

# Modeling interactions for resonant $p$ -wave scattering

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In view of recent experiments on ultra-cold polarized fermions, the zero-range potential approach is generalized to situations where two-body scattering is resonant in the  $p$ -wave channel. We introduce a modified scalar product which reveals a deep relation between the geometry of the Hilbert space and the interaction. This formulation is used to obtain a simple interpretation for the transfer rates between atomic and molecular states within a two branches picture of the many-body system close to resonance. At resonance, the energy of the dilute gas is found to vary linearly with density.

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Studies of regimes with strong correlations is actually one of the most challenging directions in the field of ultra-cold atoms. A spectacular example of such a situation is given by the BCS-BEC crossover of a two spin-component Fermi gas, obtained via tuning the scattering length of binary collisions by using Feshbach resonances [1]. Another interesting example is resonant scattering in  $p$ -wave channels [2, 3, 4, 5, 6] with spin-polarized  ${}^6\text{Li}$  and  ${}^{40}\text{K}$  atoms which opens the possibility of a BCS-BEC crossover in higher angular momentum channels in the near future. The major interest in these systems stems from the fact that the strength of the correlations can be tuned arbitrarily while the mean inter-particle distance remains large with respect to the range of interatomic forces. Consequently, low energy properties are independent of the non-universal short range physics. Ultra-cold gases can therefore be considered as model systems for accurate studies of quantum many-body problems underlying many interesting phenomena in condensed matter physics. For two spin-component fermions where the scattering amplitude in the  $s$ -wave channel dominates, several effective two-body potentials are used both in computational and analytical studies of the so-called unitary regime [7, 8, 9, 10, 11, 12], where the scattering length diverges. In this context, the zero-range pseudo-potential approach is very appealing as it captures all the effects of the interaction with only one parameter [11, 13, 14] for broad  $s$ -wave Feshbach resonances, and with two parameters in narrow  $s$ -wave Feshbach resonances [15]. Furthermore, this approach is particularly useful to obtain exact solutions of few body problems [15, 16, 17, 18], and also to improve unavoidable approximations in many-body systems [14, 19].

In this letter, a general zero-range treatment of resonant  $p$ -wave interactions is introduced. This formalism is used in the context of ultra-cold spin-polarized fermions, where binary  $s$ -wave scattering is suppressed due to the Pauli principle. We show that the Hilbert space associated with the zero-range Hamiltonian has to be defined with a new metrics. The modified scalar product illustrates nicely an intrinsic connection between the geometry of the Hilbert space and the interaction. The formalism is applied to an effective model to obtain some

physical insight into the crossover regime of a many-body system made of particles interacting in pairs via the  $p$ -wave channel. A two branches picture is obtained for the equation of state in the neighborhood of the Feshbach resonance, giving a simple interpretation for the transfer rates between atomic and molecular states. At resonance, in the dilute regime, the model predicts a ground state energy which varies linearly with respect to the atomic density.

Without any loss of generality, we introduce the formalism by considering two identical particles in absence of an external potential. The particles of mass  $m$ , positions  $(\vec{r}_1, \vec{r}_2)$  and relative coordinates  $\vec{r} = \vec{r}_1 - \vec{r}_2$  are described in their center of mass frame by the wave function  $\Psi(\vec{r})$ . The interaction between the particles occurs only in the  $p$ -wave channel of the two-body system and is modeled by the following zero-range pseudo-potential:

$$\langle \vec{r} | V | \Psi \rangle = -\frac{12\pi\hbar^2 \mathcal{V}_s}{m} (\vec{\nabla} \delta)(\vec{r}) \cdot \vec{\mathcal{R}}[\Psi] \quad , \quad (1)$$

where  $\vec{\mathcal{R}}[\cdot]$  is a regularizing operator defined by:

$$\vec{\mathcal{R}}[\Psi] = \lim_{r \rightarrow 0} \left[ \left( \frac{\partial_r^3}{2} + \alpha \partial_r^2 \right) r^2 \int_{\mathcal{S}_r} \frac{d^2\Omega \hat{e}_r}{4\pi} \Psi(\vec{r}) \right]. \quad (2)$$

In Eq.(1),  $\mathcal{V}_s$  is the scattering volume. In the resonant regime,  $|\mathcal{V}_s|$  is arbitrarily large and in contrast with the analog unitary regime in the  $s$ -wave channel, a second parameter (denoted here by  $\alpha$ ) is essential for a description of the shape of the two-body scattering amplitude [20] and has been introduced in the expression of the regularizing operator. In Eq.(2), a surface integration is performed over the sphere  $\mathcal{S}_r$  of radius  $r$  centered at  $r = 0$ ,  $d^2\Omega$  is the elementary solid angle and  $\hat{e}_r = \vec{r}/r$ . This integration ensures that the pseudo-potential acts only on the  $p$ -wave component of the wave function [21]. As a consequence, the wave function has a  $1/r^2$  singularity for  $r \rightarrow 0$  which is a general feature of the zero-range potential approach in the  $p$ -wave channel. The role of the pseudo-potential in the Schrödinger equation is two-fold: first, it imposes a specific boundary condition for the wave function in the vicinity of the  $1/r^2$   $p$ -wave sin-

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gularity:

$$\lim_{r \rightarrow 0} \left[ (\mathcal{V}_s \partial_r^3 + 2\alpha \mathcal{V}_s \partial_r^2 + 2) r^2 \int_{\mathcal{S}_r} d^2 \Omega \hat{e}_r \Psi \right] = \vec{0} \quad , \quad (3)$$

and, second, it cancels a diverging term proportional to  $(\vec{\nabla} \delta)$  coming from the action of the Laplacian on the wave function. Equation (3) is analogous to the contact condition introduced by H. Bethe and R. Peierls for a description of  $s$ -wave scattering [22] and represents an alternative way to formulate the zero-range approach. The pseudo-potential in Eq.(1) generalizes other zero-range  $p$ -wave pseudo-potentials [23, 24], where the resonant regime must be described through an energy dependent scattering volume. Contrary to these approaches, the pseudo-potential (1) can be used directly in time dependent problems or in situations where the two-body collisional energy is not explicitly defined.

As a first illustration of the formalism, we deduce the two-body eigenstates of energy  $E$  in their center of mass frame in absence of any external potential. For this purpose, we use the integral equation:

$$\Psi(\vec{r}) = \Psi_0(\vec{r}) - \int d^3 \vec{r}' G_E(\vec{r}, \vec{r}') \langle \vec{r}' | V | \Psi \rangle \quad , \quad (4)$$

where  $G_E$  is the one-body outgoing Green's function at energy  $E$ . For positive energies,  $E = \hbar^2 k^2 / m$ , Eq.(4) yields the following expression for the scattering states:

$$\Psi_{\vec{k}}(\vec{r}) = \exp(i\vec{k} \cdot \vec{r}) + 3\mathcal{V}_s \hat{e}_r \cdot \vec{\mathcal{R}}[\Psi_{\vec{k}}] \partial_r \left( \frac{\exp(ikr)}{r} \right). \quad (5)$$

Applying the regularizing operator  $\vec{\mathcal{R}}[\cdot]$  on both sides of Eq.(5) solves the problem with:

$$\vec{\mathcal{R}}[\Psi_{\vec{k}}] = \frac{i\vec{k}}{1 + \alpha k^2 \mathcal{V}_s + ik^3 \mathcal{V}_s} \quad . \quad (6)$$

In the asymptotic limit ( $kr \gg 1$ ), one obtains:

$$\Psi_{\vec{k}}(\vec{r}) \simeq \exp(i\vec{k} \cdot \vec{r}) + 3(\hat{e}_k \cdot \hat{e}_r) f_1 \frac{\exp(ikr)}{r}, \quad (7)$$

$$\text{with } , \quad -\frac{1}{f_1} = \frac{1}{k^2 \mathcal{V}_s} + \alpha + ik, \quad \text{and } \hat{e}_k = \vec{k}/k. \quad (8)$$

Eq.(8) coincides exactly with the general expansion of the inverse  $p$ -wave scattering amplitude  $f_1$  at second order in the low energy limit [20], showing that the pseudo-potential (1) provides a modeling of two-body collisions for relative momenta  $k \ll \alpha$ . The zero-range potential approach requires also that  $kR \ll 1$  where  $R$  denotes the potential range, that is the radius such that for  $r > R$  the 'real' potential term experienced by particles can be neglected in the Schrödinger equation. In actual experiments on spin-polarized fermions [2, 3, 5] an external magnetic field  $B$  tunes the energy of a two-body bound state in a closed channel which is coupled to the open channel associated with the two colliding atoms. A Feshbach resonance occurs for a vanishing value of the bound

state energy at a magnetic field  $B = B_0$ . Close to the resonance, the scattering volume takes arbitrarily large values with  $\mathcal{V}_s \propto -1/(B - B_0)$ , while the parameter  $\alpha$  is a slowly varying function of  $B$  [6, 25]. The two-body bound state in the closed channel extends on short lengths of the order of the potential range and is not described by the zero-range approach. However, in the regime where  $\alpha^3 \mathcal{V}_s$  is large and positive ( $B \lesssim B_0$ ), the pseudo-potential supports a weakly bound state of energy  $\epsilon_B \simeq -\hbar^2 / m \alpha \mathcal{V}_s \propto B - B_0$  which corresponds to the outer part (region  $r > R$ ) of the molecular state resulting from the coupling between the closed and the open channels. We anticipate that this state is populated by pairs of particles in the BEC region of the BEC-BCS crossover regime. For large and negative values of  $\alpha^3 \mathcal{V}_s$  ( $B \gtrsim B_0$ ), this state transforms into a long lived quasi-bound state [20].

Having in hand the short range behavior of the wave functions in Eq.(5), one may wonder what is the underlying structure of the Hilbert space spanned by the two-body eigenstates of the zero-range Hamiltonian. As a consequence of the  $1/r^2$  singularity, the low energy bound state is not normalizable. Moreover, the usual scalar product between two different scattering states gives an infinite result. Nevertheless, as we show in the following, it is possible to introduce a regularized scalar product such that the eigenfunctions are orthogonal to each others and the low energy bound state is normalizable. For this purpose, we perform the scalar product between two states  $|\Psi_{\vec{k}}\rangle$  and  $|\Psi_{\vec{k}'}\rangle$  with  $\vec{k} \neq \vec{k}'$ , but exclude from integration the inner volume of the sphere  $\mathcal{S}_r$ , defined above. One finds, as  $r \rightarrow 0$ :

$$\begin{aligned} & \int_{r' > r} d^3 \vec{r}' \Psi_{\vec{k}}^*(\vec{r}') \Psi_{\vec{k}'}(\vec{r}') \\ & = (r - \alpha r^2) \int_{\mathcal{S}_r} d^2 \vec{r}' \Psi_{\vec{k}}^*(\vec{r}') \Psi_{\vec{k}'}(\vec{r}') + \mathcal{O}(r). \end{aligned} \quad (9)$$

This integral is non zero and diverges in the zero-range limit due to the  $p$ -wave singularity of the scattering states. Therefore the zero-range Hamiltonian is not hermitian with respect to the usual scalar product. This feature follows from the fact that the mapping between the *true* scattering states associated with the finite range potential experienced by particles and the states  $\{|\Psi_{\vec{k}}\rangle\}$  in Eq.(5) is not valid for  $r \lesssim R$  while it is justified outside the potential range. Indeed, the singular boundary behavior imposed on wave functions in Eq.(3) is the way to reproduce the effect of the *true* finite range potential for  $r > R$  but has a formal character for interparticle distances  $r \lesssim R$ . In order to conciliate the zero-range pseudo-potential with a finite range potential of small radius  $R$ , we consider the sphere  $S_R$  which separates the outer part (region  $r > R$ ) and the inner part (region  $r \lesssim R$ ) of the *true* wave functions. Contribution in the scalar product of the outer parts of the *true* wave functions is given by Eq.(9) with  $r = R$  and due to orthogonality between the *true* scattering states, the scalar product of the inner parts cancels this term. By construction,

the inner parts of the wave functions ( $r \lesssim R$ ) are not described in the zero-range approach. However, we are free to modify the usual scalar product in order to take into account their contribution. Therefore, we define a regularized scalar product  $(\cdot|\cdot)_0$  by subtracting the surface term (*r.h.s.* of Eq.(9)) from the usual scalar product. In the formal zero-range limit, the regularized scalar product can be also written with a weight  $g(r)$  given by:

$$g(r) = 1 + \delta(r) [(\alpha r^2 - r).] \quad , \quad (10)$$

so that finally, for wave functions obeying the boundary condition Eq.(3), the scalar product reads:

$$(\Psi|\Psi')_0 = \int d^3\vec{r} g(r)\Psi^*(\vec{r})\Psi'(\vec{r}) \quad . \quad (11)$$

One can check that with this new metrics, the zero-range Hamiltonian is hermitian in the domain defined by wave-functions satisfying Eq.(3). Note that following the same reasoning, the notion of regularized scalar product has been generalized recently for zero-range interactions in all the other partial wave channels [26] in the resonant regime. Coming back to the low energy bound state of energy  $\epsilon_B = -\hbar^2 \kappa_B^2/m$  with  $\kappa_B^{-2} \simeq \alpha \mathcal{V}_s$  appearing in the regime  $\mathcal{V}_s \alpha^3 \gg 1$ , the radial part normalized with respect to Eq.(11) is:

$$\mathcal{R}_B(r) = \frac{1}{\sqrt{\alpha - 3\kappa_B/2}} \partial_r \left( \frac{\exp(-\kappa_B r)}{r} \right) \quad . \quad (12)$$

As a result, the probability of finding the molecule of vanishing binding energy outside the range of the true potential is of the order of  $1/\alpha R$ , meaning that the approach is consistent for  $\alpha > 0$  and  $\alpha R \gtrsim 1$  (for example  $\alpha R \simeq 2.8$  in  $^{40}\text{K}$  for the two resonances with  $B_0 \simeq 198.5$  G [4]). The normalization factor in Eq.(12) can be also deduced from the residue of the scattering amplitude (8) at the energy  $\hbar^2 k^2/m = \epsilon_B$  [20] and the regularized scalar product extends this method to inhomogeneous situations.

Now we turn to the case of a homogeneous system made of  $N$  spin-polarized identical fermions of mass  $m$ . For a density ( $n$ ) sufficiently small that binary processes occur at low energy ( $nR^3 \ll 1$ ) the zero-range approach is justified and the interaction between two given particles can be modeled by the pseudo-potential in Eq.(1) [27]. For a qualitative picture of the physics involved in the neighborhood of the resonant regime, we use the box model introduced in Ref.[28] in the context of *s*-wave scattering. In this effective approach, the interaction of one fermion with all the others is modeled by the interaction of a fictitious particle of mass equal to the reduced mass  $m/2$ , with a fixed scatterer at the center of a spherical box of radius  $L$ . The wave function of the fictitious particle which is non-zero in the *p*-wave channel only is an eigenstate of the pseudo-potential (1) and vanishes on the surface of the box. It represents the pair function of two fermions in their center of mass frame. The boundary condition at  $r = L$ , mimics the effects of correlations between pairs and the radius  $L$  is fixed by considering the non interacting case. In this situation, the

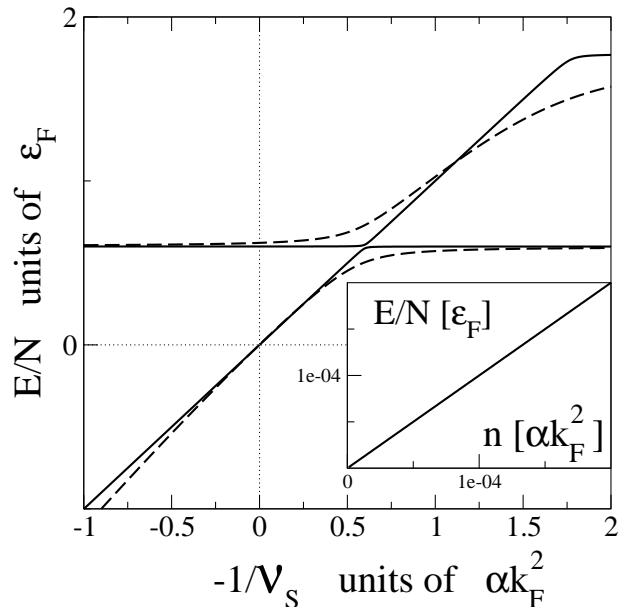


FIG. 1: Energy per particle for a homogeneous medium composed of polarized fermions as a function of  $-1/\mathcal{V}_s$  for  $\alpha = 10k_F$  (dashed line) and  $\alpha = 10^3 k_F$  (continuous line). Inset: equation of state at resonance ( $B = B_0$ ). In this regime, the energy per particle varies linearly with the atomic density.

total energy of the gas is  $E = \frac{3}{5}N\epsilon_F$ , where the Fermi energy  $\epsilon_F = \hbar^2 k_F^2/2m$  is related to the mean density  $n$ , through  $k_F^3 = 6\pi^2 n$ . The gas energy  $E$  is also related to the energy  $\epsilon$  of the fictitious particle by  $E = N\epsilon/2$ . Finally, we obtain a relation between the radius  $L$  and the Fermi momentum  $k_F$  by considering the ground state energy of the fictitious particle in the box where  $k_F L \simeq 5.8$ . Hence,  $L$  is as expected of the order of the mean interparticle distance. In the interacting case, the equation of state is deduced from the energy of the fictitious particle  $\epsilon = \hbar^2 k^2/m = 2E/N$ , where  $k$  (real for  $\epsilon > 0$  or imaginary otherwise) is a solution of the equation:

$$\frac{kL \cos(kL) - \sin(kL)}{kL \sin(kL) + \cos(kL)} = -\frac{\mathcal{V}_s k^3}{1 + \alpha \mathcal{V}_s k^2} \quad . \quad (13)$$

In current experiments [2, 3, 5], if we neglect the trap geometry, the density and the external magnetic field are the two control parameters. We consider then solutions of Eq.(13) for given values of  $-1/\mathcal{V}_s \propto B - B_0$  and of the dimensionless parameter  $\alpha/k_F \gg 1$ . In Fig.(1), we have plotted the two first branches of the energy per particle as a function of  $-1/\mathcal{V}_s$  for two values of the density ( $\alpha/k_F = 10$  and  $10^3$ ). The left part of the upper branch corresponds to the metastable weakly repulsive atomic phase. The right part of the ground branch is associated with the weakly attractive atomic phase where a BCS phase is expected at sufficiently low temperature. The left part of the ground branch represents the molecular phase composed of dimers of energy  $\epsilon/\epsilon_F \simeq -2/\mathcal{V}_s \alpha k_F^2$  [29]. As explained in Ref.[28], this two branches picture

provides the two possible scenarios for obtaining a molecular phase from the weakly interacting atomic Fermi gas by varying the external magnetic field. In the first scenario the system is initially a weakly attractive Fermi gas and follows the ground branch while the parameter  $-1/\mathcal{V}_s$  is tuned from positive to negative values. In the second scenario, the system is initially a weakly repulsive Fermi gas and is driven in the resonant regime by increasing values of  $-1/\mathcal{V}_s$ . The ground branch is then populated by three body recombination processes. At resonance ( $B = B_0$ ) the ground state energy varies linearly with density:  $E/N \propto \hbar^2 n/m\alpha \ll \epsilon_F$  (see inset of Fig.(1)). This result which has been found also in a BCS treatment [30] strongly differs from the  $n^{2/3}$  law obtained in the unitary regime for two-spin components fermions [28]. Qualitatively, a pair of interacting fermions which would have zero energy and infinite size at resonance in absence of other particles, is confined by its neighbors in a volume of the order of  $L^3 \propto 1/n$  and the box model provides an estimation of the cost in energy of this configuration which is  $\simeq \hbar^2/m\alpha L^3 \ll \hbar^2/mL^2$ . Also the level crossing between the two branches differs from the  $s$ -wave result: it is not only translated to the right of the zero energy resonance ( $B = B_0$ ) but also its amplitude tends to zero for decreasing densities. As a consequence

one may expect that in the region of the level crossing, non adiabatic transfers of atoms from the atomic branch to the ground branch resulting from inelastic three-body collisions is followed by only a small heating of the gas due to the small kinetic energy of the outgoing resulting states.

To conclude, we comment on the stability of the molecular phase which is one of the main issue for achieving the BEC-BCS crossover. Lifetime of the shallow diatomic molecules is limited by recombinations into deep bound states of energies  $\mathcal{O}(-\hbar^2/mR^2)$ . Following, the analysis of Ref.[17] the corresponding loss rate can be estimated from the probability that three atoms are confined within a volume of characteristic length  $R$ . The fact that the probability for a pair to be in the inner part of the potential ( $r < R$ ) is given by  $\sim (1 - 1/\alpha R)$  is a strong indication that this rate depends on the width of the resonance considered and could be reduced in the cases where  $\alpha R \sim 1$ . In contrast, these losses are universally suppressed in the unitary two-spin components Fermi gas [17].

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