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T-matrix and effective scattering in spin-polarized atomic deuterium ($\downarrow$D)

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ABSTRACT

The Galitskii–Migdal–Feynman (GMF) formalism is applied to spin-polarized atomic deuterium ($\downarrow$D). The effective scattering length is calculated from the GMF T-matrix, which is essentially the effective scattering amplitude dependent on the medium. It is found that the S-wave effective scattering length for $\downarrow D_2$ and $\downarrow D_3$ varies discontinuously from negative to positive values at some critical density. This indicates a crossover from a dimer-less regime to a regime with dimers. In addition, it is confirmed that $\downarrow D_1$ remains a gas down to zero Kelvin. Finally, the binding energy of the weakly bound dimers in both species $\downarrow D_2$ and $\downarrow D_3$ is computed. For completeness as well as for comparison purposes, the scattering length in the free-scattering limit is also calculated and it is found to be in a good agreement with previous calculations.

1. Introduction

Spin-polarized atomic deuterium $\downarrow$D is a composite Fermi system with nuclear spin $I=1$. Therefore, $\downarrow$D should exhibit three possible spin states: $I_Z=1, 0, -1$. There are three species of $\downarrow$D: $\downarrow D_1$, $\downarrow D_2$, and $\downarrow D_3$ [1–3]. The simplest, $\downarrow D_1$, has only one nuclear spin-state occupied, the other two being empty. In $\downarrow D_2$, two nuclear spin-states are equally occupied and the third is empty. Finally, $\downarrow D_3$ involves all three nuclear spin states, assumed to be equally occupied.

$\downarrow$D is a relatively weakly interacting neutral many-fermionic system. This makes it (spin-polarized atomic deuterium $\downarrow$D) ideal for investigating the range of validity of many-body perturbation theories, such as the Galitskii–Migdal–Feynman (GMF) formalism which is being applied in this work. $\downarrow$D has many interesting properties at high densities [3,4]. It forms a self-bound liquid at a density of order 10^{-3} Å^{-3}. The purpose of this work is to test the validity of the GMF theory for this system at high densities, and compare our results to those calculated at the same densities by different approaches.

Microscopically, there are two main tracks for studying this system. The first is the variational track, including Monte Carlo simulation [4]. Using this method, the ground-state energy of $\downarrow D_3$ has been found to be negative, implying that this system remains liquid at zero temperature and zero external pressure. The lowest-order constrained variational method has also been used to calculate the ground-state energy E [3], with the result that $E(\downarrow D_1) > E(\downarrow D_2) > E(\downarrow D_3)$. The second track is the perturbative, including the Hartree–Fock approximation [2]. In Ref. [2], the T-matrix is calculated in the Hartree–Fock limit, the input single-particle energy spectrum being $\varepsilon_\lambda(p,\omega) = p^2/2m + \Sigma_\lambda(p,\omega)$, where $\Sigma_\lambda(p,\omega)$ is the self-energy; λ, p and ω are the spin, momentum and energy of the particle, respectively. This approximation has been invoked to see how well Green-function methods can be implemented in a moderately dense Fermi liquid. We have recently used the so-called static fluctuation approximation [5] to study the thermodynamic properties of $\downarrow$D.

$\downarrow$D is expected to exhibit properties such as Cooper pairing and superfluidity [6]. This system has the special advantage that the pair potential is known to great accuracy [7]. The pairwise D–D interactions are predominantly of the triplet-potential type. The systems $\downarrow D_2$ and $\downarrow D_3$ form self-bound liquids when compressed to densities around $\rho \approx 4\times10^{-3}$ Å^{-3} at sufficiently low temperatures. The equilibrium densities for $\downarrow D_2$ and $\downarrow D_3$ are in the range 0.0035–0.004 Å^{-3} [3]. On the other hand, $\downarrow D_1$ remains gaseous down to the lowest attainable temperatures. In this paper, a wide range of densities has been used from the free-scattering limit to a density high enough to observe various quantum effects [1–4,6–9].

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In ↓D, all electrons are aligned antiparallel to the applied magnetic field and are fully polarized in fields of order 8–10 T. In this case the system is stable against recombination to the molecular state [6]. P-wave pairing has been found in $\downarrow D_1$ at extremely low temperatures [9]; whereas in $\downarrow D_2$ and $\downarrow D_3$ S-wave pairing occurs. Experimentally, the highest density attained in ↓D has been $\sim 10^{-10}$ Å^{-3} [10].

In this paper we shall apply the GMF formalism [11,12] to spin-polarized atomic deuterium ↓D to calculate the effective S-wave scattering length for $\downarrow D_2$ and $\downarrow D_3$ and the effective P-wave scattering length for $\downarrow D_1$. The GMF formalism will be used to calculate the effective phase shifts which, in turn, are used to evaluate the effective, density-dependent scattering lengths for the three species of ↓D. These scattering lengths turn out to be very useful in analyzing the critical behavior of these systems. In addition, accurate calculations of the effective S-wave scattering lengths are important in studying elastic collisions and, therefore, evaporative cooling rates [13–15].

The basic quantity in this formalism is the T-matrix whose instability is an indication of the formation of fermion pairs. This matrix is very rich in physical content. First, it is an effective ↓D–↓D interaction in momentum space taking into account the medium. Secondly, it is a generalized amplitude in the sense that, although we still have a two-body problem (an independent-pair model), it *does* incorporate the many-body medium through a Pauli exclusion operator and an energy denominator which includes a potential well reflecting the presence of all other particles. This idea is, of course, commonplace in the Hartree–Fock type of many-body theories [2], including the present formalism. Finally, the notion of multiple scattering enters into the formalism in a very fundamental way. In fact, the T-matrix can be viewed as a Lippmann–Schwinger T-matrix 'dressed up' by the medium.

The GMF t-matrix includes hole–hole scattering inside the Fermi-sea as well as particle–particle scattering outside the sea. In this work, the input single-particle energy spectrum has been approximated by the free-particle energy $\varepsilon(k) = \hbar^2 k^2/2m$. The GMF formalism has been recently applied to both spin-polarized and normal ^{3}He–He II mixtures [16,17]. It has been concluded that hole–hole scattering plays a crucial role in any possible fermion–fermion pairing in these systems.

The rest of the paper is organized as follows. Section 2 contains a brief account of the GMF formalism for spin-polarized atomic deuterium, since this theory is well-described elsewhere [12]. The results are presented and discussed in Section 3. Finally, in Section 4, the paper closes with some concluding remarks.

2. GMF formalism for spin-polarized deuterium

In this section we shall present our formalism briefly—just for reference purposes and for defining the quantities involved. The GMF T-matrix is given for a neutral Fermi system by [12]

$$T(\mathbf{p},\mathbf{p}';s,\mathbf{P}) = u(|\mathbf{p}-\mathbf{p}'|) + (2\pi)^{-3}\int \mathrm{d}\mathbf{k}\, u(|\mathbf{p}-\mathbf{k}|) \times \left[g_0(k,s)Q(\mathbf{k},\mathbf{P},\beta) - g_0^+(k,s)\overline{Q}(\mathbf{k},\mathbf{P},\beta)\right] T(\mathbf{k},\mathbf{p}';s,\mathbf{P}). \quad (1)$$

Here $\mathbf{p}$ and $\mathbf{p}'$ are the relative incoming and outgoing momenta; the parameter s is the total energy of the interacting pair in the center-of-mass frame and is given by

$$s \equiv 2\mu_D\left(2P_0 - \frac{P^2}{m_D}\right), \quad (2)$$

P_0 being the total energy of the pair and P^2 the energy carried by the center of mass; μ_D is the effective reduced mass of the interacting pair. Throughout our calculations a natural system of units is used, such that $\hbar = 1 = 2m_D$, where m_D is the D atomic mass, the conversion factor being $\hbar^2/2m_D = 12.043$ K Å^{-2}. In fully spin-polarized Fermi systems, where the fixed spin polarization prevents spin fluctuations, the enhancement of m_D^* is small; so that $m_D^* \approx m_D$ [18]. The operator $u \equiv (2\mu_D/\hbar^2)V \equiv 1/2V$, where V is the Fourier transform of a static central two-body potential. We have used three triplet-state potentials: Morse-type [7], Silvera [20] and Born–Oppenheimer [21]. Using our system of units, we have

$$s = P_0 - P^2. \quad (3)$$

The operator $Q(\overline{Q})$ is the product of particle–particle (hole–hole) occupation probabilities. In momentum space, the hole occupation probability is just the Fermi–Dirac distribution, which reduces to the unit step function at zero temperature. When subtracted from unity, this yields the particle-occupation probability. $Q(\overline{Q})$ is equal to one if both particles (holes) are outside (inside) the Fermi-sea. The angle-averaged functions Q and $\overline{Q}$ are given by

$$Q(k,\beta) = \frac{1}{\exp(-\beta(k^2-k_F^2))+1} \times \frac{1}{\exp(-\beta(k^2-k_F^2))+1}, \quad (4)$$

$$\overline{Q}(k,\beta) = \frac{1}{\exp(\beta(k^2-k_F^2))+1} \times \frac{1}{\exp(\beta(k^2-k_F^2))+1}, \quad (5)$$

k_F being the Fermi momentum for fully spin-polarized atomic deuterium and is given by

$$k_F = \left(\frac{6\pi^2\rho}{\nu}\right)^{1/3}$$

where ν is the spin degeneracy: $\nu = 1$, 2 and 3 for $\downarrow D_1$, $\downarrow D_2$ and $\downarrow D_3$, respectively.

The free two-body Green's function $g_0(s)$ is defined as

$$g_0(\vec{k},s) \equiv \frac{1}{k^2 - s - i\eta}. \quad (6)$$

The system of interacting real particles is described in terms of weakly interacting quasiparticles; this justifies the use of free Green's functions. The quantity η is a positive infinitesimal in the scattering region and zero otherwise.

The Fourier–Bessel transform of the ↓D–↓D interatomic potential was calculated using a program originally constructed by Ghassib and coworkers [19] for interhelium potentials.

The effective phase shifts can be determined by parametrizing the on-energy-shell T-matrix, $T_\ell(p,p;s,P,\beta) \equiv T_\ell(p;P,\beta)$ as follows [12]:

$$T_\ell(p;P;\beta) = -\frac{4\pi}{p}\frac{\exp(i\delta_\ell^E(p;P,\beta))\sin(\delta_\ell^E(p;P,\beta))}{Q(p;P,\beta)+\overline{Q}(p;P,\beta)}, \quad (7)$$

so that

$$\tan(\delta_\ell^E(p;P,\beta)) \equiv \frac{\mathrm{Im}\,T_\ell(p;P;\beta)}{\mathrm{Re}\,T_\ell(p;P;\beta)}, \quad (8)$$

$\mathrm{Im}\,T_\ell(p;P;\beta)$ and $\mathrm{Re}\,T_\ell(p;P;\beta)$ denoting, respectively, the imaginary and real parts of $T_\ell(p;P;\beta)$.

To calculate the real and imaginary parts of the T-matrix, it is convenient to define a real K-matrix:

$$K_\ell(p,p';s,P,\beta) \equiv u_\ell(p,p') + \frac{1}{2\pi^2}\int k^2\,\mathrm{d}k\, u_\ell(p,k) \times \left[\frac{Q(k,P,k_F)}{k^2-s} - \frac{\overline{Q}(k,P,k_F)}{k^2-s}\right] K_\ell(k,p';s,P). \quad (9)$$

Finally, the real and imaginary parts of the T-matrix are

$$\mathrm{Re}\,T_\ell(p,p';s,P,\beta) = K_\ell(p,p';s,P,\beta) - A_\ell(s,P,\beta)B_\ell(p,p';s,P,\beta), \quad (10)$$