Three-Body Problem in a Dilute Bose-Einstein Condensate

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We derive the explicit three-body contact potential for a dilute condensed Bose gas from microscopic theory. The three-body coupling constant exhibits the general form predicted by Wu [Phys. Rev. **115**, 1390 (1959)] and is determined in terms of the amplitudes of two- and three-body collisions in vacuum. In the present form, the coupling constant becomes accessible to quantitative studies which should provide the crucial link between few-body collisions and the stability of condensates with attractive two-body forces.

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Despite their diluteness, atomic Bose Einstein condensates (BECs) are significantly influenced by interatomic forces. The binary potential enters their properties mainly through two-body low energy scattering observables described by the s-wave scattering length a. Recent experiments [1] have provided the opportunity to tune the scattering length from the repulsive ($a > 0$) through the ideal gas ($a \sim 0$) to the attractive ($a < 0$) regime, where the gas finally becomes unstable with respect to collapse [2,3]. With this new technique, one can thus access a wide range of dilute gas parameters and study phenomena related to few-body collisions in the gas.

Virtually all properties of BECs at zero temperature are described by a nonlinear Schrödinger equation (NLSE) [4]

$$i\hbar\frac{\partial}{\partial t}\Psi = H_{1\mathrm{B}}\Psi + g_2|\Psi|^2\Psi + g_3|\Psi|^4\Psi + \ldots, \quad (1)$$

which, in this extended form, depends on the Hamiltonian of a single trapped atom as well as the two- and three-body coupling constants g_2 and g_3, respectively. Three-body scattering obviously becomes significant at large scattering lengths, through the increase of the dilute gas parameter $\eta = \sqrt{|\Psi|^2}|a|^3$, but also in the ideal gas regime. Small scattering lengths of only a few Å, e.g., are needed to produce stable condensates with attractive interactions and several thousands of atoms in present day atom traps. Two-body scattering alone, however, seems not sufficient to explain the experimental criterion for stability against collapse of ^{85}Rb [2], and a fit of Eq. (1) to the data gives an attractive three-body interaction with very reasonable coupling constants $|\mathrm{Re}g_3|/\hbar$ of the order of 10^{-27} cm^6/s [5]. In this way, the corresponding three-body mean field shift of the energy density, $\mathrm{Re}g_3|\Psi|^6/3$, should become directly accessible to experiments.

The determination of the three-body coupling constant in a dilute BEC, and its associated mean field energy, have a long history of theoretical research in many-body physics [6]. Already in 1959, Wu [7] discovered the general form $g_3 = 16\pi\hbar^2a^4(4\pi - 3\sqrt{3})\ln(C\eta^2)/m$ for a Bose gas of hard spheres. The constant C in the argument of the logarithm, however, remained undetermined and only recently was significant progress made. In 1999, Braaten and Nieto [8] used effective field theory to determine Wu's general result by taking into account low energy three-body scattering. They estimated the argument of the logarithm on the basis of general assumptions on the length scales set by the interatomic potential. Braaten *et al.* [9] also studied the role of parameters of the potential apart from the scattering length, through fits to many-body Monte Carlo simulations [10], as well as the properties of the effective three-body coupling constant when the scattering length is large in comparison to the range of the potential [11].

To the best of our knowledge, the three-body coupling constant has not been derived from a microscopic description of the gas and expressed in terms of the binary potential. In this Letter, we provide a microscopic theory of three-body collisions in a BEC and determine g_2 and g_3 to second order in the dilute gas parameter η. The derivation is based on the exact quantum evolution of correlation functions, i.e., quantum expectation values of products of single mode annihilation and creation operators of the form $\langle a_{\mathbf{p}}\rangle$, $\langle a_{\mathbf{p}_2}a_{\mathbf{p}_1}\rangle$, $\langle a^\dagger_{\mathbf{q}}a_{\mathbf{p}}\rangle$, etc. References [12,13] provide a general approach to transform the exact infinite hierarchy of dynamic equations for correlation functions into a more favorable form that allows for a systematic truncation in accordance with Wick's theorem. The resulting set of dynamic equations for noncommutative cumulants [13] lends itself to iteration. We apply this cumulant approach here to express the exact dynamic equation for the condensate wave function of a uniform gas through nonlinear terms in Ψ and Ψ^* and determine g_2 and g_3 in equilibrium.

According to Ref. [13], the exact quantum evolution of the condensate wave function $\Psi_{\mathbf{p}} = \langle a_{\mathbf{p}}\rangle$ depends on the pair function $\Phi_{\mathbf{p}_1\mathbf{p}_2} = \langle a_{\mathbf{p}_2}a_{\mathbf{p}_1}\rangle - \langle a_{\mathbf{p}_2}\rangle\langle a_{\mathbf{p}_1}\rangle$ and the third order cumulant Λ which is associated with the correlation function $\langle a^\dagger_{\mathbf{q}}a_{\mathbf{p}_2}a_{\mathbf{p}_1}\rangle$. We first consider the uniform gas limit. The dynamic equation for Ψ then reads [14]

$$i\hbar\frac{\partial}{\partial t}\Psi(t) = \frac{1}{(\sqrt{2\pi\hbar})^3}\int d\mathbf{q}d\mathbf{p}V(\mathbf{p}_1)\Lambda(\mathbf{q},\mathbf{p},t) + \int d\mathbf{p}V(\mathbf{p})[\Phi(\mathbf{p},t) + (\sqrt{2\pi\hbar})^3\delta(\mathbf{p})\Psi^2(t)] \times \Psi^*(t), \quad (2)$$

where the integration variables are chosen as center of mass and relative atomic momenta $\mathbf{q} = \mathbf{p}_1 + \mathbf{p}_2$ and $\mathbf{p} = (\mathbf{p}_2 - \mathbf{p}_1)/2$, respectively, and $V(\mathbf{p}) = \int d\mathbf{r}V(\mathbf{r}) \times \exp(-i\mathbf{p}\cdot\mathbf{r}/\hbar)/(\sqrt{2\pi\hbar})^3$ is the Fourier transform of the potential into momentum space. Additional terms [13] that are proportional to the density matrix of the noncondensed fraction, $\Gamma_{\mathbf{pq}} = \langle a^\dagger_{\mathbf{q}}a_{\mathbf{p}}\rangle - \langle a^\dagger_{\mathbf{q}}\rangle\langle a_{\mathbf{p}}\rangle$, neither contribute to g_2 nor to g_3 and have been omitted in Eq. (2).

The explicit dependence of Eq. (2) on higher order cumulants can be eliminated successively by solving their dynamic equations formally and inserting the solutions into Eq. (2) [13]. With this iterative procedure, Eq. (2) can be expressed exactly through nonlinear terms in Ψ, Ψ^*, and Γ up to a given order and a remainder which contains only higher order cumulants. To obtain the coupling constants g_2 and g_3, we determine all the nonlinear terms in Ψ and Ψ^* up to the fifth order.

The formal solutions of the dynamic equations of Φ and Λ [13] involve the triple function χ, i.e., the third order cumulant associated with the correlation function $\langle a_{\mathbf{p}_3}a_{\mathbf{p}_2}a_{\mathbf{p}_1}\rangle$, and the Green's function corresponding to two atoms described by the two-body Hamiltonian $H_{2B} = -\frac{\hbar^2}{m}\Delta_{\mathbf{r}} + V(\mathbf{r})$ in their center of mass frame. The relevant retarded Green's function is given by [15] $G(t) = \frac{1}{i\hbar}\theta(t)\exp(-iH_{2B}t/\hbar)$. We use $G(t,\mathbf{p},\mathbf{p}') = \langle\mathbf{p}|G(t)S|\mathbf{p}'\rangle$ in momentum space, where S projects onto the symmetrized relative momenta that correspond to two identical Bose atoms. At the initial time t_0, the gas is assumed to be prepared in a (ideal gas) coherent state of the lowest energy mode [16]. The formal solutions then read:

$$\Phi(\mathbf{p},t) = \int_{t_0}^{\infty}d\tau\int d\mathbf{p}'G(t-\tau,\mathbf{p},\mathbf{p}')V(\mathbf{p}')\Psi^2(\tau) + \int_{t_0}^{\infty}d\tau\int d\mathbf{q}'d\mathbf{p}'G(t-\tau,\mathbf{p},\mathbf{p}'_2)[V(\mathbf{p}'_1)+V(\mathbf{q}')] \times [\chi(\mathbf{q}',\mathbf{p}',\tau) + 2(\sqrt{2\pi\hbar})^3\delta(\mathbf{q}')\Phi(\mathbf{p}',\tau)\Psi(\tau)]\Psi^*(\tau), \quad (3)$$

$$\Lambda(\mathbf{q},\mathbf{p},t) = \int_{t_0}^{\infty}d\tau\int d\mathbf{q}'d\mathbf{p}'G(t-\tau,\mathbf{p},\mathbf{p}'_2-\mathbf{q}/2)[\chi(\mathbf{q}',\mathbf{p}',\tau) + 2(\sqrt{2\pi\hbar})^3\delta(\mathbf{q}')\Phi(\mathbf{p}',\tau)\Psi(\tau)] \times [V(\mathbf{p}'_1-\mathbf{q}) + V(\mathbf{q}'-\mathbf{q})]\Phi^*(\mathbf{q},\tau)e^{i(q^2/4m)(t-\tau)/\hbar} - \int_{t_0}^{\infty}d\tau\int d\mathbf{q}'d\mathbf{p}'G(t-\tau,\mathbf{p},\mathbf{p}')\chi(-\mathbf{q},\mathbf{p}',\tau)V(\mathbf{q}+\mathbf{q}') \times [\Phi(\mathbf{q}',\tau) + (\sqrt{2\pi\hbar})^3\delta(\mathbf{q}')\Psi^2(\tau)]^*e^{i(q^2/4m)(t-\tau)/\hbar}, \quad (4)$$

where $\mathbf{p}'_1 = \mathbf{q}'/2 - \mathbf{p}'$ and $\mathbf{p}'_2 = \mathbf{q}'/2 + \mathbf{p}'$. The form of Eqs. (3) and (4) is exact, save that terms that neither contribute to g_2 nor to g_3 are not given. The arguments of the triple function χ for a uniform gas are chosen here as the three-body Jacobi momenta in Fig. 1.

The dynamic equation for χ involves the Hamiltonian of three atoms interacting pairwise,

$$H_{3B} = -\frac{\hbar^2}{2m}(\Delta_{\mathbf{x}_1} + \Delta_{\mathbf{x}_2} + \Delta_{\mathbf{x}_3}) + V_{3B}, \quad (5)$$

where $V_{3B} = V(\mathbf{r}_{23}) + V(\mathbf{r}_{13}) + V(\mathbf{r}_{12})$ (see Fig. 1). The corresponding symmetrized retarded Green's function in the three-body center of mass frame is denoted here as $G_{3B}(t,\mathbf{q},\mathbf{p},\mathbf{q}',\mathbf{p}')$ in the representation through the Jacobi momenta in Fig. 1. The only relevant contribution of the triple function reads

$$\chi(\mathbf{q},\mathbf{p},t) = 6\int_{t_0}^{\infty}d\tau\int d\mathbf{q}'d\mathbf{p}'G_{3B}(t-\tau,\mathbf{q},\mathbf{p},\mathbf{q}',\mathbf{p}'_2) \times V(\mathbf{q}')\Phi(\mathbf{p}',\tau)\Psi(\tau), \quad (6)$$

where $\mathbf{p}'_2 = \mathbf{q}'/2 + \mathbf{p}'$.

All nonlinear contributions in Ψ and Ψ^* up to the fifth order are obtained by inserting Eqs. (3) and (4) into the right-hand side of Eq. (2) and then replacing χ by Eq. (6) and Φ by its leading first contribution on the right-hand side of Eq. (3). Equation (2) then becomes a non-Markovian NLSE [13] with the leading (two-body) contribution

$$i\hbar\frac{\partial}{\partial t}\Psi(t) = (2\pi\hbar)^3\int_{t_0}^{\infty}d\tau T(t-\tau,0,0)\Psi^2(\tau)\Psi^*(t) + \ldots, \quad (7)$$

where $T(t) = V\delta(t) + VG(t)V$ is the Fourier transform of the energy dependent two-body T matrix [15]. This time dependent transition matrix is sharply peaked at $t = 0$ with a width determined by the two-body collisional duration. The fifth order nonlinear terms in Ψ and Ψ^* (three-body contributions), indicated by the dots on the right-hand side of Eq. (7), involve up to four time integrals which have a similar form to the leading term.

To determine the equilibrium properties of the gas, we assume first that the scattering length is positive and the potential does not support any bound clusters of atoms. In the zero temperature equilibrium, the ansatz $\Psi(t) = \Psi\exp(-i\mu t/\hbar)$ then transforms the NLS Eq. (7), including the three-body contributions, into its stationary form in the limit $t - t_0 \to \infty$ [17]:

$$\mu = g_2(\mu)|\Psi|^2 + g_3(\mu)|\Psi|^4. \quad (8)$$

The two-body contribution to Eq. (8) is directly obtained from Eq. (7) through the Fourier transform of

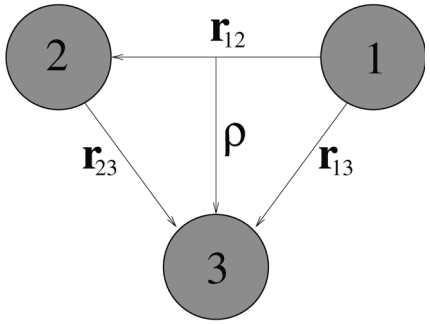

FIG. 1. Jacobi coordinates of three atoms. The spatial coordinates are chosen as the vector from atom 1 to atom 2 ($\mathbf{r}_{12}$) and the vector from the center of mass of atoms 1 and 2 to atom 3 ($\boldsymbol{\rho}$). The conjugate Jacobi momenta are $\mathbf{p} = (\mathbf{p}_2 - \mathbf{p}_1)/2$ and $\mathbf{q} = (2\mathbf{p}_3 - \mathbf{p}_1 - \mathbf{p}_2)/3$, respectively, where $\mathbf{p}_1, \mathbf{p}_2, \mathbf{p}_3$ denote the momenta of the single atoms.

$T(t - \tau, 0, 0)$ at the energy 2μ which yields the two-body T matrix $T(2\mu, 0, 0)$ [18]. The low energy expansion [19,20]

$$T(E, 0, 0) = \frac{1}{(2\pi\hbar)^3}\frac{4\pi\hbar^2}{m}a[1 - i\sqrt{mE/\hbar^2}a + \ldots] \quad (9)$$

shows that the leading contribution to μ is the mean field chemical potential $\mu_0 = 4\pi\hbar^2 a|\Psi|^2/m$. The three-body contributions to the right-hand side of Eq. (7) (not shown explicitly) can also be arranged in such a way that all bare two-body potentials are connected to two- and three-body T matrices. The general form of the real part of Eq. (8) is then obtained as ($\eta = \sqrt{|\Psi|^2 a^3}$):

$$\begin{aligned}\mathrm{Re}\mu &= (2\pi\hbar)^3 \mathrm{Re}T(2\mu, 0, 0)|\Psi|^2 \\ &\quad + 8\mu_0\left(-3\sqrt{3}\ln\left|\frac{\sqrt{m2\mu}}{p^{(3)}}\right| + 4\pi\ln\left|\frac{\sqrt{m2\mu}}{p^{(4)}}\right|\right)\eta^2 \\ &\quad + \frac{1}{2}(2\pi\hbar)^6 T_{3\mathrm{B}}^{(5)}(0, 0, 0)|\Psi|^4, \end{aligned} \quad (10)$$

where corrections smaller than $\mu_0\eta^2$ have been neglected. The first term on the right-hand side of Eq. (10) is the two-body part. All three-body contributions to Eq. (8) are at least of third order in the two-body T matrix. The real parts of the third and fourth order terms exhibit a logarithmic divergence at low energies $\mu \to 0$ as indicated in the second term on the right-hand side of Eq. (10). The respective explicit expressions read

$$\begin{aligned}\ln\left|\frac{\sqrt{m2\mu}}{p^{(3)}}\right| &= -\frac{2\pi^5\hbar^4 m}{3\sqrt{3}a^4}\mathrm{Re}\int\frac{d\mathbf{p}T(2\mu, \mathbf{p}, 0)}{2\mu - p^2/m + i0} \\ &\quad \times \sum_{\alpha=\pm1}\left\{[T(2\mu, \mathbf{p}, 0)]^*\frac{T(3\mu - \frac{3p^2}{4m}, \alpha\frac{\mathbf{p}}{2}, \frac{\mathbf{p}}{2})}{2\mu - p^2/m - i0} - [T(2\mu, \mathbf{p}, 0)]^*\frac{T(\mu + \frac{p^2}{4m}, \alpha\frac{\mathbf{p}}{2}, \frac{\mathbf{p}}{2})}{2\mu - p^2/m - i0}\right. \\ &\quad \left. + 2T(2\mu, 0, \mathbf{p})\frac{T(3\mu - \frac{3p^2}{4m}, \alpha\frac{\mathbf{p}}{2}, \frac{\mathbf{p}}{2})}{2\mu - p^2/m + i0}\right\}, \end{aligned} \quad (11)$$

$$\begin{aligned}\ln\left|\frac{\sqrt{m2\mu}}{p^{(4)}}\right| &= \frac{\pi^4\hbar^4 m}{2a^4}\mathrm{Re}\int\frac{d\mathbf{q}d\mathbf{p}T(0, 0, \mathbf{q})T(0, \mathbf{p}, 0)}{3\mu - \frac{q^2 + p^2 + \mathbf{q}\cdot\mathbf{p}}{m} + i0} \\ &\quad \times \sum_{\alpha,\beta=\pm1}\left\{\frac{T(-\frac{3q^2}{4m}, \alpha\frac{\mathbf{q}}{2}, \mathbf{p} + \frac{\mathbf{q}}{2})T(-\frac{3p^2}{4m}, \mathbf{q} + \frac{\mathbf{p}}{2}, \beta\frac{\mathbf{p}}{2})}{(2\mu - q^2/m - i0)(2\mu - p^2/m + i0)} + 2\frac{T(-\frac{3q^2}{4m}, \alpha\frac{\mathbf{q}}{2}, \mathbf{p} + \frac{\mathbf{q}}{2})T(-\frac{3p^2}{4m}, \mathbf{q} + \frac{\mathbf{p}}{2}, \beta\frac{\mathbf{p}}{2})}{(2\mu - q^2/m + i0)(2\mu - p^2/m + i0)}\right\}. \end{aligned} \quad (12)$$

The logarithmic behavior of the real parts of the integrals in Eqs. (11) and (12) was determined with the methods in Ref. [20]. The momentum units $p^{(3)}$ and $p^{(4)}$ are found using the regular parts of the integrals in the limit $\mu \to 0$.

The last contribution to the right-hand side of Eq. (10) involves the T matrix for three asymptotically free incoming and outgoing atoms, $T_{3\mathrm{B}}(E) = V_{3\mathrm{B}} + V_{3\mathrm{B}}G_{3\mathrm{B}}(E)V_{3\mathrm{B}}$. The regular part of $T_{3\mathrm{B}}$, denoted here by $T_{3\mathrm{B}}^{(5)}$, consists of all multiple scattering contributions to $T_{3\mathrm{B}}$ from the fifth order upward [21]. $T_{3\mathrm{B}}^{(5)}(E)$ can be evaluated at $E = 0$ [20] and is the only contribution to g_3 that depends on the complete zero energy three-body scattering state.

Equation (8) also exhibits an imaginary part

$$\mathrm{Im}\mu = \mu_0\left[-\sqrt{\frac{m2\mu}{\hbar^2}}a + \frac{8\pi\hbar}{\sqrt{m2\mu}a}\eta^2 + \mathcal{O}(\eta^2\ln\eta)\right] \quad (13)$$

whose first leading term stems from Eq. (9). The second term is the leading contribution to the imaginary part of the integral in Eq. (11). The imaginary part of μ describes the exchange of atoms between the condensed and thermal fraction [13] and is thus required to vanish exactly in equilibrium as soon as all few-body scattering contributions are taken into account. The right-hand sides of Eqs. (10) and (13) change by an amount smaller than $\mu_0\eta^2$ if μ is replaced by its leading contribution μ_0. The square root terms in Eq. (13) then, indeed, cancel each other and Eqs. (10) and (8) yield

$$\begin{aligned} g_2 &= (2\pi\hbar)^3\mathrm{Re}T(2\mu_0, 0, 0), \\ g_3 &= \frac{32\pi\hbar^2}{m}a^4\left(-3\sqrt{3}\ln\left|\frac{\sqrt{m2\mu_0}}{p^{(3)}}\right| + 4\pi\ln\left|\frac{\sqrt{m2\mu_0}}{p^{(4)}}\right|\right) \\ &\quad + \frac{1}{2}(2\pi\hbar)^6 T_{3\mathrm{B}}^{(5)}(0, 0, 0). \end{aligned} \quad (14)$$

A trapped dilute BEC can usually be divided into regions with an extent much larger than the range of the interatomic forces but still much smaller than the scale of the spatial variation of the condensate wave function $\Psi(\mathbf{x})$. In these regions, the gas can be considered as locally homogeneous and the coupling constants in Eq. (14) remain valid when μ_0 is replaced by the local chemical potential $\mu_0(\mathbf{x}) = 4\pi\hbar^2 a|\Psi(\mathbf{x})|^2/m$.

A realistic molecular potential $V(\mathbf{r})$ usually supports two-body bound states. The coupling constant g_3 then acquires an imaginary part through $T_{3B}^{(5)}$. According to three-body collision theory, this imaginary part corresponds to the thresholdless formation of dimer molecules and was determined here via an optical theorem with the methods of Ref. [22]. We thus obtained $2\mathrm{Im}g_3/\hbar = -K_3/6$ where K_3 is the three-body recombination rate constant for an ultracold noncondensed Bose gas. This was determined in Ref. [23] using classical probability arguments, by assuming that three atoms are lost in each event. The factor of $1/6$ expresses the fact that all three condensed atoms share the same quantum state [24] and was verified in subsequent experiments [25]. In the presence of bound states, the condensate can assume only a metastable state. The change of its density, however, is negligible on time scales comparable to collisional durations so that the present results remain valid.

If a is negative but the trapped gas is still stable with respect to collapse, the above analysis slightly modifies: $\mu_0(\mathbf{x})$ then becomes negative and instead of Eq. (13) one obtains real contributions, $\mu_0\sqrt{m2|\mu|}a/\hbar$ and $\mu_0 8\pi\hbar|\Psi|^2a^2/\sqrt{m2|\mu|}$, through Eq. (9) and the integral in Eq. (11), respectively. The contribution of Eq. (11), with $|\mu|$ replaced by $|\mu_0|$, revises the two-body coupling constant to $g_2 = (2\pi\hbar)^3T(2\mu_0, 0, 0) - 4\pi\hbar a^2\sqrt{2|\mu_0|/m}$. This leads to $g_2 = \frac{4\pi\hbar^2}{m}a[1 + \mathcal{O}(\eta^2)]$ by Eq. (9).

When a three-body bound state emerges close to the zero energy threshold, g_3 is dominated by the residue of the corresponding pole through $T_{3B}^{(5)}$ [20]. The real part of g_3 can then assume all positive and negative values in complete analogy to the two-body case. This phenomenon was discussed in Ref. [11] in connection with the Efimov effect in the three-body energy spectrum [26].

The three-body coupling constant in Eq. (14) has the form predicted by Wu [7] and Braaten *et al.* [8,11] and can be determined quantitatively by solving the two- and three-body scattering problem in vacuum [27]. The explicit representation in Eq. (14) also allows us to directly relate all our current knowledge about two- and three-body transition amplitudes to properties of the gas. The present theory is valid for all (nonsingular) molecular potentials and avoids divergences. Convergence at high energies has been achieved by taking into account the exact binary potential which enters the coupling constants through two- and three-body T matrices. At low energies, the arguments of the infrared divergent contributions to g_3 have been determined to multiples of μ_0, which is the energy scale that corresponds to the healing length [4].

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