Rigorous Approach to the Problem of Ultraviolet Divergencies in Dilute Bose Gases

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In this Letter we consider a system of N pairwise finite-range interacting atoms and prove rigorously that in the zero-range interaction limit all the eigenstates and eigenenergies of the Hamiltonian converge to those corresponding to N atoms interacting via the Fermi-Huang regularized pseudopotential. Next, we show that the latter eigensystem (if treated exactly) is *invariant* under a nontrivial transformation of the interaction potential. Finally, we realize that most of the approximate schemes of many-body physics do not exhibit this invariance: We use this property to resolve all inconsistencies of the Hartree-Fock-Bogoliubov variational formalism known thus far.

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The realization of Bose Einstein Condensate [1] has brought an enormous interest in developing new theoretical approaches and refining the existing ones. The mean-field formalism with contact interactions has been shown to provide a powerful tool for analyzing the properties of trapped Bose gases [2]. Unfortunately, the most general variational mean-field approach, the Hartree-Fock-Bogoliubov approximation (HFB), is not yet quite satisfactory if used with contact interactions: It exhibits UV divergencies, inconsistencies with the Hugenholtz-Pines theorem [3], many-body T-matrix calculations [4], and even with the very existence of atomic condensates themselves [5]. Several heuristic modifications of the theory were suggested [3,4,6,7], showing a good agreement with the experimental data [8]. In this Letter, we propose a novel, quite straightforward way to cure these inconsistencies.

First, we prove rigorously that the regularized Fermi-Huang pseudopotential [9] is not just an ansatz, but provides the exact zero-range limit of the many-body observables along with a cancellation of all the UV divergencies. Second, we introduce a new family of pseudopotentials parametrized by a free parameter Λ (so-called Λ potentials): No *exact* (after the zero-range approximation has been made) observable depends on it, while some *approximate* treatments differ for different Λ. The above conclusions are general and they do not rely on any particular approximation. Finally, as an application of this new potential, we find a particular value for Λ such that HFB equations are entirely free of all inconsistencies known thus far.

An explicit expression for the Λ potential reads

$$\hat{V}^{\Lambda}(\vec{r}) = g_{\Lambda}\delta(\vec{r})[\partial_r + \Lambda](r\cdot) \qquad \text{with } g_{\Lambda} = \frac{g_0}{1 - a\Lambda}, \tag{1}$$

where $\vec{r} = \vec{r}_1 - \vec{r}_2$ is the relative coordinate of two atoms, a is the s-wave scattering length, $g_0 = 2\pi\hbar^2 a/\tilde{\mu}$ is the usual effective coupling constant, and $\tilde{\mu} = m/2$ is the reduced mass. When $\Lambda = 0$, $\hat{V}^{\Lambda=0}$ coincides with the Fermi-Huang pseudopotential. For a $1/r$-divergent wave function $\psi(\vec{r}) = \tilde{\alpha}/r + \eta(\vec{r})$ [10], the action of the Λ potential is

$$\hat{V}^{\Lambda}\psi(\vec{r}) = g_{\Lambda}\delta(\vec{r})[\eta(\vec{0}) + \Lambda\tilde{\alpha}]. \tag{2}$$

For a low-energy two-body body scattering process, the eigenstates of the Λ potential coincide with the asymptotic form of the s-wave eigenstates of any other interaction potential of a scattering length a. However, for energies of the order $(\hbar^2/ma^2)$ or higher, the actual finite size structure of the potentials comes into play, and the range of the applicability of the zero-range approximation reduces to the particular case of a zero-energy resonance.

Now, we consider a system of N atoms of mass m and coordinates $\{\mathbf{r}\} \equiv \{\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N\}$ interacting via $\hat{V}^{\Lambda}$. The Hamiltonian reads

$$\hat{\mathcal{H}}^{\text{p.p.}} = \sum_{i=1}^{N} \frac{p_i^2}{2m} + \sum_{\alpha=1}^{\alpha_{\max}} \hat{V}^{\Lambda}(r_\alpha), \tag{3}$$

where $\alpha = 1, \ldots, \alpha_{\max} \equiv N(N-1)/2$ labels ordered pairs of atoms (i_α, j_α), and $\vec{r}_\alpha = \vec{r}_{i_\alpha} - \vec{r}_{j_\alpha}$ is the relative position of the members of the αth pair. As a direct consequence of Eq. (2), any eigenstate $\Psi(\{\mathbf{r}\})$ of (3) is a solution of an interaction-free Schrödinger equation subject to the following contact conditions for all pairs α:

$$\lim_{r_\alpha \to 0} \frac{\partial}{\partial r_\alpha}\Big|_{\{\mathcal{R}_\alpha\}} \ln[r_\alpha \Psi] = -\frac{1}{a}, \tag{4}$$

where $\{\mathcal{R}_\alpha\} \equiv \{\vec{R}_\alpha, \{\vec{r}_i | i \neq i_\alpha, j_\alpha\}\}$ is a set composed of the coordinate of the center of mass $\vec{R}_\alpha = (\vec{r}_{i_\alpha} + \vec{r}_{j_\alpha})/2$ of the αth pair and all other coordinates not belonging to this pair. Indeed, it is easy to show that the δ singularities in the action of the Hamiltonian (3) on a many-body state $\Psi(\{\vec{r}\})$ cancel each other if and only if Ψ satisfies the contact conditions (4). Notice that these contact conditions *do not depend on* Λ, and thus no *exact* (after the zero-range approximation has been made) eigenstate does.

Now, we are going to show how regularized pseudopotentials arise in the limit of zero-range interactions. For this purpose, we consider N particles of mass m, interacting via a potential which belongs to a one-parameter family of square-well potentials: $v^R(r) = -v_0^R \Theta(R - r)$. The depth of the potential $v_0^R > 0$ is chosen in such a way that the scattering length a is the same for all members of the family, and each of them supports the same number of s-wave bound states, either one or none depending on the sign of the scattering length [11]. The Hamiltonian of the system reads

$$\hat{\mathcal{H}}^R = \sum_{i=1}^{N} \frac{p_i^2}{2m} + \sum_{\alpha=1}^{\alpha_{\max}} v^R(r_\alpha). \tag{5}$$

We wish to prove the following.

Statement.—In the limit of the infinitely small potential range, the Green function of the finite-range-interaction Hamiltonian (5) converges to the Green function of the pseudopotential Hamiltonian (3):

$$\lim_{R\to 0}(E - \hat{\mathcal{H}}^R)^{-1} = (E - \hat{\mathcal{H}}^{\text{p.p.}})^{-1}. \tag{6}$$

Proof.—As we saw above [see (4)], all the Λ potentials lead to the same eigenstates (and thus the same Green function): Hence, without loss of generality, we can limit our proof to the case of the Fermi-Huang pseudopotential $\hat{V}^0$.

Let us define two operator-valued functions:

$$\hat{\mathcal{G}}_{\hat{a}}^E = (E + i\epsilon - \hat{a})^{-1}, \qquad \hat{\mathcal{T}}_{\hat{a},\hat{b}}^E = (1 - \hat{b}\hat{\mathcal{G}}_{\hat{a}}^E)^{-1}\hat{b}. \tag{7}$$

The former is the retarded Green function at energy E for a Hamiltonian $\hat{a}$. The latter is the T matrix of a perturbation $\hat{b}$ in the presence of the background Hamiltonian $\hat{a}$. Two relations will be heavily used in what follows. First is the Lippman-Schwinger relation between the Green function of the "full Hamiltonian" $\hat{a} + \hat{b}$ and the one of the background:

$$\hat{\mathcal{G}}_{\hat{a}+\hat{b}}^E = \hat{\mathcal{G}}_{\hat{a}}^E + \hat{\mathcal{G}}_{\hat{a}}^E \hat{\mathcal{T}}_{\hat{a},\hat{b}}^E \hat{\mathcal{G}}_{\hat{a}}^E. \tag{8}$$

The second is the Lupu-Sax formula [12] relating the T matrices of the same perturbation but in two different background Hamiltonians $\hat{a}_1$ and $\hat{a}_2$:

$$\hat{\mathcal{T}}_{\hat{a}_2,\hat{b}}^E = [1 - \hat{\mathcal{T}}_{\hat{a}_1,\hat{b}}^E(\hat{\mathcal{G}}_{\hat{a}_2}^E - \hat{\mathcal{G}}_{\hat{a}_1}^E)]^{-1}\hat{\mathcal{T}}_{\hat{a}_1,\hat{b}}^E. \tag{9}$$

Introduce also a family of "reduced Hamiltonians" $\hat{\mathcal{H}}_{\{\alpha\}}^R$ and a family of reference Hamiltonians $\hat{h}_\alpha^E$:

$$\hat{\mathcal{H}}_{\{\alpha\}}^R = \sum_{i=1}^{N} \frac{p_i^2}{2m} + \sum_{\beta=1}^{\alpha} v^R(r_\beta) \quad \text{and} \quad \hat{h}_\alpha^E = \frac{p_\alpha^2}{2\tilde{\mu}} + E, \tag{10}$$

where $\vec{p}_\alpha = (\vec{p}_{i_\alpha} - \vec{p}_{j_\alpha})/2$ is the relative momentum for the αth pair. Each reference Hamiltonian is just a sum of the relative kinetic energy for the corresponding pair and the energy E at which the Green functions (6) are compared. The Green function of the αth reference Hamiltonian is proportional to the zero-energy Green function for the relative motion of two particles:

$$\langle\{\mathbf{r}\}|\hat{\mathcal{G}}_{\hat{h}_\alpha^E}^E|\{\mathbf{r}'\}\rangle = -\frac{\tilde{\mu}}{2\pi\hbar^2|\vec{r}_\alpha - \vec{r}'_\alpha|}\,\delta(\{\mathcal{R}_\alpha - \mathcal{R}_{\boldsymbol{\alpha}}{}'\}). \tag{11}$$

In turn, the T matrix of the interaction potential $\hat{v}_\alpha^R \equiv v^R(r_\alpha)$ in the presence of $\hat{h}_\alpha^E$ can be expressed through the *zero-energy two-body T matrix* of it:

$$\langle\{\mathbf{r}\}|\hat{\mathcal{T}}_{\hat{h}_\alpha^E,\hat{v}_\alpha^R}^E|\{\mathbf{r}'\}\rangle = g_0 D^R(\vec{r}_\alpha,\vec{r}'_\alpha)\delta(\{\mathcal{R}_\alpha - \mathcal{R}'_\alpha\}). \tag{12}$$

The kernel D^R is zero when $r_\alpha > R$ or $r'_\alpha > R$ and is normalized to unity as $\int d^3\vec{r}\, d^3\vec{r}'\, D^R(\vec{r},\vec{r}') = 1$. An explicit expression for it can be found in Ref. [13]. In the limit of zero-range interaction, the kernel obviously converges to a product of delta functions, and, hence, the T matrix converges to

$$\hat{\mathcal{T}}_{\hat{h}_\alpha^E,\hat{v}_\alpha^R}^E \overset{R\to 0}{\to} g_0\delta(\vec{r}_\alpha). \tag{13}$$

Notice that by construction of the reference Hamiltonian $\hat{h}_\alpha^E$ neither the Green function $\hat{\mathcal{G}}_{\hat{h}_\alpha^E}^E$ nor the T matrix $\hat{\mathcal{T}}_{\hat{h}_\alpha^E,\hat{v}_\alpha^R}^E$ depends on energy E.

Using relations (8) and (9), the full many-body Green function of the system can be rigorously expressed through the zero-energy two-body T matrices (12) of the interaction potential $v^R(r)$. Removing from the Hamiltonian (5) one pair interaction after another, we obtain the following chain relation:

$$\begin{aligned}
&(E - \hat{\mathcal{H}}^R)^{-1} \equiv \hat{\mathcal{G}}_{\hat{\mathcal{H}}^R}^E \equiv \hat{\mathcal{G}}_{\hat{\mathcal{H}}_{\{\alpha_{\max}\}}^R}^E \\
&\uparrow\cdots \\
&\hat{\mathcal{G}}_{\hat{\mathcal{H}}_{\{\alpha\}}^R}^E = \hat{\mathcal{G}}_{\hat{\mathcal{H}}_{\{\alpha-1\}}^R}^E \\
&\qquad + \hat{\mathcal{G}}_{\hat{\mathcal{H}}_{\{\alpha-1\}}^R}^E [1 - \hat{\mathcal{T}}_{\hat{h}_\alpha^E,\hat{v}_\alpha^R}^E(\hat{\mathcal{G}}_{\hat{\mathcal{H}}_{\{\alpha-1\}}^R}^E - \hat{\mathcal{G}}_{\hat{h}_\alpha^E}^E)]^{-1} \\
&\qquad \times \hat{\mathcal{T}}_{\hat{h}_\alpha^E,\hat{v}_\alpha^R}^E \hat{\mathcal{G}}_{\hat{\mathcal{H}}_{\{\alpha-1\}}^R}^E \\
&\uparrow\cdots \\
&\hat{\mathcal{G}}_{\hat{\mathcal{H}}_{\{0\}}}^E \equiv \left(E - \sum_{i=1}^{N} \frac{p_i^2}{2m}\right)^{-1}.
\end{aligned} \tag{14}$$

This relation is the cornerstone of the proof.

Imagine now that the full Green function $\hat{\mathcal{G}}_{\hat{\mathcal{H}}^R}^E$ acts on a state $|\Psi\rangle$ whose wave function $\Psi(\{\mathbf{r}\})$ is regular everywhere. Computation of the result of this action $\langle\{\mathbf{r}\}|\hat{\mathcal{G}}_{\hat{\mathcal{H}}^R}^E|\Psi\rangle$ involves expressions of a form $\hat{\mathcal{T}}_{\hat{h}_\alpha^E,\hat{v}_\alpha^R}^E \times (\hat{\mathcal{G}}_{\hat{\mathcal{H}}_{\{\alpha-1\}}^R}^E - \hat{\mathcal{G}}_{\hat{h}_\alpha^E}^E)\hat{\mathcal{T}}_{\hat{h}_\alpha^E,\hat{v}_\alpha^R}^E \Xi$, where $\Xi(\{\mathbf{r}\})$ is a regular function, and, in the limit $R \to 0$, leads to the expressions of the following type:

$$g_0\delta(\vec{r}_\alpha)\left[\Gamma(\vec{r}_\alpha) - \frac{\tilde{\alpha}}{r_\alpha}\right]. \tag{15}$$

[In Eq. (15), both $\Gamma(\vec{r}_\alpha)$ and $\tilde{\alpha}$ depend also on $\{\mathcal{R}_\alpha\}$.] Γ is given by

$$\Gamma(\vec{r}_\alpha) = \int d^{3N}\{\mathbf{r}'\}\langle\{\mathbf{r}\}|\hat{\mathcal{G}}^E_{\hat{\mathcal{H}}^{R\to 0}_{\{\alpha-1\}}}|\{\mathbf{r}'\}\rangle g_0\delta(\vec{r}'_\alpha)\Xi(\{\mathbf{r}'\}),$$

and $\tilde{\alpha} = -g_0(\tilde{\mu}/2\pi\hbar^2)\Xi(\{\mathbf{r}\})|_{\vec{r}_\alpha=0}$. Now using the definition of the Green function $\hat{\mathcal{G}}^E_{\hat{\mathcal{H}}^R_{\{\alpha-1\}}}$, we find that $\Gamma(\vec{r}_\alpha)$ has an UV singularity of form $\tilde{\alpha}/r_\alpha$ [the same as the second term in expression (15)] (see [14]). This leads to

$$g_0\delta(\vec{r}_\alpha)\left[\Gamma(\vec{r}_\alpha) - \frac{\tilde{\alpha}}{r_\alpha}\right] = \hat{V}^0_\alpha\Gamma(\vec{r}_\alpha), \qquad (16)$$

i.e., the expression (15) involves the Fermi-Huang pseudopotential $\hat{V}^0_\alpha \equiv \hat{V}^0(r_\alpha)$ [cf. (2) at $\Lambda = 0$]. This justifies the following limit:

$$\hat{\mathcal{T}}^E_{\hat{h}^E_\alpha,\hat{v}^R_\alpha}(\hat{\mathcal{G}}^E_{\hat{\mathcal{H}}^R_{\{\alpha-1\}}} - \hat{\mathcal{G}}^E_{\hat{h}^E_\alpha}) \overset{R\to 0}{\to} \hat{V}^0_\alpha\hat{\mathcal{G}}^E_{\hat{\mathcal{H}}^{R\to 0}_{\{\alpha-1\}}}. \qquad (17)$$

Inserting the above substitution at every level of the chain procedure (14) and collecting all the terms [15], one finally arrives at $\lim_{R\to 0}\hat{\mathcal{G}}^E_{\hat{\mathcal{H}}^R} = \hat{\mathcal{G}}^E_{\hat{\mathcal{H}}^{\text{p.p.}}}$, Q.E.D.

Notice that the relation (17) clearly shows that the role of the regularizing operator in the pseudopotential expression (1) is to subtract the free propagators $\hat{\mathcal{G}}^E_{\hat{h}^E_\alpha}$ already taken into account by the two-body T matrix $\hat{\mathcal{T}}^E_{\hat{h}^E_\alpha,\hat{v}^R_\alpha}$. As a result, UV divergencies disappear at each level of the chain recursion (14).

As an application of the Λ potential, we consider now the HFB theory for N bosons interacting via V^Λ with $a > 0$, in a box of size L. As we will see, the Λ freedom in choosing the effective Hamiltonian (3) offers the following advantages: (a) unlike for the conventional HFB formalism ($\Lambda = 0$), there exists a range of Λ such that the *atomic* condensate constitutes the minimum of the HFB functional in the low density regime [16]; (b) for a particular value, $\Lambda = \Lambda^\star$, HFB equations are consistent with the results of the ladder approximation for the many-body T matrix [4] and the Hugenholtz-Pines theorem is satisfied; (c) in the vicinity of $\Lambda^\star$, the ground state energy of the system is consistent with Bogoliubov's predictions.

The HFB approximation is twofold. First, it breaks the U(1) symmetry: The atomic field $\hat{\psi}$ is split into a classical field Φ and a quantum fluctuation $\hat{\phi} = \hat{\psi} - \Phi$. Second, the exact density operator is replaced by a Gaussian variational ansatz: $\hat{D} \equiv \exp(-\hat{K}/k_BT)/Z$, where Z is the partition function and the quadratic variational Hamiltonian is

$$\hat{K}[h,\Delta,\Phi] = \frac{1}{2}\int\int d^3\vec{r}_1\, d^3\vec{r}_2[\hat{\phi}^\dagger(\vec{r}_1)h(\vec{r}_1,\vec{r}_2)\hat{\phi}(\vec{r}_2) + \hat{\phi}^\dagger(\vec{r}_1)\Delta(\vec{r}_1,\vec{r}_2)\hat{\phi}^\dagger(\vec{r}_2) + \text{H.c.}]. \qquad (18)$$

For what follows, we introduce the coordinates $\vec{R} = (\vec{r}_1 + \vec{r}_2)/2$ and $\vec{r} = \vec{r}_1 - \vec{r}_2$. The second-quantized form of the full Hamiltonian (3) reads

$$\hat{\mathcal{H}}^\Lambda = \int d^3\vec{R}\left\{\hat{\psi}^\dagger\left(-\frac{\hbar^2}{2m}\Delta\right)\hat{\psi} + \frac{g_\Lambda}{2}\hat{\psi}^\dagger\hat{\psi}^\dagger\overset{\Lambda}{\hat{\psi}\hat{\psi}}\right\}, \qquad (19)$$

where

$$F(\vec{R},\vec{R}) = \lim_{r\to 0}\{\partial_r + \Lambda\}[rF(\vec{R} + \vec{r}/2, \vec{R} - \vec{r}/2)] \qquad (20)$$

is a shortened notation for the action of the regularizing operator [see (1)]. Using Wick's theorem, we obtain an approximate grand canonical potential $J \equiv E^\Lambda - \mu N - TS$, where $E^\Lambda = \text{Tr}[\hat{\mathcal{H}}^\Lambda\hat{D}]$ is the energy, N is the number of particles, and $S = -k_B\text{Tr}[\ln(\hat{D})\hat{D}]$ is the entropy. Minimization of J with respect to the three variational fields h, Δ, and Φ leads to the following implicit equations for these fields:

$$\begin{aligned} h(\vec{r}_1,\vec{r}_2) &= -\frac{\hbar^2}{2m}(\vec{\nabla}^2\delta)(\vec{r}) + [\hbar\Sigma^\Lambda_{11} - \mu]\delta(\vec{r}), \\ \Delta(\vec{r}_1,\vec{r}_2) &= \hbar\Sigma^\Lambda_{12}\delta(\vec{r}), \\ -\frac{\hbar^2}{2m}\Delta\Phi &+ [g_\Lambda(2\tilde{n} + |\Phi|^2) - \mu]\Phi + g_\Lambda\tilde{\kappa}_\Lambda\Phi^* = 0, \end{aligned} \qquad (21)$$

where $\hbar\Sigma^\Lambda_{11} = 2ng_\Lambda$ and $\hbar\Sigma^\Lambda_{12} = g_\Lambda(\Phi^2 + \tilde{\kappa}_\Lambda)$ are the self-energies, $\tilde{n} = \text{Tr}[\hat{\phi}^\dagger(\vec{R})\hat{\phi}(\vec{R})\hat{D}]$ is the noncondensed density, $n = |\Phi|^2 + \tilde{n}$ is the total density, and

$$\tilde{\kappa}_\Lambda = \tilde{\kappa}(\vec{R},\vec{R})^\Lambda$$

results from the action of the regularizing operator (20) on the anomalous density $\tilde{\kappa}(\vec{r}_1,\vec{r}_2) = \text{Tr}[\hat{\phi}(\vec{r}_1)\hat{\phi}(\vec{r}_2)\hat{D}]$.

The diagonalization of the variational Hamiltonian $\hat{K}$ leads to the following quasiparticle spectrum:

$$\hbar\omega_k = \left(\frac{\hbar^2k^2}{2m} + 2g_\Lambda\Phi^2\right)^{1/2}\left(\frac{\hbar^2k^2}{2m} - 2g_\Lambda\tilde{\kappa}_\Lambda\right)^{1/2}. \qquad (22)$$

Equations (21) and (22) clearly show that HFB is Λ dependent. As it has been shown in Ref. [4], this approach is able only to provide a Born approximation for the diagonal self-energy $\hbar\Sigma_{11}$; hence, its explicit Λ dependence. However, this is not the case for $\hbar\Sigma_{12}$; indeed, the total pairing field reproduces the contact conditions (4) of a two-body wave function,

$$\langle\hat{\psi}(\vec{r}_1)\hat{\psi}(\vec{r}_2)\rangle = (\Phi^2 + \tilde{\kappa}_0)\left(1 - \frac{a}{r}\right) + \mathcal{O}(r), \qquad (23)$$

and as a result $\hbar\Sigma^\Lambda_{12} = g_0(\Phi^2 + \tilde{\kappa}_0)$ for all Λ.

Requiring that all the eigenenergies (22) are real, we find that, for zero temperature and densities below a value of $n_{\text{crit}} = \frac{\pi}{192a^3}$, the existence of an atomic condensate ($\Phi \neq 0$) implies the following constraint on Λ:

$$\Lambda^\star a \leq \Lambda a < 1 \qquad \text{with } \Lambda^\star a = \frac{\tilde{\kappa}_0}{\Phi^2 + \tilde{\kappa}_0}. \qquad (24)$$

At the lower limit $\Lambda = \Lambda^\star$, the Λ-regularized anomalous density disappears, and the theory becomes *fully consistent* with the results of the many-body T-matrix calculations in the ladder diagrams approximation [4]:

$$\tilde{\kappa}_{\Lambda^\star} = 0; \qquad \hbar\Sigma_{11}^{\Lambda^\star} = 2ng_{\Lambda^\star}; \qquad \hbar\Sigma_{12}^{\Lambda^\star} = g_{\Lambda^\star}\Phi^2,$$
$$g_{\Lambda^\star} = g_0\left[1 + \frac{\tilde{\kappa}_0}{\Phi^2}\right] = T^{\mathrm{MB}}(\vec{0},\vec{0},\vec{0};0), \tag{25}$$

yielding a gapless spectrum [17,18].

Consider now the zero-temperature low-density limit of our equations. Assuming Λa to be of the order of $\sqrt{na^3}$ and neglecting all the terms of order na^3 or higher, the energy E^Λ is *independent* of Λ and coincides with the well-known Bogoliubov result

$$E^\Lambda = \frac{g_0}{2}\, nN\left(1 + \frac{128}{15\sqrt{\pi}}\sqrt{na^3} + \ldots\right). \tag{26}$$

The Λ-potential based variational HFB model is therefore consistent with the perturbative Bogoliubov approach. As the density increases, the parameter $\Lambda^\star$ increases as well, and at a critical density $n_{\mathrm{crit}} = \frac{\pi}{192a^3}$ we find $\Lambda^\star a = 1$: The energy diverges and the mean-field treatment breaks down.

Note in conclusion that the Λ invariance described in our Letter holds even if the constant Λ is replaced by an arbitrary field $\Lambda(\vec{R})$. The generalization of our HFB theory to the case of the trapped gases is thus straightforward: One has simply to fix Λ as $\Lambda(\vec{R}) = \Lambda^\star[\tilde{\kappa}_0(\vec{R}), \Phi^2(\vec{R})]$ according to (24) at every point $\vec{R}$ of the trap.

As an extension of this work, we mention that, using a procedure similar to the 3D case, it is possible to obtain the low-dimensional analogs of the Λ potential:

$$V_{2\mathrm{D}}^\Lambda(\vec{\rho}) = -\frac{\pi\hbar^2}{\tilde{\mu}}\,\frac{1}{\log(q\Lambda R)} \times \delta(\vec{\rho})\left\{1 - \log(q\Lambda\rho)\rho\,\frac{\partial}{\partial\rho}\right\},$$
$$V_{1\mathrm{D}}^\Lambda(z) = -\frac{\hbar^2}{\tilde{\mu}}\,\frac{\Lambda}{\Lambda a_{1\mathrm{D}} - 1} \times \delta(z)\left\{1 + \frac{1}{2\Lambda}\,\frac{\partial}{\partial z}\left(\Big|_{0+} - \Big|_{0-}\right)\right\},$$

where $q = e^C/2$, C is the Euler's constant, R is the 2D effective hard disk radius, and $a_{1\mathrm{D}}$ is the 1D scattering length [19,20].

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[15] This calculation also involves expressions of a form $\hat{\mathcal{T}}^E_{\hbar\tilde{k}^E_\alpha,\hat{v}^R_\alpha}\Xi$, where the limit $\hat{\mathcal{T}}^E_{\hbar\tilde{k}^E_\alpha,\hat{v}^R_\alpha}\Xi \overset{R\to 0}{\to} \hat{V}^0_\alpha\Xi$ is also well justified.
[16] The ground state of a real many-body Hamiltonian is not an atomic condensate, due to the presence of two-body bound states. For $a > 0$, the pseudopotential also supports a bound state which coincides with the asymptotic form of the highest s-wave bound state of the real two-body potential. As a result, at $\Lambda = 0$ (and more generally at $\Lambda < \Lambda^\star$) HFB describes a *molecular* condensate, instead of the *atomic* one [5].
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