LETTER TO THE EDITOR

Stability of Trapped Ultracold Fermi Gases
Using Effective s- and p-Wave Contact-Interactions

R. Roth and H. Feldmeier
Gesellschaft für Schwerionenforschung (GSI)
Planckstr. 1, 64291 Darmstadt, Germany
E-mail: r.roth@gsi.de, h.feldmeier@gsi.de

Abstract. The stability of trapped dilute Fermi gases against collapse towards large densities is studied. A hermitian effective contact-interaction for all partial waves is derived, which is particularly suited for a mean-field description of these systems. Including the s- and p-wave parts explicit stability conditions and critical particle numbers are given as function of the scattering lengths. The p-wave contribution determines the stability of a single-component gas and can substantially modify the stability of a two-component gas. Moreover it may give rise to a novel p-wave stabilized high-density phase.

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Since the first realization of a Bose-Einstein condensate of $^{87}$Rb atoms in 1995 [1], the field of trapped ultracold atomic gases experienced great experimental progress. This raised the question if a Fermi gas can be prepared under similar conditions and whether a transition to a superfluid state can be achieved. An important step towards a possible super-fluid state of trapped Fermi gases was the cooling of $^{40}$K atoms to a temperature regime where degeneracy dominates [2].

A major problem for the evaporative cooling of fermions is the Pauli exclusion principle. The relative wave-function of two indistinguishable fermions has odd parity and hence they do not feel the s-wave part of the interaction which dominates the force between bosons at low kinetic energies. This limits the efficiency of evaporative cooling. Several techniques are under discussion to circumvent this problem, e.g., simultaneous trapping of two fermionic species [2, 3], sympathetic cooling of a fermion-boson mixture [4], and the use of p-wave resonances to enable efficient cooling via p-wave interactions [5, 6, 7].

In this letter we investigate the question how p-wave interactions influence the properties of degenerate Fermi gases. The Thomas-Fermi approximation together with a new hermitian effective contact-interaction is employed to describe the effects of the atom-atom interaction in a dilute gas including s- and p-wave contributions. We use this formalism to investigate the influence of p-wave interactions on the stability of trapped one- and two-component Fermi gases against collapse towards high densities where the atoms escape from the trap due to three-body collisions and the formation of bound dimers.

In the standard description of trapped atomic gases one uses point interactions in the s-wave channel only. In the following we present a hermitian effective contact-interaction (ECI) for all partial waves, which is derived to be an effective mean-field interaction.

Consider two particles of mass $m$ which interact via a spherical potential with a range much smaller than their relative wave length. An auxiliary boundary condition at a large radius leads to a discrete energy spectrum $\tilde{E}_{nl}$, where $n$ numbers the positive energy eigenstates and $l$ denotes the relative angular momentum. Negative energy states, i.e., bound states, need not be taken into account since the ECI is used for the description of systems that are not self-bound. The energy shift $\Delta E_{nl} = \tilde{E}_{nl} - E_{nl}$ with respect to the eigenvalues $E_{nl} = \frac{k^2}{2m}$ of the kinetic energy without interaction can be expressed in terms of the phase shift $\eta_l(k)$ for the $l$-th partial wave [8].

For mean-field type calculations we require that the expectation value of the ECI calculated with mean-field states, i.e., free two-body states $|nlm_l\rangle$, equals the exact energy shift $\langle nlm_l| v^{\text{eff}}_l |nlm_l\rangle = \Delta E_{nl}$.

We choose the following hermitian ansatz for the operator of the ECI in a particular $l$-channel

$$v^{\text{eff}}_l = \int d^3r \langle \vec{r}^* \frac{\partial}{\partial \vec{r}^*} \frac{\partial}{\partial \vec{r}} g_l \frac{\delta(\vec{r})}{4\pi r^2} \frac{\partial}{\partial \vec{r}} \rangle.$$  

The arrows above the derivatives indicate to which side they act. Using this ansatz in condition (1) we obtain an explicit expression for the interaction strength $g_l$

$$g_l = \frac{4\pi}{m} \left[ \frac{(2l+1)!!}{l!} \right]^2 \eta_l(k) \frac{k^{2l+1}}{k^{2l+1}} \approx \frac{4\pi}{m} \frac{(2l+1)}{(l!)^2} a_l^{2l+1},$$  

where $a_l$ is a normalization constant.
where \( a_l \) is the scattering length of the \( l \)-th partial wave. It turns out that (3) does not depend explicitly on the auxiliary boundary condition and hence we generalized the result to continuous momenta and energies. Approximation of the phase shifts \( \eta_l(k) \) in terms of the scattering lengths \( a_l \), so that \( g_l \) is momentum independent, leads to deviations of at most 5\% in the energy shift up to \( |k a_l| \sim 3 \). For the s-wave and p-wave component this reduces to \( g_0 = 4\pi a_0/m \) and \( g_1 = 12\pi a_1^3/m \), respectively.

The s-wave part is identical to the widely used local contact interaction. Another way to include higher partial wave terms is the pseudo-potential of K. Huang and C.N. Yang \[9, 10\]. This approach leads to non-hermitian interactions for \( l > 0 \). The two-body energy shift induced by this pseudo-potential is by a factor \( l + 1 \) smaller than the exact one, and is therefore not suited for mean-field calculations beyond s-waves.

Using the s- and p-wave contributions of the ECI we calculate the Hartree-Fock energy-density functional of interacting Fermi gases composed of \( \Xi \) distinguishable components in an external potential \( U(\vec{x}) \). We use the Thomas-Fermi approximation, which is excellent for these systems \[11\]. The local energy density of the Fermi gas as a function of the local Fermi momenta \( \kappa_\xi(\vec{x}) = [6\pi^2 \rho_\xi(\vec{x})]^{1/3} \) of the different components \( \xi = 1, \ldots, \Xi \) reads

\[
\mathcal{E}[\kappa_1(\vec{x}), \ldots, \kappa_\Xi(\vec{x})] = \frac{1}{6\pi^2} \sum_\xi U_\xi(\vec{x}) \kappa_\xi^2(\vec{x}) + \beta_1 \sum_\xi \kappa_\xi^2(\vec{x}) \kappa_\xi^5(\vec{x}) + \beta_0 \sum_{\xi' > \xi} \kappa_\xi^2(\vec{x}) \kappa_{\xi'}^2(\vec{x})
+ \beta_1 \sum_\xi \kappa_\xi^8(\vec{x}) + \beta_1 \sum_{\xi' > \xi} \frac{1}{2} [\kappa_\xi^2(\vec{x}) \kappa_\xi^5(\vec{x}) + \kappa_{\xi'}^5(\vec{x}) \kappa_{\xi'}^3(\vec{x})],
\]

(4)

with coefficients

\[
\beta_t = \frac{1}{20\pi^2 m}, \quad \beta_0 = \frac{a_0}{9\pi^3 m}, \quad \beta_1 = \frac{a_1^3}{30\pi^3 m}.
\]

(5)

The first two terms are caused by the external potential and the kinetic energy, respectively. The remaining ones are the contributions of the s- and p-wave parts of the ECI. As a direct consequence of the Pauli principle, fermions of one kind interact only via the p-wave part, while fermions belonging to different components feel s- and p-wave interactions. The coefficient of the last term may be modified by effective range corrections of the s-wave channel. Since in the following applications \( a_1 \) is treated as a parameter this effect and others which contribute to the same order in \( \kappa_\xi \) are absorbed in \( a_1 \).

The ground state properties of the system are determined by minimization of the energy with respect to the local Fermi momentum under the constraint of a fixed particle number \( N_\xi \) for each component. Implementing the constraints by means of chemical potentials \( \mu_\xi \) the variational problem reduces to an algebraic equation for the local Fermi momentum.

First we consider a single-component Fermi gas, where the extremum condition is given by

\[
m[\mu - U(\vec{x})] = \frac{1}{2} \kappa^2(\vec{x}) + \frac{8}{15\pi} a_1^3 \kappa^5(\vec{x}).
\]

(6)

Usually the s-wave contribution dominates at low energies, but since s-wave scattering is excluded here only p-wave scattering contributes to the mean-field energy.

From the extremum condition (3) we get the following upper bound for the local Fermi momentum of a single-component gas

\[
- a_1 \kappa(\vec{x}) \leq \frac{(3\pi)^{1/3}}{2}.
\]

(7)
beyond which no energy minimum exists anymore. Condition (7) can also be expressed as an upper bound for the chemical potential

\[ a_1^2 m[\mu - U(\vec{x})] \leq \frac{3(3\pi)^{3/2}}{40}. \]  

This limits the particle number \( N \) of a stable single-component condensate for attractive p-wave interactions.

The stability condition (7) involves the local Fermi momentum or density at some point in space, which is not easy to access experimentally. Therefore, we express the stability condition by a phenomenological parameterization as function of particle number, scattering length and trap size. For simplicity we restrict ourselves to an external potential \( U(\vec{x}) \) with the shape of a deformed harmonic oscillator, where \( \ell = (\ell_x \ell_y \ell_z)^{1/3} = (m^3 \omega_x \omega_y \omega_z)^{-1/6} \) is the geometric mean of the oscillator lengths. The parameterization is fitted to the critical particle numbers obtained from the numerical solution of the extremum condition (6) for a given scattering length using the maximum chemical potential (8) for a stable condensate. We find that the parameterized stability condition

\[ C\left(\sqrt{\frac{N a_1}{\ell}}\right) \leq 1 \quad \text{with} \quad C = -2.246, \]  

for the single-component gas reproduces the numerically calculated stability limit within errors of 1%.

The critical particle number \( N_c = [\ell/(Ca_1)]^6 \) of a single-component gas for a typical set of experimental parameters (\( a_1 = -200a_B, \ell = 1\mu m \)) is about \( 8 \times 10^9 \). This is much larger than the particle numbers achieved in present experiments. Nevertheless, this stability limit could be exceeded in near future, e.g., by increased interaction strength or by the use of tightly confining traps [12].

In the following we consider a gas composed of two fermionic species residing in two magnetic substates of hyperfine splitting. Although the s-wave interaction between the species usually dominates, we show that p-wave interactions cannot be neglected in general.

The energy minimization using the energy-density functional (4) for a two-component system leads to two coupled equations for \( \kappa_1(\vec{x}) \) and \( \kappa_2(\vec{x}) \)

\[ m[\mu_1 - U_1(\vec{x})] = \frac{1}{2} \kappa_1^2(\vec{x}) + \frac{2}{3\pi} a_0 \kappa_2^3(\vec{x}) \]
\[ + \frac{1}{30\pi} a_1^2 \left[ 16 \kappa_1^5(\vec{x}) + 3 \kappa_2^5(\vec{x}) + 5 \kappa_1^2(\vec{x}) \kappa_2^3(\vec{x}) \right]. \]  

The second equation is generated by the exchange \([\mu_1 - U_1(\vec{x})] \leftrightarrow [\mu_2 - U_2(\vec{x})]\) and \( \kappa_1(\vec{x}) \leftrightarrow \kappa_2(\vec{x}) \). These two equations have a great variety of possible solutions, depending on the signs and the relative strength of \( a_0 \) and \( a_1 \). In this letter we restrict ourselves to equal particle numbers or \( [\mu - U(\vec{x})] = [\mu_1 - U_1(\vec{x})] = [\mu_2 - U_2(\vec{x})] \) which leads to equal local Fermi momenta \( \kappa(\vec{x}) = \kappa_1(\vec{x}) = \kappa_2(\vec{x}) \) and the single extremum condition for both components:

\[ m[\mu - U(\vec{x})] = \frac{1}{2} \kappa^2(\vec{x}) + \frac{2}{3\pi} a_0 \kappa^3(\vec{x}) + \frac{4}{5\pi} a_1^2 \kappa^5(\vec{x}). \]  

The generalization to different chemical potentials, different interaction strengths or more components is straightforward.
For the two-component system with s-wave interactions only, the stability condition was studied in [11]. Using (11) which includes the p-wave interaction we obtain the more general condition

\[-a_0 \kappa(\vec{x}) - 2 (a_1 \kappa(\vec{x}))^3 \leq \frac{\pi}{2}\] (12)

for each component not to collapse just because of mean-field effects. For $a_1 = 0$ this reduces to the stability condition given in [11], while for $a_1 < 0$ the condition limits the particle number of a metastable two-component fermion condensate even more. It also shows, that a repulsive s-wave interaction ($a_0 > 0$) does not guarantee a stable condensate at larger densities if an attractive p-wave component is present. In this context it is also interesting to study the transition to spatially separated components.

Several very interesting effects appear for interactions with attractive s-wave ($a_0 < 0$) and repulsive p-wave components ($a_1 > 0$). Here $a_1$ need not be the true p-wave scattering length but may include effective range and other effects which contribute to the $\kappa^3$-order in the energy density. In figure 1 the r.h.s. of the extremum condition (11) is depicted as function of the local Fermi momentum $\kappa$. For an attractive pure s-wave interaction (lower curve) the r.h.s. exhibits an absolute maximum which leads to an upper bound for the chemical potential as discussed for the single-component gas. If a repulsive p-wave contribution is added, then the r.h.s. of (11) grows at large Fermi momenta due to the leading $\kappa^5$ contribution. For values of the s- and p-wave scattering lengths which satisfy the condition

\[\frac{a_1}{|a_0|} \geq \frac{2}{3\pi^{2/3}} \approx 0.311\] (13)

the stability condition (12) is fulfilled for all values of the local Fermi momentum, i.e., the r.h.s. of the extremum condition is a monotonic function of $\kappa$ and the maximum does not appear anymore (upper curve). Thus the repulsive p-wave interaction stabilizes the condensate for any particle number even though the s-wave interaction is attractive.

If the ratio of the scattering lengths is below the limit given by (13), then the r.h.s. of the extremum condition exhibits a low and a high density branch, as shown by the middle curve of figure 1. For chemical potentials $\mu$ below the value of the local maximum one obtains the regular low-density solution everywhere in the potential $U(\vec{x})$. An example is shown in insert (a) of figure 1. For larger $\mu$ novel high-density solutions exist in areas of the trap where $m[\mu - U(\vec{x})]$ is larger than the value of the local maximum. As depicted in insert (b) the density shows a discontinuous jump from the outer low-density to the central high-density phase. This phase is stabilized only due to the presence of the repulsive p-wave interaction and occurs when the condition (12) is violated. For values of $\mu$ in between the maximum and the minimum a Maxwell construction with equal pressure in the high- and low-density regime may be used to identify the equilibrium density.

However, when $a_1/|a_0|$ drops below $2/(3\pi^{3/2})$ the density in the high-density regime grows rapidly so that the three-body recombination rate and thus the trap loss is not small anymore. If $a_1/|a_0| < \sqrt{160}/(729\pi^2) \approx 0.281$ the local minimum of the r.h.s. of (11) occurs at negative values, so that even a self-bound solution exists. In this case the product $|a_0| \kappa(\vec{x} = 0) > \frac{\pi}{4}$, which means that in the self-bound area in the center of the trap the mean distance $\rho^{-1/3}$ between the atoms gets close to the scattering length $|a_0|$ and the underlying approximations break down. Nevertheless we expect that for interactions with $a_1/|a_0| \approx 0.3$ a metastable high-density phase
occurs, where the central densities are by one order of magnitude higher than in the outer low-density region.

Like for the single-component gas we express the stability condition in terms of the particle number $N$ of each component, the mean oscillator length $\ell$ of a harmonic trap, and the scattering lengths $a_0$ and $a_1$. We use the following slightly more complicated parameterization for the stability condition

$$C_0 \left( \sqrt[6]{N a_0 / \ell} \right) + C_1 \left( \sqrt[6]{N a_1 / \ell} \right)^3 + C_{01} \left( \sqrt[6]{N a_0 / \ell} \right) \left( \sqrt[6]{N a_1 / \ell} \right)^n \leq 1. \quad (14)$$

The fit has to be done separately for each type of attractive interaction. The resulting optimal coefficients are summarized in table 1 and reproduce the numerical stability limit again with deviations of less than 1%.

The critical particle numbers $N_c$ resulting from the stability condition (14) are shown in figure 2 as function of $a_0$ and $a_1$. For negative $p$-wave scattering length $N_c$ describes the maximum particle number of a metastable condensate. The white area in the figure marks the region where from the mean-field point of view a metastable condensate with smooth density exists for all particle numbers. In principle a positive $a_1$ always leads to a stable mean-field solution. But for $a_0 < 0$ and values of $a_1 / |a_0| \lesssim 0.28$ this solution is at a density which is too large for the metastable state. Therefore, the limit for $N_c$ resulting from (14) is plotted. The bending over of

| interaction type | $C_0$ | $C_1$ | $C_{01}$ | $n$ |
|------------------|------|------|--------|----|
| $a_0 \leq 0$, $a_1 \leq 0$ | -1.835 | -2.570 | 0.656 | 1  |
| $a_0 \geq 0$, $a_1 < 0$  | -1.378 | -2.570 | 1.360 | 1  |
| $a_0 < 0$, $a_1 \geq 0$  | -1.835 | -1.940 | 2.246 | 3  |
As an example for estimating from figure 2 the critical particle number we take a two-component \( ^6\text{Li} \) condensate in a trap with \( \ell = 1\,\mu\text{m} \). The extraordinary large attractive s-wave scattering length of \( a_0 = -2160a_B \) \cite{13}, i.e. \( a_0/\ell \approx -0.1 \), leads to the rather small critical particle number \( N_c = 26000 \) for each of the two components. As also seen from figure 2 the p-wave interaction will change \( N_c \) significantly whenever \( |a_1|/|a_0| \gtrsim 0.2 \).

We conclude that for Fermi gases p-wave scattering should not be neglected from the outset. If attractive it constrains the total particle number in the metastable condensate, if repulsive it helps to stabilize multi-component systems with attractive s-wave interactions. In special cases even a novel high-density phase may occur in the center of the trap which should not be confused with Bose condensation of Cooper pairs.

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