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LETTER TO THE EDITOR

Stability of trapped ultracold Fermi gases using effective s- and p-wave contact interactions

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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 a 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.

Since the first realization of a Bose–Einstein condensate of ^{87}Rb atoms in 1995 [1] the field of trapped ultracold atomic gases has experienced great experimental progress. This raised the question of whether 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 superfluid 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 wavefunction 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 [5–7].

In this letter we investigate the question of 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 wavelength. An auxiliary boundary condition at a large radius leads to a discrete energy spectrum $\bar{E}_{nl}$, 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 $\Delta E_{nl} = \bar{E}_{nl} - E_{nl}$ with respect to the eigenvalues $E_{nl} = k_{nl}^2/m$ of the kinetic energy without interaction can be expressed in terms of the phase shift $\eta_l(k)$ for the lth 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

$$\langle nlm_l | v_l^{\text{eff}} | nlm_l \rangle \stackrel{!}{=} \Delta E_{nl}. \tag{1}$$

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

$$v_l^{\text{eff}} = \int \mathrm{d}^3 r \; |\vec{r}\rangle \frac{\overleftarrow{\partial^l}}{\partial r^l} \; g_l \; \frac{\delta(r)}{4\pi r^2} \; \frac{\overrightarrow{\partial^l}}{\partial r^l} \langle \vec{r}|. \tag{2}$$

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

$$g_l = -\frac{4\pi}{m} \left[\frac{(2l+1)!!}{l!} \right]^2 \frac{\eta_l(k)}{k^{2l+1}} \approx \frac{4\pi}{m} \frac{(2l+1)}{(l!)^2} \; a_l^{2l+1}, \tag{3}$$

where a_l is the scattering length of the lth 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 $|ka_l| \sim 3$. For the s-wave and p-wave components 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 Huang and Yang [9, 10]. This approach leads to non-Hermitian interactions for $l > 0$. The two-body energy shift induced by this pseudo-potential is a factor $\frac{l+1}{2l+1}$ 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 Ξ 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

$$\begin{aligned}\mathcal{E}[\kappa_1(\vec{x}), \ldots, \kappa_\Xi(\vec{x})] = \frac{1}{6\pi^2} \sum_\xi U_\xi(\vec{x})\, \kappa_\xi^3(\vec{x}) + \beta_t \sum_\xi \kappa_\xi^5(\vec{x}) + \beta_0 \sum_{\xi' > \xi} \kappa_\xi^3(\vec{x})\, \kappa_{\xi'}^3(\vec{x}) \\ + \beta_1 \sum_\xi \kappa_\xi^8(\vec{x}) + \beta_1 \sum_{\xi' > \xi} \frac{1}{2} \big[\kappa_\xi^3(\vec{x})\, \kappa_{\xi'}^5(\vec{x}) + \kappa_\xi^5(\vec{x})\, \kappa_{\xi'}^3(\vec{x}) \big],\end{aligned} \tag{4}$$

with coefficients

$$\beta_t = \frac{1}{20\pi^2 m}, \qquad \beta_0 = \frac{a_0}{9\pi^3 m}, \qquad \beta_1 = \frac{a_1^3}{30\pi^3 m}. \tag{5}$$

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 κ_ξ 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_ξ, for each component. Implementing the constraints by means of chemical potentials, μ_ξ, 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

$$m[\mu - U(\vec{x})] = \frac{1}{2}\,\kappa^2(\vec{x}) + \frac{8}{15\pi}\,a_1^3\,\kappa^5(\vec{x}). \tag{6}$$

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 (6) we get the following upper bound for the local Fermi momentum of a single-component gas

$$-a_1\,\kappa(\vec{x}) \leqslant \frac{(3\pi)^{1/3}}{2}, \tag{7}$$

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

$$a_1^2\,m[\mu - U(\vec{x})] \leqslant \frac{3(3\pi)^{3/2}}{40}. \tag{8}$$

This limits the particle number, N, of a stable single-component Fermi gas 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 parametrization as a 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 parametrization 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 gas. We find that the parametrized stability condition

$$C\left(\sqrt[6]{N}\,\frac{a_1}{\ell}\right) \leqslant 1 \qquad \text{with} \quad C = -2.246, \tag{9}$$

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

The critical particle number $N_\mathrm{c} = [\ell/(Ca_1)]^6$ of a single-component gas for a typical set of experimental parameters ($a_1 = -200a_\mathrm{B}$, $\ell = 1\ \mu$m) is about 8×10^9. This is much larger than the particle numbers achieved in present experiments. Nevertheless, this stability limit could be exceeded in the 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 $\kappa_2(\vec{x})$

$$m[\mu_1 - U_1(\vec{x})] = \frac{1}{2}\,\kappa_1^2(\vec{x}) + \frac{2}{3\pi}\,a_0\,\kappa_2^3(\vec{x}) + \frac{1}{30\pi}\,a_1^3\big[16\,\kappa_1^5(\vec{x}) + 3\,\kappa_2^5(\vec{x}) + 5\,\kappa_1^2(\vec{x})\kappa_2^3(\vec{x})\big]. \tag{10}$$

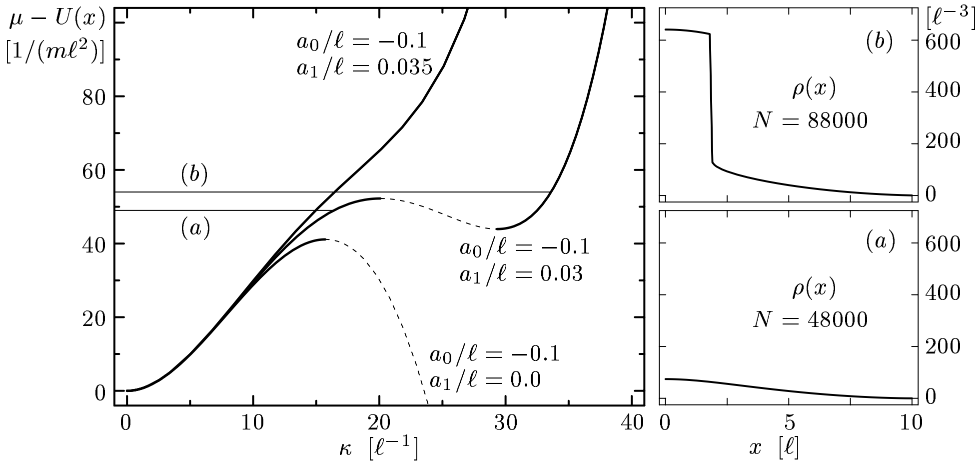

Figure 1. The r.h.s. of equation (11) as a function of the local Fermi momentum κ. The three curves correspond to different interaction parameters as labelled. Solutions of (11) on the dotted parts of the curves correspond to maxima of the energy density, while the full branches denote (local) minima. The inserts (*a*) and (*b*) show the densities for two values of μ indicated by the thin lines for a harmonic trap with mean oscillator length ℓ.

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 strengths 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:

$$m[\mu - U(\vec{x})] = \frac{1}{2}\kappa^2(\vec{x}) + \frac{2}{3\pi}a_0\,\kappa^3(\vec{x}) + \frac{4}{5\pi}a_1^3\,\kappa^5(\vec{x}). \tag{11}$$

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

$$-a_0\kappa(\vec{x}) - 2\,(a_1\kappa(\vec{x}))^3 \leqslant \frac{\pi}{2} \tag{12}$$

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 Fermi gas even more. It also shows that a repulsive s-wave interaction ($a_0 > 0$) does not guarantee a stable gas 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 κ^8-order in the energy density. In figure 1 the r.h.s. of the extremum condition (11) is depicted as a function of the local Fermi momentum κ. 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

Table 1. Parameters of the fitted stability condition (14) for the two component Fermi gas for different interaction types.

Interaction type	C_0	C_1	C_{01}	n
$a_0 \leqslant 0,\ a_1 \leqslant 0$	−1.835	−2.570	0.656	1
$a_0 \geqslant 0,\ a_1 < 0$	−1.378	−2.570	1.360	1
$a_0 < 0,\ a_1 \geqslant 0$	−1.835	−1.940	2.246	3

the r.h.s. of (11) grows at large Fermi momenta due to the leading κ^5 contribution. For values of the s- and p-wave scattering lengths which satisfy the condition

$$\frac{a_1}{|a_0|} \geqslant \frac{2}{3\pi^{2/3}} \approx 0.311 \tag{13}$$

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 κ and the maximum does not appear anymore (upper curve). Thus the repulsive p-wave interaction stabilizes the gas 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 μ 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 inset (*a*) of figure 1. For larger μ, 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 inset (*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 μ 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 $a_1/|a_0| < \sqrt[3]{160/(729\pi^2)} \approx 0.281$ 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 $|a_0|\,\kappa(\vec{x}=0) > \frac{9}{8}\pi$, which means that in the self-bound area in the centre 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 one order of magnitude higher than in the outer low-density region.

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

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

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 a function of a_0 and a_1. For negative p-wave scattering length, N_c describes the maximum particle number of a metastable Fermi gas. The white area in the figure marks the

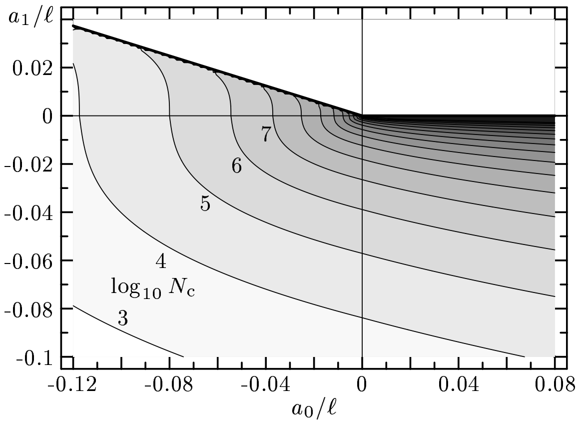

Figure 2. Logarithmic contour plot of the critical particle number N_c as a function of the s- and p-wave scattering length for the two-component Fermi gas. Neighbouring contours are separated by a factor of 10 in particle number, selected ones are labelled with $\log_{10} N_c$. The white area indicates the parameter region where the particle number is not limited.

region where, from the mean-field point of view, a metastable gas 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 the contour lines close to $a_1/|a_0| \approx 0.3$ indicates the onset of the novel high-density phase.

As an example for estimating the critical particle number from figure 2, we take a two-component ^{6}Li gas in a trap with $\ell = 1\ \mu$m. The extraordinarily large attractive s-wave scattering length of $a_0 = -2160 a_B$ [13], i.e. $a_0/\ell \approx -0.1$, leads to the rather small critical particle number $N_c = 26\,000$ 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 Fermi gas. 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 centre of the trap which should not be confused with Bose condensation of Cooper pairs.

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