D6}$$

for which the sum in Eq. (D2) is approximately 0. It should be noted that we have assumed the Thomas-Fermi limit $\zeta \ll 1$, which is essential for the analytic solution of the Gross-Pitaevskii and Bogoliubov–de Gennes equations.

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