Effective Contact Interaction for Dilute Ultra-Cold Quantum Gases in Traps

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In the last years great experimental progress has been achieved in the field of ultra-cold trapped atomic gases. In 1995 a Bose-Einstein condensate of ^{87}Rb atoms was realized [1]. The cooling of a trapped gas of fermionic ^{40}K atoms to a temperature equal to half of the Fermi energy [2] could be accomplished in autumn 1999.

In these dilute systems the inter-particle distance is much larger than the range of their interaction, and, due to the low temperature, their relative velocities are very small so that only s-wave scattering occurs between bosons. Therefore one uses a zero-range s-wave pseudo-potential to calculate energies and densities [3].

However, identical fermions (same m-state) cannot interact through a zero-range potential because their relative wave-function has to be antisymmetric and hence vanishes at the origin where the point-like interaction is nonzero. The first non-vanishing scattering comes from low energy p-waves. Thus one needs a derivation for a contact p-wave interaction from the p-wave phase-shifts in analogy to the s-wave case in order to calculate mean-field properties of the dilute fermi gas.

We present a hermitean effective contact interaction (ECI) for arbitrary partial waves with strengths given by the respective scattering lengths. The attribute "contact" means that they are δ-distributions at the origin but contain radial derivatives for $l > 0$. The word "effective" relates to the demand that the ECI yields effectively they same mean energy calculated with uncorrelated free states as the true two-body interaction with correlated eigenstates.

In order to enumerate the scattering states we first discretize the two-body problem by putting the system in a large spherical container with radius Λ in the relative coordinate. Λ will drop out at the end. Second, we demand that the expectation value of the ECI calculated with nth free scattering state $|nlm\rangle$ with angular momentum l equals the nth positive energy eigenvalue of the true interaction with the same l.

The free radial wave function of $|nlm\rangle$ is given by

$$R_{nl}(r) = A_{nl}\; j_l(k_{nl} r) \tag{1}$$

with quantized free momenta $k_{nl} = \xi_{nl}/\Lambda$, where ξ_{nl} is the nth zero of the spherical Bessel function of angular momentum l. A_{nl} is the normalization of the free states.

In presence of an interaction with range λ the radial wave function of the correlated scattering state $|\overline{nlm}\rangle$ can be written for $r > \lambda$ as

$$\bar{R}_{nl}(r) = \bar{A}_{nl}\,[j_{nl}(\bar{k}_{nl} r) - \tan\eta_l(\bar{k}_{nl})\; n_{nl}(\bar{k}_{nl} r)]. \tag{2}$$

Inside the potential, $r < \lambda$, the shape of $\bar{R}_{nl}(r)$ depends on the details of the potential. For example the number of nodes is given by the number of bound states with the same angular momentum. The quantized relative momentum $\bar{k}_{nl}$ in presence of the interaction is related to the phase shift $\eta_l(\bar{k}_{nl})$ through the boundary condition $\bar{R}_{nl}(\Lambda) = 0$:

$$j_{nl}(\bar{k}_{nl}\Lambda) = \tan\eta_l(\bar{k}_{nl})\; n_{nl}(\bar{k}_{nl}\Lambda). \tag{3}$$

With the assumption

$$\tan\eta_l(k) \ll 1 \qquad \text{or} \qquad \Delta k_{nl}/k_{nl} \ll 1 \tag{4}$$

expansion of both sides of (3) in momentum around the free momentum k_{nl} using the momentum shift $\Delta k_{nl} = \bar{k}_{nl} - k_{nl}$ yields in first order approximation

$$\frac{\Delta k_{nl}}{k_{nl}} = \frac{\Delta E_{nl}}{2E_{nl}} = \tan\eta_l(k_{nl})\,\frac{n_l(\xi_{nl})}{\xi_{nl}\, j_l'(\xi nl)}, \tag{5}$$

with $E_{nl} = \hbar^2 k_{nl}^2/(2\mu)$, μ=reduced mass. All terms of second or higher order in the small quantities (4) are neglected.

The last factor can be reformulated by using the norm constant A_{nl} of the free radial wave function, thus the final expression for the energy shift between the eigenvalues of the hamiltonian with and without interaction reads

$$\Delta E_{nl} = -\frac{\hbar^2}{2\mu}\,\frac{\tan\eta_l(k_{nl})}{k_{nl}}\,A_{nl}^2. \tag{6}$$

The next step is to construct an effective zero-range potential $\mathbf{v}^{\text{eff}}$ which reproduces this energy shift for the free states (1) in the sense

$$\langle nlm|\,\mathbf{v}^{\text{eff}}\,|nlm\rangle \stackrel{!}{=} \Delta E_{nl}. \tag{7}$$

According to the angular momentum structure of the energy shifts it is convenient to write the hermitian operator of the ECI in a partial-wave decomposed fashion:

$$\mathbf{v}^{\text{eff}} = \sum_l \mathbf{v}_l^{\text{eff}} = \sum_l g_l \int \mathrm{d}^3 r\;\; |\vec{r}\rangle \frac{\overleftarrow{\partial}^l}{\partial r^l}\delta^{(3)}(\vec{r})\frac{\overrightarrow{\partial}^l}{\partial r^l}\langle\vec{r}|\,, \tag{8}$$

where g_l is the interaction strength and $\delta^{(3)}(\vec{r})$ is the 3-dimensional delta function. This operator describes a zero-range, non-local, hermitian interaction, which automatically projects onto the angular momentum under consideration. The interaction strength can be determined by inserting the ansatz into condition (7) as

$$g_l = -\frac{4\pi\hbar^2}{2\mu}\left[\frac{(2l+1)!!}{l!}\right]^2 \frac{\tan\eta_l(k)}{k^{2l+1}} = \frac{4\pi\hbar^2}{2\mu}\,\frac{(2l+1)}{(l!)^2}\,a_l^{2l+1}. \tag{9}$$

The last equation uses the parameterization of the phase shifts in terms of the scattering lengths a_l, which is valid under the assumption (4). For $l = 0$ we obtain the well known result $g_0 = 2\pi\hbar^2 a_0/\mu$ and for $l = 1$ we get $g_1 = 6\pi\hbar^2(a_1)^3/\mu$.

Equations (8) and (9) give the analytic form of the effective contact interaction (ECI) in all partial waves.

Now the ECI can be used to set up a mean-field type many-body calculation to investigate the properties of trapped ultra-cold fermionic gases as function of the interaction strength, i.e. the scattering length a_l, and the other parameters like trap size, particle number, etc. This investigation as well as the details of the ECI are subject of a forthcoming paper.

[1] M.H. Anderson, J.R.Ensher et al.; Science 269 (1995) 198.

[2] B. DeMarco and D.S. Jin; Science 285 (1999) 1703.

[3] F. Dalfovo, S. Giorgini et al.; Rev. Mod. Phys. 71 (1999) 463.