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# BCS theory for trapped ultracold fermions

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**Abstract.** We develop an extension of the well-known BCS-theory to systems with trapped fermionic atoms. The theory fully includes the quantized energy levels in the trap. The key ingredient is to model the attractive interaction between two atoms by a pseudo-potential which leads to a well defined scattering problem and consequently to a BCS-theory free of divergences. We present numerical results for the BCS critical temperature and the temperature dependence of the gap. They are used as a test of existing semi-classical approximations.

**PACS.** 05.30.Fk Fermion systems and electron gas – 03.75.Fi Phase coherent atomic ensembles; quantum condensation phenomena – 32.80.Pj Optical cooling of atoms; trapping

## 1 Introduction

Considerable interest in the field of ultracold atomic gases has been sparked by the achievement of Bose-Einstein condensation in the bosonic systems $^{87}$Rb, $^{23}$Na and $^{7}$Li [1]. Recently, several experimental groups have extended these experiments to the case of trapped fermions [2]. As a first step, it is attempted to achieve a degenerate Fermi gas. In a possible next step, the celebrated Bardeen-Cooper-Schrieffer (BCS) phase transition could be observed. A promising candidate for achieving this transition is the isotope $^{6}$Li: by trapping $^{6}$Li in two hyperfine states, one can take advantage of the strong (attractive) interactions due to $s$-wave scattering between atoms in different hyperfine states to achieve pair creation at a reasonably high temperature [3].

BCS-pairing occurs in a multitude of physical systems (*e.g.* electrons in metals, electron-hole exciton systems and neutron-proton systems) which share the characteristic that the formation of bound states (Cooper pairs) between the strongly coupled constituents is energetically favorable [4]. For ultracold atoms in traps, the interactions are much better-known than in most of the above mentioned systems [5]. Therefore, the achievement of a superfluid state in these systems opens up the possibility of testing our theoretical models, in particular, the validity of the BCS theory itself. Furthermore, the interaction strength and the density of the gas are experimentally tunable which, in principle, makes it possible to study the crossover from BCS pairing to Bose-Einstein condensation of bosonic pairs [6].

To describe experiments with trapped fermionic atoms, one has to extend present theories (i) to include the discrete nature of the quantum energy levels of the particles in the trap, and (ii) to take into account the interactions specific to the atomic case. We consider a model of trapped fermions with two internal states. At low energies, the $p$-wave interaction between atoms in the same internal state is negligible compared to the $s$-wave interaction between atoms in different internal states. The latter interaction is characterized at low energies and for dilute gases ($k_{\rm F} r_{\rm e} < 1$, where $r_{\rm e}$ is the effective range of the interaction, $k_{\rm F}$ the Fermi wavevector) by a single parameter, the scattering length $a$. In order to achieve pair formation the interaction has to be strong; here we assume $|a| \gg r_{\rm e}$, a so-called zero-energy resonance [7]. In this case, an excellent model for the atomic interactions is provided by the pseudo-potential discussed in [8]. This model potential allows us to obtain an extension of the BCS theory to inhomogeneous atomic systems.

We use this theory to calculate various observables including the critical BCS temperature and the density distribution of the gas. We predict that this transition occurs at experimentally accessible densities and temperatures, due to the large negative scattering length for $^{6}$Li atoms. We also carefully compare the results of this general theory to those of a semi-classical theory based on the Thomas-Fermi approximation [9] (see also [10]). In that way, we establish a region of validity of this approximation.

## 2 Hamiltonian and BCS equations of motion

Our model Hamiltonian for the trapped atomic gas includes only the dominant $s$-wave interactions between

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atoms in different internal states:

$$\hat{H} = \sum_\sigma \int \mathrm{d}^3 r \psi_\sigma^\dagger(\mathbf{r}) \mathcal{H}_0 \psi_\sigma(\mathbf{r}) + \frac{1}{2}\sum_\sigma \int \mathrm{d}^3 R \mathrm{d}^3 r \mathrm{d}^3 r' \langle \mathbf{r}'|\hat{V}_{\mathrm{RM}}|\mathbf{r}\rangle \times \psi_\sigma^\dagger(\mathbf{R}+\frac{\mathbf{r}'}{2})\psi_{-\sigma}^\dagger(\mathbf{R}-\frac{\mathbf{r}'}{2})\psi_{-\sigma}(\mathbf{R}-\frac{\mathbf{r}}{2})\psi_\sigma(\mathbf{R}+\frac{\mathbf{r}}{2}). \quad (1)$$

Here the fermion field operator $\psi_\sigma(\mathbf{r})$ annihilates a fermion in the position eigenstate $|\mathbf{r}\rangle$ with an internal state $\sigma = +, -$. The single particle Hamiltonian

$$\mathcal{H}_0 = -\frac{\hbar^2}{2m}\nabla^2 + U_0(\mathbf{r}) - \mu \quad (2)$$

includes the trapping potential $U_0(\mathbf{r})$ and the chemical potential $\mu$. We assume there is an equal number of particles $N_\sigma$ in each state and hence a single chemical potential $\mu$ [11]. In equation (1), we keep a general non-local interaction $\hat{V}_{\mathrm{RM}}$ assuming only that it does not affect the center of mass motion $\mathbf{R}$ of the interacting particles.

We follow the steady-state mean-field approach of BCS theory: the quartic terms of $\hat{H}$ are replaced by quadratic terms taking into account all possible binary contractions in the spirit of Wick's theorem [4]. This leads to linear equations for the field operators [12]:

$$\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}\psi_\pm(\mathbf{r}) = \mathcal{H}_0\psi_\pm(\mathbf{r}) + \int \mathrm{d}^3 r' W(\mathbf{r},\mathbf{r}')\psi_\pm(\mathbf{r}') \pm \int \mathrm{d}^3 r' \Delta(\mathbf{r},\mathbf{r}')\psi_\mp^\dagger(\mathbf{r}'). \quad (3)$$

The Hartree field $W(\mathbf{r},\mathbf{r}')$ is defined as:

$$W(\mathbf{r},\mathbf{r}') \equiv \int \mathrm{d}^3 y \langle \mathbf{r}-\mathbf{r}'+\frac{\mathbf{y}}{2}|\hat{V}_{\mathrm{RM}}|\mathbf{r}'-\mathbf{r}+\frac{\mathbf{y}}{2}\rangle \times \langle \psi_\pm^\dagger(\mathbf{r}'-\frac{\mathbf{y}}{2})\psi_\pm(\mathbf{r}-\frac{\mathbf{y}}{2})\rangle \quad (4)$$

($W$ is the same for both internal states). The pairing field describes correlations due to Cooper pairing:

$$\Delta(\mathbf{r},\mathbf{r}') \equiv \int \mathrm{d}^3 y \langle \mathbf{r}-\mathbf{r}'|\hat{V}_{\mathrm{RM}}|\mathbf{y}\rangle \times \langle \psi_-\left(\frac{\mathbf{r}'+\mathbf{r}}{2}-\frac{\mathbf{y}}{2}\right)\psi_+\left(\frac{\mathbf{r}'+\mathbf{r}}{2}+\frac{\mathbf{y}}{2}\right)\rangle. \quad (5)$$

Equations (3, 4, 5) form a non-linear self-consistent problem.

## 3 BCS theory for atoms: the pseudo-potential

The interaction between atoms is often approximated in the center of mass frame by a contact potential, that is $\hat{V}_{\mathrm{RM}} = 4\pi a\hbar^2\delta(\hat{\mathbf{r}})/m$. However, this approximation leads to an ultra-violet divergent theory. This reflects the fact that the contact interaction is an effective low-energy interaction invalid for high energies. One way to remove this divergence is to introduce an energy cut-off in the interaction. This approach has been used to describe superconductivity in metals where a natural cut-off in the form of the Debye frequency exists. Another method is to express the coupling constant in terms of the two-body scattering matrix obtained from the Lippman-Schwinger equation. This renormalization scheme has been implemented in the literature only in the homogeneous case [6]. Here, we put forward a technique valid also in the inhomogeneous case. We use the pseudo-potential $\hat{V}_{\mathrm{RM}}$ [8] defined for an arbitrary function $\phi(\mathbf{r})$ by

$$\langle \mathbf{r}|\hat{V}_{\mathrm{RM}}|\phi\rangle \equiv g\delta(\mathbf{r})\partial_r[r\phi(\mathbf{r})] \quad (6)$$

with $g = 4\pi a\hbar^2/m$. We first note that in contrast to the usual contact potential the pseudo-potential leads to a well defined two-body scattering problem; the scattering state in the center of mass frame for two particles with a relative momentum $\mathbf{p} = (\mathbf{p}_1 - \mathbf{p}_2)/2$ and a relative position $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$ is

$$\phi(\mathbf{r}) = \mathrm{e}^{\mathrm{i}\mathbf{p}\cdot\mathbf{r}/\hbar} - \frac{a}{1+\mathrm{i}pa/\hbar}\frac{\mathrm{e}^{\mathrm{i}pr/\hbar}}{r}\cdot \quad (7)$$

For a potential of finite range $r_{\mathrm{e}}$ the above form, diverging as $1/r$ for $r \to 0$, is only valid for $r \gg r_{\mathrm{e}}$ and for $pr_{\mathrm{e}}/\hbar \ll 1$ [7]. The pseudo-potential has an effective range $r_{\mathrm{e}} = 0$; this does not lead to any mathematical problem as the $1/r$ divergence is regularized by the operator $\partial_r[r\cdot]$ in equation (6).

We now introduce the pseudo-potential of equation (6) in the equations of motion equation (3) [13]. As it introduces a $\delta(\mathbf{r})$, we have $\Delta(\mathbf{r},\mathbf{r}') = \delta(\mathbf{r}-\mathbf{r}')\Delta(\mathbf{R})$ and $W(\mathbf{r},\mathbf{r}') = \delta(\mathbf{r}-\mathbf{r}')W(\mathbf{R})$, with $\mathbf{R} = (\mathbf{r}+\mathbf{r}')/2$, so that equation (3) becomes local:

$$\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}\psi_\pm(\mathbf{R}) = [\mathcal{H}_0 + W(\mathbf{R})]\psi_\pm(\mathbf{R}) \pm \Delta(\mathbf{R})\psi_\mp^\dagger(\mathbf{R}). \quad (8)$$

The regularizing operator $\partial_r[r\cdot]$ on the right-hand side of equation (6) plays no role for the self-consistent Hartree field, which is given by

$$W(\mathbf{R}) \equiv g\langle\psi_\sigma^\dagger(\mathbf{R})\psi_\sigma(\mathbf{R})\rangle. \quad (9)$$

The pertinence of the regularizing operator becomes clear for the pairing field: using equation (6) with $\phi(\mathbf{y}) = \langle\psi_-(\mathbf{R}-\mathbf{y}/2)\,\psi_+(\mathbf{R}+\mathbf{y}/2)\rangle$ we obtain

$$\Delta(\mathbf{R}) \equiv -g\lim_{r\to 0}\partial_r[r\langle\psi_+(\mathbf{R}+\frac{\mathbf{r}}{2})\psi_-(\mathbf{R}-\frac{\mathbf{r}}{2})\rangle]. \quad (10)$$

Here the operator $\partial_r[r\cdot]$ is necessary as the expectation value $\langle\psi_+\psi_-\rangle$ in equation (10) diverges as $1/r$ for $r \to 0$. To see this, we calculate from equation (8) the time derivative of $\langle\psi_+\psi_-\rangle$ which vanishes as the system

is in a steady state:

$$0 = \left[-\frac{\hbar^2}{m}[\nabla_{\mathbf{r}}^2 + \frac{1}{4}\nabla_{\mathbf{R}}^2] + U(\mathbf{R}-\frac{1}{2}\mathbf{r}) + U(\mathbf{R}+\frac{1}{2}\mathbf{r})\right] \times\langle\psi_+(\mathbf{R}+\frac{\mathbf{r}}{2})\psi_-(\mathbf{R}-\frac{\mathbf{r}}{2})\rangle + \Delta(\mathbf{R}+\frac{1}{2}\mathbf{r})\langle\psi_-^\dagger(\mathbf{R}+\frac{\mathbf{r}}{2})\psi_-(\mathbf{R}-\frac{\mathbf{r}}{2})\rangle + \Delta(\mathbf{R}-\frac{1}{2}\mathbf{r})\langle\psi_+^\dagger(\mathbf{R}-\frac{\mathbf{r}}{2})\psi_+(\mathbf{R}+\frac{\mathbf{r}}{2})\rangle - \Delta(\mathbf{R})\delta(\mathbf{r}) \quad (11)$$

where $U = U_0 + W - \mu$. The presence of $\delta(\mathbf{r})$ imposes a $1/r$ divergence in the pairing field ($\nabla^2(1/r) = -4\pi\delta(\mathbf{r})$):

$$\langle\psi_+(\mathbf{R}+\frac{\mathbf{r}}{2})\psi_-(\mathbf{R}-\frac{\mathbf{r}}{2})\rangle = \frac{m}{4\pi\hbar^2 r}\Delta(\mathbf{R}) + F_{\rm reg}(\mathbf{R}) + O(r). \quad (12)$$

The $1/r$ behavior of the pairing field could actually be expected from the $1/r$ behavior of the two-body scattering wavefunction equation (7). Since the pseudo-potential removes this divergence, equation (10) yields the gap equation:

$$\Delta(\mathbf{R}) = -gF_{\rm reg}(\mathbf{R}). \quad (13)$$

## 4 Gap equation in the homogeneous case

We now compare the prediction of the present theory with the standard theory for a homogeneous system. In this case $U_0 \equiv 0$, and $W$, $\Delta$ do not depend on the position $\mathbf{R}$. The pairing field for a temperature $T$ can then be expressed as an integral (see [4]):

$$\langle\psi_+(\mathbf{R}+\frac{\mathbf{r}}{2})\psi_-(\mathbf{R}-\frac{\mathbf{r}}{2})\rangle = \frac{\Delta}{2}\int\frac{{\rm d}^3k}{(2\pi)^3}\frac{{\rm e}^{{\rm i}\mathbf{k}\cdot\mathbf{r}}}{E_{\mathbf{k}}}[1-2f(E_{\mathbf{k}})] \quad (14)$$

with

$$f(E) = [\exp(E/k_{\rm B}T)+1]^{-1} \quad (15)$$

and $E_{\mathbf{k}} = [\Delta^2 + (\hbar^2k^2/2m - \tilde{\mu})^2]^{1/2}$ where $\mu = \tilde{\mu} + W$. This integral diverges for $r = 0$ as in equation (12). To calculate $F_{\rm reg}$ we add and subtract from $\langle\psi_+\psi_-\rangle$ the integral of a function having the same large $k$ behavior as the integrand in equation (14), that is we add and subtract $G_{\tilde{\mu}}(\mathbf{r})\Delta/2$, where $G_{\tilde{\mu}}(\mathbf{r})$ is the single free particle Green's function:

$$G_{\tilde{\mu}}(\mathbf{r}) = \int\frac{{\rm d}^3k}{(2\pi)^3}\frac{{\rm e}^{{\rm i}\mathbf{k}\cdot\mathbf{r}}}{\left[\frac{\hbar^2k^2}{2m} - \tilde{\mu} - {\rm i}0^+\right]} = \frac{m}{2\pi\hbar^2}\frac{{\rm e}^{{\rm i}\tilde{k_{\rm F}}r}}{r} \quad (16)$$

with $\hbar^2\tilde{k_{\rm F}}^2/2m = \tilde{\mu}$. The contribution of $G_{\tilde{\mu}}\Delta/2$ to $F_{\rm reg}$ is now easy to calculate. The remaining integral $\langle\psi_+\psi_-\rangle - G_\mu\Delta/2$ converges for $r \to 0$. Using $1/(X+{\rm i}\epsilon) = \mathcal{P}(1/X) - {\rm i}\pi\delta(X)$, we finally obtain:

$$F_{\rm reg}(\mathbf{R}) = \frac{\Delta}{2}\int\frac{{\rm d}^3k}{(2\pi)^3}\left[\frac{1-2f(E_{\mathbf{k}})}{E_{\mathbf{k}}} - \mathcal{P}\left(\frac{1}{\frac{\hbar^2k^2}{2m}-\tilde{\mu}}\right)\right]. \quad (17)$$

The gap equation $\Delta = -gF_{\rm reg}$ coincides with the gap equation obtained by renormalizing *via* the Lippman-Schwinger equation [6].

## 5 Gap equation in a trap

We now turn to the inhomogeneous case, for which we have to use a numerical approach. The atoms are trapped in the potential $U_0(\mathbf{r})$, so that the single particle Hamiltonian $\mathcal{H}_0$ has a purely discrete spectrum $E_\eta^0$, where $\eta$ is a set of quantum numbers. Following the Bogoliubov technique [4], we expand the field operator in eigenmodes $(u_\eta, v_\eta)$ [14]:

$$\psi_+(\mathbf{r}) = \sum_\eta b_{\eta,+}u_\eta(\mathbf{r}) - b_{\eta,-}^\dagger v_\eta^*(\mathbf{r}), \quad (18)$$

$$\psi_-(\mathbf{r}) = \sum_\eta b_{\eta,-}u_\eta(\mathbf{r}) + b_{\eta,+}^\dagger v_\eta^*(\mathbf{r}). \quad (19)$$

The mode functions $(u_\eta, v_\eta)$ solve the eigenvalue problem:

$$E_\eta u_\eta(\mathbf{R}) = [\mathcal{H}_0 + W(\mathbf{R})]u_\eta(\mathbf{R}) + \Delta(\mathbf{R})v_\eta(\mathbf{R})$$
$$E_\eta v_\eta(\mathbf{R}) = -[\mathcal{H}_0 + W(\mathbf{R})]v_\eta(\mathbf{R}) + \Delta^*(\mathbf{R})u_\eta(\mathbf{R}). \quad (20)$$

with $E_\eta$ positive. The mode functions are normalized as $\langle u_\eta|u_\eta\rangle + \langle v_\eta|v_\eta\rangle = 1$. The operators $b_{\eta,\pm}, b_{\eta,\pm}^\dagger$ then annihilate and create an elementary excitation of energy $E_\eta$, respectively. They satisfy the usual fermionic anticommutation relations.

For thermal equilibrium, the only non-vanishing averages of a product of two elementary excitation operators are $\langle b_{\eta,\pm}^\dagger b_{\eta,\pm}\rangle = 1 - \langle b_{\eta,\pm}b_{\eta,\pm}^\dagger\rangle = f(E_\eta)$, where the Fermi distribution function is given in equation (15). The pairing function is therefore given by

$$\langle\psi_+(\mathbf{R}+\frac{\mathbf{r}}{2})\psi_-(\mathbf{R}-\frac{\mathbf{r}}{2})\rangle = \sum_\eta u_\eta(\mathbf{R}+\frac{\mathbf{r}}{2})v_\eta^*(\mathbf{R}-\frac{\mathbf{r}}{2})[1-f(E_\eta)] - \sum_\eta v_\eta^*(\mathbf{R}+\frac{\mathbf{r}}{2})u_\eta(\mathbf{R}-\frac{\mathbf{r}}{2})f(E_\eta). \quad (21)$$

A similar expression holds for $W$:

$$W(\mathbf{R}) = \sum_\eta |u_\eta|^2(\mathbf{R})f(E_\eta) + |v_\eta|^2(\mathbf{R})[1-f(E_\eta)]. \quad (22)$$

Inspired by the homogeneous case, we introduce the single particle Green's function

$$G_\mu(\mathbf{R},\mathbf{r}) \equiv \langle \mathbf{R}+\frac{\mathbf{r}}{2}|\frac{1}{\mathcal{H}_0}|\mathbf{R}-\frac{\mathbf{r}}{2}\rangle. \quad (23)$$

To determine the divergence of $G_\mu(\mathbf{R},\mathbf{r})$ for $r \to 0$ we use the defining equation for a Green's function:

$$\left[-\frac{\hbar^2}{2m}\nabla^2_{\mathbf{r}_1} + U_0(\mathbf{r}_1) - \mu\right]\langle \mathbf{r}_1|\frac{1}{\mathcal{H}_0}|\mathbf{r}_2\rangle = \delta(\mathbf{r}_1-\mathbf{r}_2). \quad (24)$$

As $\nabla^2_{\mathbf{r}_1}(1/|\mathbf{r}_1-\mathbf{r}_2|) = -4\pi\delta(\mathbf{r}_1-\mathbf{r}_2)$ this imposes a divergence of $\langle \mathbf{r}_1|\mathcal{H}_0^{-1}|\mathbf{r}_2\rangle$ as $m/2\pi\hbar^2|\mathbf{r}_1-\mathbf{r}_2|$ in the limit $\mathbf{r}_1 \to \mathbf{r}_2$, irrespective of the trapping potential $U_0$ and of the position $\mathbf{r}_2$. In the limit $r \to 0$ we then split $G_\mu$ in a diverging part and a regular part:

$$G_\mu(\mathbf{R},\mathbf{r}) = \frac{m}{2\pi\hbar^2 r} + G^{\mathrm{reg}}_\mu(\mathbf{R}) + O(r). \quad (25)$$

From equation (12) we see that the quantity $\Delta(\mathbf{R})G_\mu(\mathbf{R},\mathbf{r})/2$ diverges in the limit $r \to 0$ in exactly the same way as the pairing field. Therefore we subtract and add from equation (21) the quantity $\Delta(\mathbf{R})G_\mu(\mathbf{R},\mathbf{r})/2$:

$$\langle \psi_+(\mathbf{R}+\frac{\mathbf{r}}{2})\psi_-(\mathbf{R}-\frac{\mathbf{r}}{2})\rangle = \left[\langle \psi_+(\mathbf{R}+\frac{\mathbf{r}}{2})\psi_-(\mathbf{R}-\frac{\mathbf{r}}{2})\rangle - \frac{1}{2}\Delta(\mathbf{R})G_\mu(\mathbf{R},\mathbf{r})\right] + \frac{1}{2}\Delta(\mathbf{R})G_\mu(\mathbf{R},\mathbf{r}). \quad (26)$$

The second line of equation (26) has a $1/r$ diverging part eliminated by the pseudopotential, and a regular part determined from equation (25). The first line of equation (26) is free of $1/r$ divergences; we express $G_\mu(\mathbf{R},\mathbf{r})$ as an infinite sum over the eigenvectors $|\phi^0_\eta\rangle$ of the single particle Hamiltonian $\mathcal{H}_0$ and we use equation (21) to get the gap equation:

$$\Delta(\mathbf{R}) = -g\sum_\eta \left\{u_\eta(\mathbf{R})v^*_\eta(\mathbf{R})[1-2f(E_\eta)] - \frac{\Delta(\mathbf{R})}{2}\frac{|\phi^0_\eta(\mathbf{R})|^2}{E^0_\eta}\right\} - \frac{g}{2}\Delta(\mathbf{R})G^{\mathrm{reg}}_\mu(\mathbf{R}). \quad (27)$$

In a practical numerical calculation, the infinite sum in equation (27) is, of course, replaced by a finite one. The regular part of the Green's function has to be calculated numerically once, for a given value of the chemical potential $\mu$.

## 6 Numerical results for a gas in a harmonic trap

Equation (20) for the $(u_\eta, v_\eta)$'s, the self-consistent determination of $\Delta(\mathbf{R})$ given by equation (27) and of $W(\mathbf{R})$ given by equation (22) constitute a non-linear problem. To obtain the critical temperature $T_\mathrm{c}$, one linearizes this problem for small $\Delta(\mathbf{R})$ which leads to the integral equation $\Delta(\mathbf{s}) = \int \mathrm{d}^3 r M(\mathbf{s},\mathbf{r})\Delta(\mathbf{r})$. The temperature for which the highest eigenvalue $\lambda$ of the kernel $M$ crosses 1, is then $T_\mathrm{c}$ [4]. The kernel is given as

$$M(\mathbf{S},\mathbf{R}) = \lim_{r\to 0}\left[K(\mathbf{S}+\frac{\mathbf{r}}{2},\mathbf{R}-\frac{\mathbf{r}}{2}) - \delta(\mathbf{R}-\mathbf{S})\frac{m}{4\pi\hbar^2 r}\right] \quad (28)$$

with [4]

$$K(\mathbf{S}+\frac{\mathbf{r}}{2},\mathbf{R}-\frac{\mathbf{r}}{2}) = -\frac{g}{2}\sum_{\eta,\eta'}\frac{\tanh(\beta\frac{\xi_\eta}{2})+\tanh(\beta\frac{\xi_{\eta'}}{2})}{\xi_\eta+\xi_{\eta'}} \times \phi^*_\eta(\mathbf{R}-\frac{\mathbf{r}}{2})\phi^*_{\eta'}(\mathbf{R}-\frac{\mathbf{r}}{2})\phi_\eta(\mathbf{S}+\frac{\mathbf{r}}{2})\phi_{\eta'}(\mathbf{S}+\frac{\mathbf{r}}{2}). \quad (29)$$

Here, $\phi_\eta(\mathbf{r}) = \langle \mathbf{r}|\phi_\eta\rangle$ are the single particle eigenstates of $\mathcal{H}_0 + W(\mathbf{r})$ with energy $\xi_\eta$.

In the experiments with atomic gases the particles are kept in harmonic traps; for simplicity we have assumed an isotropic harmonic trap $U_0(\mathbf{r}) = (1/2)m\omega^2 r^2$ in our calculations. We give in the Appendix a derivation of the regular part $G^{\mathrm{reg}}_\mu$ of the single particle Green's function for this case. We have performed a numerical diagonalization of the kernel $M$ for a varying chemical potential $\mu$. For the interaction, we took the parameters of $^6$Li that is $a = -1140$ Å [15] and a trapping frequency of 820 Hz which gives $g/(l^3\hbar\omega) \simeq -1$ with $l = (\hbar/m\omega)^{1/2}$. In Figure 1, we plot $T_\mathrm{c}$ as a function of $N_\sigma$. As $\hbar\omega/k_\mathrm{B} \simeq 40$ nK the calculated critical temperature seems experimentally obtainable.

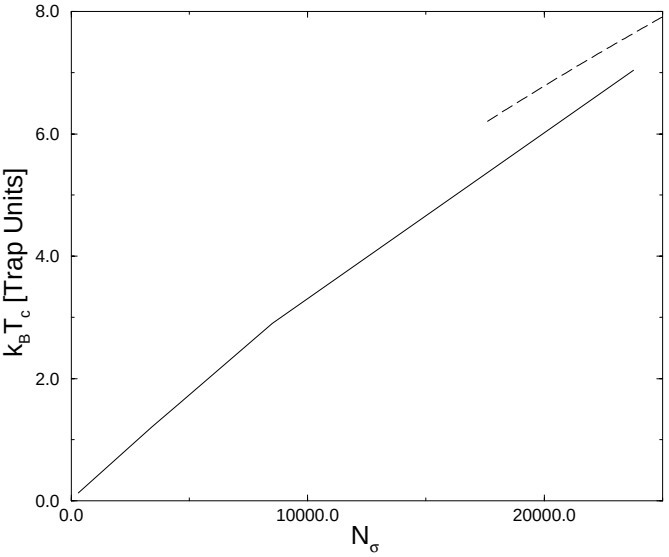


**Fig. 1.** The critical temperature $k_\mathrm{B}T_\mathrm{c}/\hbar\omega$, where $\omega$ is the trap frequency, as a function of the number of particles $N_\sigma$ in each of the internal states for $g/(l^3\hbar\omega) = -1$ where $l = \sqrt{\hbar/m\omega}$. The solid line is obtained from numerical solution of the linearized gap equation. The dashed line depicts the result of the TFA in the parameter space where it is valid (*i.e.* $k_\mathrm{B}T_\mathrm{c} \gg \hbar\omega$).

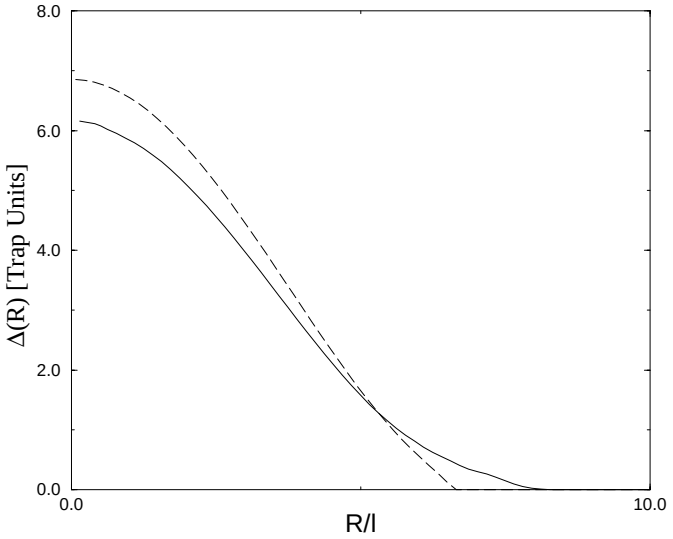


**Fig. 2.** Gap function $\Delta(\mathbf{R})/\hbar\omega$ as function of $R/l$ for $g = -l^3\hbar\omega$ where $l = \sqrt{\hbar/m\omega}$. We have $\mu = 31.5\hbar\omega$ (yielding $N_\sigma \simeq 8000$) and $k_\mathrm{B}T = k_\mathrm{B}T_\mathrm{c}/10 = 0.28\hbar\omega$. Solid line: numerical solution of the complete BCS theory. Dashed line: TFA.

To obtain the spatial structure of the gap function $\Delta(\mathbf{R})$ for arbitrary temperatures, we solve numerically the whole self-consistent non-linear problem. We plot in Figure 2 the gap function as function of $R$ for a relatively large number of particles and a temperature much smaller than $T_\mathrm{c}$. In this low temperature regime the Cooper pairing takes place over the whole trapped cloud.

In both of the above figures, we also compare with the Thomas-Fermi approximation (TFA), in which the system is treated as being locally homogeneous [9], neglecting the discrete nature of the energy spectrum. There are two conditions for the validity of the TFA. First, the correlation length between the unpaired fermions $\simeq 1/k_\mathrm{F}$ should be much shorter than the spatial radius $r_\mathrm{TF} = \sqrt{2\mu/m\omega^2}$ of the cloud, requiring $\mu \gg \hbar\omega$. Also, the size $\xi$ of the Cooper pairs must be much smaller than $r_\mathrm{TF}$ making a local theory for the pairing reasonable. For $T = 0$, $k_\mathrm{F}\xi \simeq \mu/\Delta_{T=0} \simeq \mu/k_\mathrm{B}T_\mathrm{c}$ where we have used $\Delta_{T=0} = 1.76k_\mathrm{B}T_\mathrm{c}$ [4] valid in the TFA. For $T = T_\mathrm{c}$, we have the same estimate $k_\mathrm{F}\xi \simeq \mu/k_\mathrm{B}T_\mathrm{c}$. For any $T$ below $T_\mathrm{c}$ the inequality $\xi \ll r_\mathrm{TF}$ then reduces to the requirement that the critical temperature must be much larger than the trap level spacing for the TFA to work; *i.e.* $k_\mathrm{B}T_\mathrm{c}/\hbar\omega \gg 1$.

We see from Figures 1 and 2 that the agreement with the TFA is reasonably good for $k_\mathrm{B}T_\mathrm{c} > \hbar\omega$. To determine the region of validity of the TFA more clearly, we plot in Figure 3 the quantity $S \equiv \int \mathrm{d}^3R\ \Delta(\mathbf{R})$ as a function of temperature. In Figure 3a, we chose a small number of trapped particles; in Figure 3b a much larger number of particles are trapped. The temperature where the gap, that is $S$, vanishes, determines $T_\mathrm{c}$. For (a), we find $k_\mathrm{B}T_\mathrm{c} = 0.13\hbar\omega$. This value for $T_\mathrm{c}$ is confirmed in Figure 4, where we plot the highest eigenvalue of the kernel $M(\mathbf{r},\mathbf{s})$ given in equation (28) as a function of $T$. We see that the eigenvalue crosses the value 1 at $T_\mathrm{c} \simeq 0.13\hbar\omega/k_\mathrm{B}$. Since

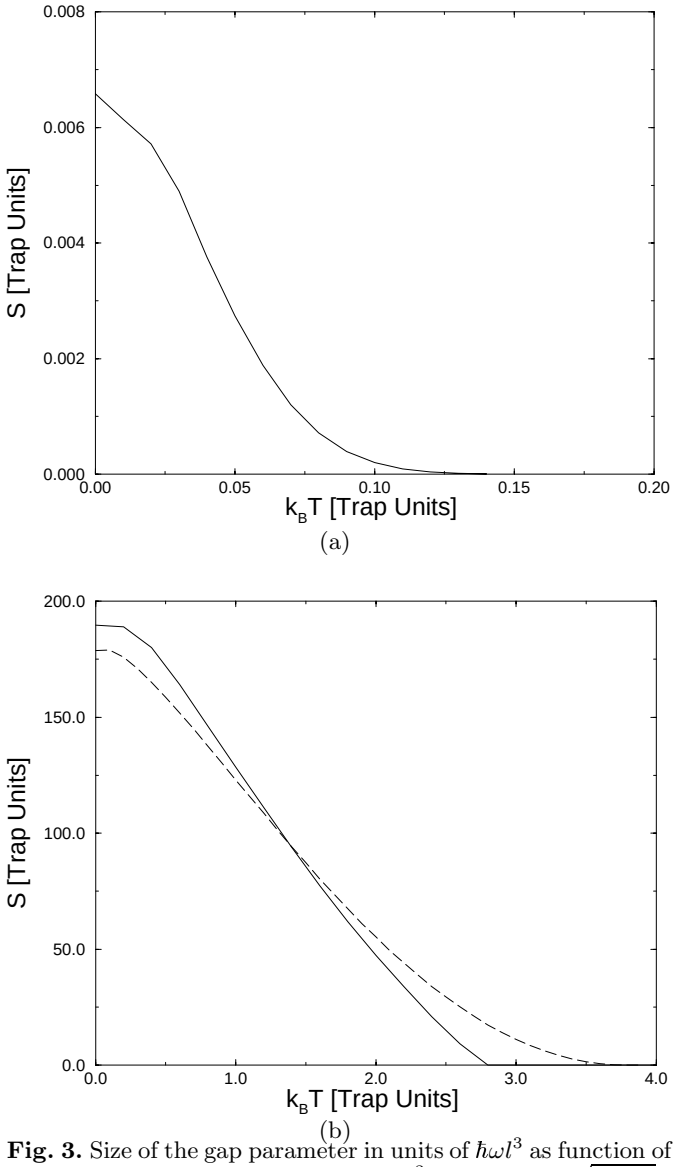


**Fig. 3.** Size of the gap parameter in units of $\hbar\omega l^3$ as function of $k_\mathrm{B}T/\hbar\omega$ for a scattering length $g = -l^3\hbar\omega$ (with $l = \sqrt{\hbar/m\omega}$), and for (a) $\mu = 11.5\hbar\omega$ yielding $N_\sigma \simeq 300$, and (b) $\mu = 31.5\hbar\omega$ yielding $N_\sigma \simeq 8000$. Solid line: numerical solution of the complete BCS theory. Dotted line in (b): TFA.

the value of the critical temperature is relatively small in the sense that $k_\mathrm{B}T_\mathrm{c}/\hbar\omega \ll 1$, the TFA breaks down for this set of parameters; it yields a $S$ which is larger by two orders of magnitude as compared to the result in Figure 3a. For the parameters in Figure 3b we have $k_\mathrm{B}T_\mathrm{c} = 2.8\hbar\omega$ and the agreement with the TFA is reasonably good as expected.

## 7 Conclusion

In conclusion, we have implemented a BCS theory for a dilute gas of weakly interacting fermionic atoms in a trap. It reproduces the well-known regularized gap

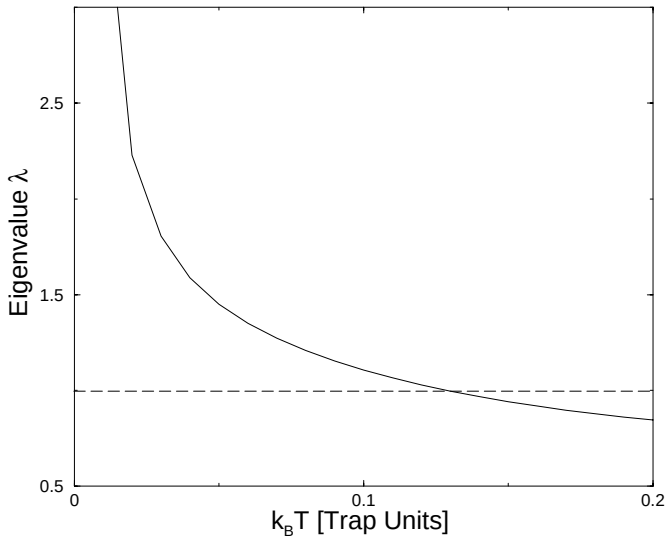


**Fig. 4.** The highest eigenvalue $\lambda$ of the kernel $M(\mathbf{s},\mathbf{r})$ as a function of $k_{\rm B}T/\hbar\omega$ for $g=-l^3\hbar\omega$ and $\mu=11.5\hbar\omega$.

equation for the homogeneous case, and it provides a method for achieving a finite theory for a trapped gas taking into account the discrete nature of the normal state trap levels. Based on this theory, we intend in a next step to include time dependence in our treatment to study the response of the system to external perturbations, in a search for observable signatures of the BCS transition.

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## Appendix: Green's function for the harmonic oscillator

In this part we calculate the regular part $G_\mu^{\rm reg}$ of the single particle Green's function for the 3D isotropic harmonic oscillator $U_0(\mathbf{r})=(1/2)m\omega^2r^2$. For simplicity we use $\hbar\omega$ as a unit of energy and $(\hbar/m\omega)^{1/2}$ as a unit of length, which amounts to setting $m=\hbar=\omega=1$.

The Green's function is well defined in the case of a chemical potential $\mu$ differing from the energies of the bound states in the trap. Here we assume that $\mu\neq n+(1/2)$, where $n$ is any positive integer. We can then use the following integral representation of the resolvant of the harmonic oscillator Hamiltonian $\mathcal{H}_0=-(1/2)\nabla^2+(1/2)r^2-\mu$:

$$\frac{1}{\mathcal{H}_0}=\frac{\mathrm{i}}{1+\mathrm{e}^{2\mathrm{i}\pi\mu}}\int_0^{2\pi}\mathrm{d}t\,\mathrm{e}^{-\mathrm{i}\mathcal{H}_0t} \tag{A.1}$$

as can be checked directly in the eigenbasis of $\mathcal{H}_0$.

The Feynman propagator of the 1D harmonic oscillator is given by [16]:

$$\langle x_2|\mathrm{e}^{-\frac{\mathrm{i}}{2}[-\partial_x^2+x^2]t}|x_1\rangle=\frac{\mathrm{e}^{-\mathrm{i}\pi/4}}{\sqrt{2\pi|\sin t|}}\mathrm{e}^{\mathrm{i}S}\quad\text{for } 0<t<\pi \tag{A.2}$$

$$=\frac{\mathrm{e}^{-3\mathrm{i}\pi/4}}{\sqrt{2\pi|\sin t|}}\mathrm{e}^{\mathrm{i}S}\quad\text{for } \pi<t<2\pi \tag{A.3}$$

where $S=(x_1^2+x_2^2)/(2\tan t)-x_1x_2/\sin t$ is the action of the classical path linking $(x_1,0)$ to $(x_2,t)$.

We apply this result to the 3D case; we split the integration over $t$ in equation (A.1) in the two intervals $[0,\pi]$ and $[\pi,2\pi]$; in the second integral we change the integration variable from $t$ to $2\pi-t$. Setting $u=1/\sqrt{\tan(t/2)}$ we obtain

$$G_\mu(\mathbf{R},\mathbf{r})=\frac{\sqrt{2}}{(2\pi)^{3/2}}\mathrm{Re}\left[\frac{\mathrm{e}^{-\mathrm{i}\pi(\mu+1/4)}}{\cos\pi\mu}\times\int_0^{+\infty}\mathrm{d}u\;F(u;R)\mathrm{e}^{\mathrm{i}r^2u^2/4}\right] \tag{A.4}$$

where we have introduced the function

$$F(u;R)=(1+u^{-4})^{1/2}\mathrm{e}^{2\mathrm{i}\mu\arctan(1/u^2)}\mathrm{e}^{-\mathrm{i}R^2/u^2}. \tag{A.5}$$

If we substitute $r$ by 0 in equation (A.4) we get a integral diverging in $u=+\infty$, as $F(u;R)$ converges to 1 for $u\to+\infty$. We therefore split $F(u;R)$ as $[F(u;R)-1]+1$; the difference $F(u;R)-1$ tends to 0 for $u\to\infty$ as $1/u^2$, so that the integral of $[F(u;R)-1]$ now converges and $r$ can be set to 0. The contribution of the constant term 1 can be calculated exactly from the known integral

$$\int_0^{+\infty}\mathrm{d}\rho\,\mathrm{e}^{\mathrm{i}\rho^2}=\frac{\sqrt{\pi}}{2}\mathrm{e}^{\mathrm{i}\pi/4}. \tag{A.6}$$

We are therefore led to the following $r$-expansion:

$$G_\mu(\mathbf{R},\mathbf{r})=\frac{1}{2\pi r}+\frac{\sqrt{2}}{(2\pi)^{3/2}}\mathrm{Re}\left[\frac{\mathrm{e}^{-\mathrm{i}\pi(\mu+1/4)}}{\cos\pi\mu}\int_0^{+\infty}\mathrm{d}u[F(u;R)-1]\right]+O(r). \tag{A.7}$$

Numerically we split the integration over $u$ in the two intervals $[0,1]$ and $[1,+\infty[$. In the first interval we introduce the change of variables $v=1/u$. We are then facing integrals with rapidly ($R\gg1$) oscillating integrands, of the type:

$$I=\int_1^U\mathrm{d}u\;G(u)\mathrm{e}^{-\mathrm{i}R^2/u^2} \tag{A.8}$$

$$J=\int_1^V\mathrm{d}v\;H(v)\mathrm{e}^{-\mathrm{i}R^2v^2} \tag{A.9}$$

where $G$, $H$ are slowly varying functions. We split the interval of integration in $n$ intervals of size $\delta = (U-1)/n$ and use the approximate formula:

$$I \simeq \sum_{k=0}^{n-1} \frac{1}{2}[G(u_k) + G(u_{k+1})] \int_{u_k}^{u_{k+1}} \mathrm{d}u\, \mathrm{e}^{-\mathrm{i}R^2/u^2} \quad \text{(A.10)}$$

with $u_k = 1 + k\delta$. Similar expressions hold for $J$. The integrals over $u$ in equation (A.10) can be expressed exactly in terms of the complementary error-function with a complex argument. The missing piece from $U$, $V$ to $+\infty$ is approximated analytically from an asymptotic expression of $G(u), H(v)$.

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11. This gives the highest critical BCS temperature [9].
12. The Hamiltonian is symmetric under the unitary transform $U\psi_\pm(\mathbf{r})U^\dagger = \mathrm{i}\psi_\mp(\mathbf{r})$. In this paper we have assumed a BCS state obeying this symmetry so that we get $\langle\psi_-(\mathbf{r}_1)\psi_+(\mathbf{r}_2)\rangle = -\langle\psi_+(\mathbf{r}_1)\psi_-(\mathbf{r}_2)\rangle$ and hence the change of sign $\pm$ in the last term of equation (3). If the $|\pm\rangle$ atomic internal states are viewed formally as the states $m = \pm 1/2$ of a spin 1/2, $U$ corresponds to the spin rotation of angle $\pi/2$ around the $x$ axis.
13. As we use here the BCS theory as a mean field theory for an interaction potential given by the pseudo-potential the BCS theory applies when the pseudo-potential can be treated in the Born approximation. This requires $p|a|/\hbar < 1$; as $p \simeq \hbar k_\mathrm{F}$ and $k_\mathrm{F} \simeq (3\pi^2\rho)^{1/3}$, the density $\rho$ at the center of the trap should satisfy $\rho|a|^3 < 1/3\pi^2$. As $k_\mathrm{F} = (2m\mu)^{1/2}/\hbar$, $\mu$ should satisfy $\mu < \hbar^2/2ma^2$.
14. The minus sign in front of one the $v$'s comes from the symmetry relation [12] which leads to $Ub_{\eta,\pm}U^\dagger = \mathrm{i}b_{\eta,\mp}$.
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