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Superfluid Thomas–Fermi Approximation for Trapped Fermi Gases

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Abstract. We present a generalization of fermionic fluiddynamics to the case of two trapped fermion species with a contact interaction. Within a mean field approximation, we derive coupled equations of motion for the particle densities, particle currents, and anomalous pair density. For an inhomogeneous system, the equilibrium situation with vanishing currents is described by a generalized Thomas–Fermi relation that includes the superfluid gap, together with a new nonlocal gap equation that replaces the usual BCS one. These equations are numericaly solved resorting to a local density approximation (LDA). Density and gap profiles are analyzed in terms of the scattering length, revealing that the current frame can exhibit microscopic details of quantum origin that are frequently absent in more macroscopic scenarios.

1. Introduction

The use of mean–field theories to establish the equation of state (EOS) of trapped Fermi gases goes back to the first application of the Thomas–Fermi (TF) theory to fermions confined in harmonic traps with potential $V(\mathbf{r})$ [1]. When two fermion species are coupled by pairing interactions, the BCS theory for homogeneous systems combined with the local–density approximation (LDA), by replacing the chemical potential μ by the local shift $\mu - V(r)$ in the expressions for the TF particle densities and for the superfluid gap, become one of the most popular tools to look for the appearance and characteristics of a superfluid phase [2]. The TF+BCS can be used in harmonic traps if the superfluid critical temperature T_c satifies $\hbar\omega \ll T_c \ll \varepsilon_F$ [3]; accordingly one could not, in principle, take its validity for granted at very low temperatures, where the Cooper pairs are large in units of the oscillator length. Since pairing correlations involve a small fraction of particles around the Fermi level, the density and related quantities are expected to be weakly influenced by this coupling [4]; however, the validity of LDA–like descriptions cannot be fully trusted in the unitary regime [5] where the trapped atoms are strongly correlated.

The usual TF+BCS treatment that derives the density of a trapped fermion species ignoring any coupling to the superfluid gap, computed separately, has not been tested so far by comparison with other mean field treatments. In a recent paper [6] we have proposed an alternative scheme to TF+BCS in the presence of harmonic traps, by means of an extension of the fluiddynamical (FD) scheme of nuclear physics [8, 9, 10], starting from a two–body Hamiltonian with pairing

interactions. We are able to construct a set of coupled equations of motion for the particle and pair densities and for the particle currents in coordinate representation, and generalize the TF description of normal fluids through a chemical potential that depends on particle kinetic energies, mutual interaction and pairing energy.

In Sec. 2 we shortly review our FD description of paired fermions and in Sec. 3 we analyze the equilibrium densities and gap, compared with TF+BCS results for different values of the scattering length. The results and perspectives are summarized in Sec. 4.

2. Theory

Our starting point is a zero–temperature grand potential operator for two mutually interacting fermion species with spin projections $\sigma = \pm$, described by field operators $\Psi_\sigma(\mathbf{r})$, with populations N_σ trapped in harmonic potentials $V_\sigma(\mathbf{r})$ that interact with a contact force of strength g corresponding to a negative scattering length a

$$\hat{\Omega} = \int d\mathbf{r} \left\{ \sum_\sigma \left[-\frac{\hbar^2}{2m} \Psi_\sigma^\dagger \nabla^2 \Psi_\sigma + [V_\sigma - \mu_\sigma] \Psi_\sigma^\dagger \Psi_\sigma \right] + g \Psi_+^\dagger \Psi_-^\dagger \Psi_- \Psi_+ \right\} \tag{1}$$

We introduce the one-body density and current operators for each fermion species, and the anomalous pair density or pairing tensor

$$\hat{\rho}_\sigma(\mathbf{r},\mathbf{r}') = \Psi_\sigma^\dagger(\mathbf{r}') \Psi_\sigma(\mathbf{r}) \tag{2}$$

$$\hat{\mathbf{j}}_\sigma(\mathbf{r},\mathbf{r}') = \frac{\hbar}{2m\imath}(\nabla - \nabla') \hat{\rho}_\sigma(\mathbf{r},\mathbf{r}') \tag{3}$$

$$\hat{\kappa}_\sigma(\mathbf{r},\mathbf{r}') = \Psi_\sigma(\mathbf{r}) \Psi_{-\sigma}(\mathbf{r}') \equiv -\hat{\kappa}_{-\sigma}(\mathbf{r}',\mathbf{r}) \tag{4}$$

From the equation of motion (EOM) of the field operators, we construct the mean field EOM's for the spatial matrix elements of the operators (2) to (4). Since the gap matrix is defined in terms of the regular part of the pairing tensor as $\Delta(\mathbf{r},\mathbf{r}') = -g\kappa_{reg}(\mathbf{r},\mathbf{r}')$, care has to be taken with respect to regularization of the anomalous pair density, *i.e.*, by adopting the prescription in Ref. [3]. The details of this derivation are given in Ref. [6] and the final set of equations read

$$\frac{\partial}{\partial t}\rho_\sigma(\mathbf{r}) = -\nabla \cdot \mathbf{j}_\sigma(\mathbf{r}) \tag{5}$$

$$\imath\hbar \frac{\partial \Delta_\sigma(\mathbf{r})}{\partial t} = \left[-\frac{\hbar^2}{4m}\nabla^2 + V_{total}(\mathbf{r})) - \mu_{total} \right] \Delta_\sigma(\mathbf{r}) + \mu^{(0)}_{total}[\rho(\mathbf{r})] \, \Delta^{(0)}_\sigma[\rho(\mathbf{r})] \tag{6}$$

$$\frac{\partial}{\partial t}\mathbf{j}_\sigma = -\frac{\rho_\sigma}{m} \nabla \mu_\sigma \tag{7}$$

The main hypothesis of this approach are: (1) the last term in the right–hand–side of Eq. (6) is an inhomogeneous contribution to the gap evolution, approximated by a local function of the chemical potentials $\mu^{(0)}_\sigma[\rho]$ and gaps $\Delta^{(0)}_\sigma[\rho]$ of the homogeneous system and (2) the local Bernoulli potential that drives the particle current is the thermodynamical chemical potential

$$\mu_\sigma(\mathbf{r}) \equiv \mu^{STF}_\sigma(\mathbf{r}) = \frac{\partial \tau_\sigma}{\partial \rho_\sigma} + V_\sigma + g\,\rho_{-\sigma} + \frac{1}{g}\frac{\partial |\Delta|^2}{\partial \rho_\sigma} \tag{8}$$

Then, the equilibrium situation of the paired system is described by the coupled set

$$\nabla \mu^{STF}_\sigma(\mathbf{r}) = 0 \tag{9}$$

$$\left[-\frac{\hbar^2}{4m}\nabla^2 + V_{total} - \mu_{total} \right] \Delta^{FD}_\sigma + \mu^{(0)}_{total}[\rho] \, \Delta^{(0)}_\sigma[\rho] = 0 \tag{10}$$

with the superfluid Thomas–Fermi (STF) chemical potential depending on density as well as on the real FD gap $\Delta_\sigma^{FD}(\mathbf{r})$. Equation (9) together with (8) defines the STF particle density, which for vanishing gap reproduces the standard TF density of a normal Fermi gas. We note that STF is the simplest generalization of TF, and that the more important difference between this formalism and approaches based on local BCS is the definition of the superfluid gap via Eq. (10), that includes a quantum gap pressure through the kinetic operator.

3. Results and Discussion

In Ref. [6] we provide details of our procedure to solve Eq. (9) within the LDA by adopting several forms of the EOS and gap for homogeneous systems. In the present work we report results for (i) the full EOS for paired fermions with arbitrary coupling in the form calculated by Papenbrock and Bertsch [11] (PB) hereafter noted as STF+PB, and (ii) the standard TF+BCS in the weak coupling limit, with EOS and gap defined by

$$\mu_\sigma^{TF} = \frac{\hbar^2 k_F^2}{2m} + g\rho_{-\sigma}, \tag{11}$$

$$\Delta^{BCS} = \frac{8}{e^2}\frac{\hbar^2 k_F^2}{2m}\exp\left(-\frac{\pi}{2k_F|a|}\right) \tag{12}$$

with local Fermi momentum $k_F = (6\pi^2\rho_\sigma)^{1/3}$.

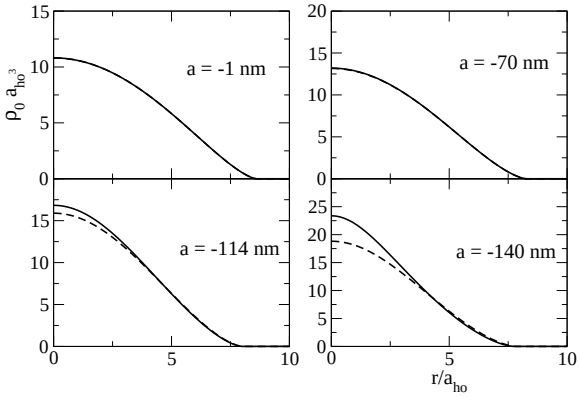

Figure 1. Density profiles for each species in a ^{6}Li mixture with $N_\pm = 8500$ atoms for several values of scattering length. Full and dashed lines respectively correspond to the STF+PB and to the TF+BCS calculations.

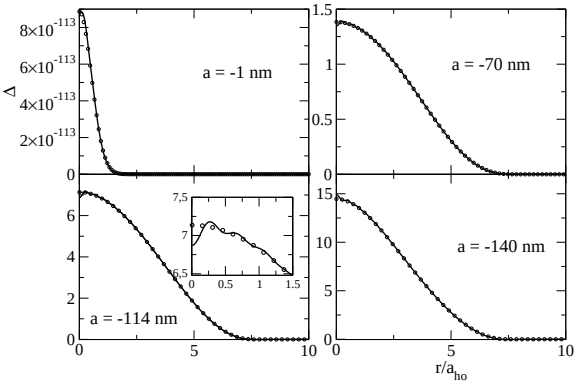

Figure 2. Gap profiles for the same lithium mixture. Full lines and circles respectively correspond to the STF+PB and to the TF+BCS calculations

In Fig. 1 we show the density profiles for a ^{6}Li mixture with $N_+ \equiv N_- = 8.5\times10^3$ atoms, and for several scattering lengths a as shown in the four panels. As a rule, we observe that for each interaction strength the particle densities predicted by these EOS's mainly differ at the trap center, whereas the widths of the profiles are roughly the same for all EOS's. These differences are not noticeable for weak interaction strengths and become visible for $|a|$ above several tens of nm. The increase of the density in the STF+PB calculation is more important, the larger the magnitude of $|a|$, and can be attributed to the contribution of the gap density to the EOS; as seen in Eq. (8), the term Δ_σ^2 provides an additional negative pressure which is stronger at larger densities, i.e., at the trap center. For larger $|a|$ both the STF+PB and the TF+BCS EOS's predict a transition to a collapsed phase, as discussed in Ref. [6]; actually, the derivative of the

chemical potential with respect to density vanishes –and changes sign afterwards– at a = -148 nm within the STF approach, and at -173 nm for standard TF in the current system.

Using the particle densities and total chemical potential μ_{total} as inputs for the FD gap equation (10), we solve the latter according to the numerical procedure described in Ref. [6]. Figure 2 displays the spatial profiles of the gap for the same parameters as in Fig. 1. We see that for intermediate and high scattering lengths, the quantum gap pressure induces oscillations in the gap profile near the origin, with wavelength comparable with the trap size, without modifying the spatial spread. The inset in the lower left panel of Fig. 2 permits a clear view of these oscillations. This quantum gap pressure represents a perturbation to the TF+BCS gap equation (12), that decreases exponentially fast for ρ approaching zero, while it can be sizeable at the trap center for large number of particles. This is consistent with the shape of the profiles depicted in Fig. 2 and differs from the smooth BCS results in Ref. [3], where the gap oscillations are suppressed.

4. Summary

In this contribution, our aim has been to illustrate the changes in density and gap profiles in an equilibrated two fermion species in a harmonic trap, with equal populations, for increasing absolute values of the (negative) scattering length of ^{6}Li atoms. This analysis complements results presented in Ref. [6], where only global quantities such as the densities at the trap center and the total gap strength are shown as functions of $|a|$. Comparisons with quantum Monte Carlo results and studies of the behavior of the various magnitudes with the number of atoms can be found in Ref. [6]. Our main conclusion here is that for weakly interacting systems, the new STF+PB gives essentially the same particle densities and gap profiles as the traditional TF+BCS procedure. As the magnitude of the scattering length increases, larger densities appear near the trap center, while the gap presents oscillations within a wavelength comparable with the trap size. These effects are microscopic and of quantum origin, and can be entirely attibuted to the pairing energy present in the STF definition of the chemical potential, and to the quantum pairing pressure associated with the kinetic operator in the FD gap. These differences can, in fact, bear interesting consequences in the spectrum of small amplitude motion, that in configurations of trapped atoms consist of coupled density and pairing vibrations [6], as well as in assessing the superfluid properties of moderately large ^{3}He droplets in the submillikelvin regime. These topics are under study and results will be reported soon.

4.1. Acknowledgments

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