Microscopic many-body theory of atomic Bose gases near a Feshbach resonance

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Abstract
A Feshbach resonance in the s-wave scattering length occurs if the energy of
the two atoms in the incoming open channel is close to the energy of a
bound state in a coupled closed channel. Starting from the microscopic
Hamiltonian that describes this situation, we derive the effective
atom–molecule theory for a Bose gas near a Feshbach resonance. In order to
take into account all two-body processes, we have to dress the bare
couplings of the atom–molecule model with ladder diagrams. This results in
a quantum field theory that exactly reproduces the scattering amplitude of
the atoms and the bound-state energy of the molecules. Since these
properties are incorporated at the quantum level, the theory can be applied
both above and below the critical temperature of the gas. Moreover, making
use of the true interatomic potentials ensures that no divergences are
encountered at any stage of the calculation. We also present the mean-field
theory for the Bose–Einstein condensed phase of the gas.

Keywords: Bose–Einstein condensation, Feshbach resonance,
coherent matter waves, many-body theory

1. Introduction

The recent experiment by Donley *et al* [1] has made it clear
that near a Feshbach resonance the coherence between atoms
and molecules can have a profound effect on the dynamics of
an atomic Bose–Einstein condensate (BEC). As a result, it has
become an urgent problem to understand from first principles
how to properly incorporate the possible coherence between
atoms and molecules into the theory of an interacting Bose gas.
In the last four years important progress towards a solution
of this problem has been made by a number of groups [2–
7]. Nevertheless, it appears that a fully satisfactory theory,
which obeys all the requirements that on physical grounds can
a priori be imposed upon the theory, still needs to be developed.
It is with this goal in mind that the present paper has been
written.

A first requirement for the theory is that it is based on an
adequate microscopic description of a Feshbach resonance.
Feshbach resonances have been known for a long time in
nuclear physics [8], but have only more recently been predicted
to occur in ultracold atomic gases [9, 10]. The defining feature
of such resonances is that they can only occur in a multichannel
scattering problem. More precisely, a Feshbach resonance
occurs when the kinetic energy of the particles in the incoming
open channel is equal to the energy of a bound state in a closed
channel that is (weakly) coupled to the incoming channel. It
is important for our purposes that the physics of a Feshbach
resonance is quite different from the physics of a resonance in
a single-channel scattering problem with a bound state near the
continuum threshold of the particles. This can most easily be
seen from the fact that in the latter case the bound state in the
incoming channel is only very weakly bound and the extent
of its wavefunction is, therefore, always much larger than the
range of the interaction between the particles. For a Feshbach
resonance the extent of the closed-channel contribution to the
bound-state wavefunction is generally of the same size as the
range of the interactions, because it usually corresponds to a
deeply bound state in the potential of another, closed, channel.
As a result also, the quantum numbers of this part of the bound-
state wavefunction are different from the quantum numbers of
the incoming particles, which is clearly not the case for the
single-channel scattering problem.

A second requirement follows from the fact that the many-body theory based on the microscopic description envisaged above is free of ultraviolet divergences at any level of approximation, and in particular for both the normal and superfluid phases of the atomic Bose gas. The reason for this is that microscopically the interatomic interactions responsible for the Feshbach resonance are determined by short-range potentials, which cut off all the momentum integrals that arise when we diagrammatically include the effects of the interactions. As a result the desired effective atom–molecule Hamiltonian of the gas can contain only terms with coefficients that are finite and cut-off. Moreover, the coefficients are determined by only a small number of experimental parameters such as the position and the width of the Feshbach resonance, for instance.

The most crucial additional requirement for the effective atom–molecule Hamiltonian is that it must exactly reproduce the two-body physics of the atomic gas, i.e. by solving the Hamiltonian in the Hilbert space of two atoms we must recover the correct scattering amplitude of the atoms and also the correct binding energy and quantum numbers of the molecule. Note that in this manner the molecular properties are exactly incorporated at the quantum level, which is important for several reasons. First, the theory can now be applied both in the normal and in the superfluid phase of the gas. Second, we are not restricted to a mean-field description of the gas and are now also able to systematically study fluctuation effects, which we have recently shown to be of importance under the experimental conditions of interest [11]. Finally, the theory can be immediately generalized to atomic Fermi gases near a Feshbach resonance, which are of great current interest in view of the prospect of creating new neutral Bardeen–Cooper–Schrieffer (BCS) superfluids [12–14]. Also in this case fluctuation effects are known to be significant [15, 16] and can only be accounted for after the molecular properties are exactly incorporated in the quantum theory.

As already implicitly mentioned, the effective atom–molecule Hamiltonian is in first instance the most convenient way to arrive at a mean-field description of the gas. In the case of a Bose–Einstein condensed atomic gas, an exact property of the system is that it has a gapless excitation. Therefore, any physically reasonable mean-field theory must have the same property. From a fundamental point of view the gapless excitation is due to the fact that a BEC spontaneously breaks the global $U(1)$ symmetry associated with the conservation of the total number of atoms. For the mean-field theory to fulfil this requirement automatically it must be formulated such that it does not contain an anomalous density or pairing field [17, 18]. Including an anomalous density in general leads to double counting of the interaction effects because the anomalous density is proportional to the condensate density and its effect is, therefore, already largely included in the mean-field terms due to the condensate. As a result, the gaplessness of the mean-field theory is lost.

In agreement with the above discussion, this paper is organized as follows. In section 2 we start from a microscopic Hamiltonian for an atomic Bose gas with a Feshbach resonance and derive from this a bare atom–molecule theory. To make contact with the experimentally known parameters of the Feshbach resonance, we then carry out in section 3 a complete ladder summation to arrive at the desired effective atom–molecule Hamiltonian that exactly incorporates all the relevant two-atom physics. In section 4 we show in particular how the correct properties of the molecule are recovered. After that we discuss in section 5 how to arrive at the simplest mean-field theory that is appropriate at the low temperatures of interest experimentally, where the thermal component of the gas can be neglected. We finally end in section 6 with our conclusions.

2. Bare atom–molecule theory

Without loss of generality we can consider the simplest situation in which a Feshbach resonance arises, i.e. we consider a homogeneous gas of identical atoms with two internal states denoted by $|\uparrow\rangle$ and $|\downarrow\rangle$. The atoms in the two states interact via the potentials $V_{\uparrow\uparrow}(x - x')$ and $V_{\downarrow\downarrow}(x - x')$ respectively. The state $|\downarrow\rangle$ has an energy $\Delta\mu B/2$ with respect to the state $|\uparrow\rangle$ due to the Zeeman interaction with the magnetic field B. The coupling between the two states, which from the atomic physics point of view is due to the hyperfine interaction, is denoted by $V_{\uparrow\downarrow}(x - x')$. Putting everything together our microscopic Hamiltonian is thus given by

$$
\begin{aligned}
\hat{H} = \int \mathrm{d}x\, \hat{\psi}_{\uparrow}^{\dagger}(x) \Bigg[&-\frac{\hbar^2 \boldsymbol{\nabla}^2}{2m} \\
&+ \frac{1}{2} \int \mathrm{d}x'\, \hat{\psi}_{\uparrow}^{\dagger}(x') V_{\uparrow\uparrow}(x - x') \hat{\psi}_{\uparrow}(x') \Bigg] \hat{\psi}_{\uparrow}(x) \\
&+ \int \mathrm{d}x\, \hat{\psi}_{\downarrow}^{\dagger}(x) \Bigg[-\frac{\hbar^2 \boldsymbol{\nabla}^2}{2m} + \frac{\Delta\mu B}{2} \\
&+ \frac{1}{2} \int \mathrm{d}x'\, \hat{\psi}_{\downarrow}^{\dagger}(x') V_{\downarrow\downarrow}(x - x') \hat{\psi}_{\downarrow}(x') \Bigg] \hat{\psi}_{\downarrow}(x) \\
&+ \frac{1}{2} \int \mathrm{d}x \int \mathrm{d}x'\, [\hat{\psi}_{\uparrow}^{\dagger}(x) \hat{\psi}_{\uparrow}^{\dagger}(x') V_{\uparrow\downarrow}(x - x') \\
&\times \hat{\psi}_{\downarrow}(x') \hat{\psi}_{\downarrow}(x) + \text{h.c.}],
\end{aligned}
\tag{1}
$$

where the potential $V_{\downarrow\downarrow}(x - x')$ is assumed to contain the bound state responsible for the Feshbach resonance. Using a Hubbard–Stratonovich transformation to decouple this part of the Hamiltonian [19, 20], we introduce the molecular field operator $\hat{\psi}_{\mathrm{m}}(x)$ that annihilates a molecule at position x. In the approximation that we are close to resonance, only a single bound state contributes and this operator has the property that

$$
\langle \hat{\psi}_{\downarrow}(x) \hat{\psi}_{\downarrow}(x') \rangle = \sqrt{2} \langle \hat{\psi}_{\mathrm{m}}((x + x')/2) \rangle \chi_{\mathrm{m}}(x - x'). \tag{2}
$$

The properly normalized and symmetrized bound-state wavefunction in the potential $V_{\downarrow\downarrow}(x - x')$, which we choose to be real for simplicity, obeys the Schrödinger equation

$$
\left[-\frac{\hbar^2 \boldsymbol{\nabla}^2}{m} + V_{\downarrow\downarrow}(x) \right] \chi_{\mathrm{m}}(x) = E_{\mathrm{m}} \chi_{\mathrm{m}}(x). \tag{3}
$$

Note that the wavefunction $\chi_{\mathrm{m}}(x)$ represents the bare molecular wavefunction. Due to the coupling $V_{\uparrow\downarrow}(x - x')$ the true or dressed molecular wavefunction acquires also a non-zero component in the open channel. This distinction is especially important near the Feshbach resonance as is discussed in detail in section 4. After the Hubbard–Stratonovich transformation we obtain the bare Hamiltonian for the coupled atom–molecule system. It reads

$$\hat{H} = \int d\boldsymbol{x}\, \hat{\psi}_\uparrow^\dagger(\boldsymbol{x}) \left[-\frac{\hbar^2 \boldsymbol{\nabla}^2}{2m} \right.$$

$$+ \frac{1}{2} \int d\boldsymbol{x}' \hat{\psi}_\uparrow^\dagger(\boldsymbol{x}') V_{\uparrow\uparrow}(\boldsymbol{x} - \boldsymbol{x}') \hat{\psi}_\uparrow(\boldsymbol{x}') \Big] \hat{\psi}_\uparrow(\boldsymbol{x})$$

$$+ \int d\boldsymbol{x}\, \hat{\psi}_m^\dagger(\boldsymbol{x}) \left[-\frac{\hbar^2 \boldsymbol{\nabla}^2}{4m} + \Delta\mu B + E_m \right] \hat{\psi}_m(\boldsymbol{x})$$

$$+ \int d\boldsymbol{x} \int d\boldsymbol{x}'\, [g_{\uparrow\downarrow}(\boldsymbol{x} - \boldsymbol{x}') \hat{\psi}_m^\dagger((\boldsymbol{x} + \boldsymbol{x}')/2)$$

$$\times\, \hat{\psi}_\uparrow(\boldsymbol{x}') \hat{\psi}_\uparrow(\boldsymbol{x}) + \text{h.c.}], \tag{4}$$

where $g_{\uparrow\downarrow}(\boldsymbol{x}) = V_{\uparrow\downarrow}(\boldsymbol{x}) \chi_m(\boldsymbol{x})/\sqrt{2}$ is the bare atom–molecule coupling. The molecule–molecule and atom–molecule interactions also follow from the above procedure but will be neglected in the following, since under the experimental conditions of interest [1, 21] the density of molecules is very small.

3. Ladder summations

For an the application of the Hamiltonian in (4) to realistic atomic gases we have to include all two-body processes, because at the relevant low densities three-body (and more) processes can in the first instance be neglected. These are most conveniently included by a renormalization of the bare potential $V_{\uparrow\uparrow}(\boldsymbol{x} - \boldsymbol{x}')$ and the bare coupling $g_{\uparrow\downarrow}(\boldsymbol{x})$. Moreover, the molecules acquire a self-energy.

The interaction potential of the atoms in principle renormalizes to the many-body T (transition) matrix. This renormalization is determined by a Bethe–Salpeter equation which, within the (for our purposes) sufficiently accurate Hartree–Fock approximation [17], reads

$$T^{MB}(\boldsymbol{k}, \boldsymbol{k}', \boldsymbol{K}, z) = V_{\uparrow\uparrow}(\boldsymbol{k} - \boldsymbol{k}') + \frac{1}{V} \sum_{\boldsymbol{k}''} V_{\uparrow\downarrow}(\boldsymbol{k} - \boldsymbol{k}')$$

$$\times\, \frac{[1 + N(\epsilon_{K/2+k''} - \mu) + N(\epsilon_{K/2-k''} - \mu)]}{z - \epsilon_{K/2+k''} - \epsilon_{K/2-k''}}$$

$$\times\, T^{MB}(\boldsymbol{k}'', \boldsymbol{k}', \boldsymbol{K}, z), \tag{5}$$

where $N(x) = [e^{\beta x} - 1]^{-1}$ is the Bose distribution function of the atoms, μ their chemical potential and $1/k_B T$ the inverse thermal energy. This equation describes the scattering of a pair of atoms from relative momentum $\boldsymbol{k}'$ to relative momentum $\boldsymbol{k}$ at energy z. Due to the fact that the scattering takes place in a medium the many-body T matrix also depends on the centre-of-mass momentum $\boldsymbol{K}$. The energy of a single atom is equal to $\epsilon_k = \hbar^2 k^2/2m$. In the Hartree–Fock approximation the energy in principle also contains a mean-field correction which we neglect in the first instance. We come back to this point in section 4, however. The diagrammatic representation of (5) is given in figure 1.

For temperatures not too close to the critical temperature we are allowed to neglect the many-body effects [17], and (5) reduces to the Lippmann–Schwinger equation for the two-body T matrix. The effective interaction between the atoms thus becomes $T^{2B}(\boldsymbol{k}, \boldsymbol{k}', z - \epsilon_K/2)$. For the realistic conditions of the atomic gases under consideration here, i.e. small external momenta and energies, the two-body T matrix is independent of momentum and energy and equal to $4\pi a_{\uparrow\uparrow} \hbar^2/m$, with $a_{\uparrow\uparrow}$ the s-wave scattering length of the potential $V_{\uparrow\uparrow}(\boldsymbol{x} - \boldsymbol{x}')$.
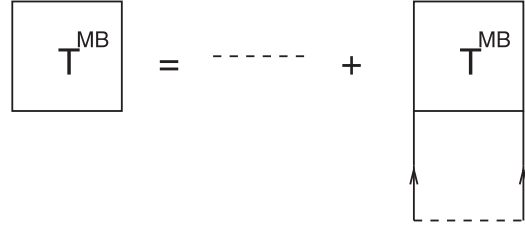
Figure 1. Diagrammatic representation of the many-body T matrix. The solid lines correspond to single-atom propagators. The dashed lines corresponds to the interatomic interaction $V_{\uparrow\uparrow}$.

Therefore, we conclude that the renormalization of this potential is given by

$$V_{\uparrow\uparrow}(\boldsymbol{x} - \boldsymbol{x}') \to \frac{4\pi a_{\uparrow\uparrow} \hbar^2}{m} \delta(\boldsymbol{x} - \boldsymbol{x}'). \tag{6}$$

The renormalization of the bare atom–molecule coupling is determined by the equation

$$g^{MB}(\boldsymbol{k}, \boldsymbol{K}, z) = g_{\uparrow\downarrow}(\boldsymbol{k}) + \frac{1}{V} \sum_{\boldsymbol{k}'} T^{MB}(\boldsymbol{k}, \boldsymbol{k}', \boldsymbol{K}, z)$$

$$\times\, \frac{[1 + N(\epsilon_{K/2+k'} - \mu) + N(\epsilon_{K/2-k'} - \mu)]}{z - \epsilon_{K/2+k'} - \epsilon_{K/2-k'}} g_{\uparrow\downarrow}(\boldsymbol{k}'), \tag{7}$$

and is presented diagrammatically in figure 2. Neglecting many-body effects, the coupling constant becomes $g^{2B}(\boldsymbol{k}, z - \epsilon_K/2)$ with

$$g^{2B}(\boldsymbol{k}, z) = g_{\uparrow\downarrow}(\boldsymbol{k})$$

$$+ \frac{1}{V} \sum_{\boldsymbol{k}'} T^{2B}(\boldsymbol{k}, \boldsymbol{k}', z) \frac{1}{z - 2\epsilon_{k'}} g_{\uparrow\downarrow}(\boldsymbol{k}'). \tag{8}$$

For the relevant small momenta and energies we are thus led to the substitution

$$g_{\uparrow\downarrow}(\boldsymbol{x} - \boldsymbol{x}') \to g\delta(\boldsymbol{x} - \boldsymbol{x}'), \tag{9}$$

where g can be related to experimentally known parameters as follows. The resonance is characterized experimentally by a width ΔB and a position B_0. More precisely, the s-wave scattering length of the atoms as a function of magnetic field is given by

$$a(B) = a_{bg} \left(1 - \frac{\Delta B}{B - B_0} \right), \tag{10}$$

where a_{bg} denotes the so-called background scattering length. To correspond with the experiment we thus have that $a_{\uparrow\uparrow} = a_{bg}$. In order to reproduce the experimentally observed width of the resonance we have that $g = \hbar\sqrt{2\pi a_{bg} \Delta B \Delta\mu/m}$, since an elimination of the molecular field shows that $a_{bg} \Delta B = mg^2/(2\pi\hbar^2 \Delta\mu)$.

The self-energy of the molecules, shown diagrammatically in figure 3, is given by

$$\hbar\Sigma^{MB}(\boldsymbol{K}, z) = \frac{2}{V} \sum_{\boldsymbol{k}} g_{\uparrow\downarrow}(\boldsymbol{k})$$

$$\times\, \frac{[1 + N(\epsilon_{K/2+k} - \mu) + N(\epsilon_{K/2-k} - \mu)]}{z - \epsilon_{K/2+k} - \epsilon_{K/2-k}}$$

$$\times\, g^{MB}(\boldsymbol{k}, \boldsymbol{K}, z). \tag{11}$$

In the first instance we neglect again many-body effects which reduces the self-energy in (11) to $\hbar\Sigma^{2B}(z - \epsilon_K/2)$ with

$$\hbar\Sigma^{2B}(z) = \langle\chi_{\rm m}|\hat{V}_{\uparrow\downarrow}\hat{G}_{\uparrow\uparrow}(z)\hat{V}_{\uparrow\downarrow}|\chi_{\rm m}\rangle, \qquad (12)$$

where the propagator $\hat{G}_{\uparrow\uparrow}(z)$ is given by

$$\hat{G}_{\uparrow\uparrow}(z) = \frac{1}{z - \hat{H}_{\uparrow\uparrow}}, \qquad (13)$$

with the Hamiltonian

$$\hat{H}_{\uparrow\uparrow} = \frac{\hat{p}^2}{m} + \hat{V}_{\uparrow\uparrow} \equiv \hat{H}_0 + \hat{V}_{\uparrow\uparrow}. \qquad (14)$$

We insert in (12) a complete set of bound states $|\phi_\kappa\rangle$ with energies E_κ and scattering states $|\phi_{\mathbf{k}}^{(+)}\rangle$. The latter obey the Lippmann–Schwinger equation

$$|\phi_{\mathbf{k}}^{(+)}\rangle = |\mathbf{k}\rangle + \frac{1}{2\epsilon_k^+ - \hat{H}_0}\hat{V}_{\uparrow\uparrow}|\phi_{\mathbf{k}}^{(+)}\rangle, \qquad (15)$$

where $\epsilon_k^+ = \epsilon_k + {\rm i}0$ denotes the usual limiting procedure. This reduces the self-energy $\hbar\Sigma^{2B}(z)$ to

$$\hbar\Sigma^{2B}(z) = \sum_\kappa |\langle\chi_{\rm m}|\hat{V}_{\uparrow\downarrow}|\phi_\kappa\rangle|^2 \frac{1}{z - E_\kappa}$$
$$+ \int \frac{{\rm d}\mathbf{k}}{(2\pi)^3}|\langle\chi_{\rm m}|\hat{V}_{\uparrow\downarrow}|\phi_{\mathbf{k}}^{(+)}\rangle|^2 \frac{1}{z - 2\epsilon_k}, \qquad (16)$$

where we replaced the sum over the momenta $\mathbf{k}$ by an integral. Using (8) and the Lippmann–Schwinger equation we have that

$$g^{2B}(k, 2\epsilon_k^+) = \frac{1}{\sqrt{2}}\langle\chi_{\rm m}|\hat{V}_{\uparrow\downarrow}|\phi_{\mathbf{k}}^{(+)}\rangle. \qquad (17)$$

As a result we have for the retarded self-energy $\hbar\Sigma^{(+)}(\hbar\omega)$, i.e. the self-energy $\hbar\Sigma^{2B}(z)$ evaluated at the physically relevant energy $z = \hbar\omega^+$,

$$\hbar\Sigma^{(+)}(\hbar\omega) \simeq -g^2 \frac{m^{3/2}}{2\pi\hbar^3}{\rm i}\sqrt{\hbar\omega} - (\Delta\mu B_0 + E_{\rm m}), \qquad (18)$$

where we have denoted the energy-independent shift, that results from the $z = 0$ part of the right-hand side of (16), in such a manner that the position of the resonance in the magnetic field is precisely at the experimentally observed magnetic field value B_0.

4. Molecular binding energy and density of states

Putting the results of the previous sections together, we find that the Bose gas near a Feshbach resonance is described by a coupled set of equations of motion for the atomic and molecular Heisenberg operators $\hat{\psi}_{\rm a}(\mathbf{x}, t) \equiv \hat{\psi}_\uparrow(\mathbf{x}, t)$ and $\hat{\psi}_{\rm m}(\mathbf{x}, t)$ respectively. Within our approximations, these coupled equations are given by

$${\rm i}\hbar\frac{\partial\hat{\psi}_{\rm a}(\mathbf{x}, t)}{\partial t} = \left[-\frac{\hbar^2\nabla^2}{2m} + T_{\rm bg}^{2B}\hat{\psi}_{\rm a}^\dagger(\mathbf{x}, t)\hat{\psi}_{\rm a}(\mathbf{x}, t)\right]\hat{\psi}_{\rm a}(\mathbf{x}, t)$$
$$+ 2g\hat{\psi}_{\rm a}^\dagger(\mathbf{x}, t)\hat{\psi}_{\rm m}(\mathbf{x}, t),$$

$${\rm i}\hbar\frac{\partial\hat{\psi}_{\rm m}(\mathbf{x}, t)}{\partial t} = \left[-\frac{\hbar^2\nabla^2}{4m} + \delta(B(t))\right.$$
$$\left. - g^2\frac{m^{3/2}}{2\pi\hbar^3}{\rm i}\sqrt{{\rm i}\hbar\frac{\partial}{\partial t} + \frac{\hbar^2\nabla^2}{4m}}\right]\hat{\psi}_{\rm m}(\mathbf{x}, t) + g\hat{\psi}_{\rm a}^2(\mathbf{x}, t), \qquad (19)$$
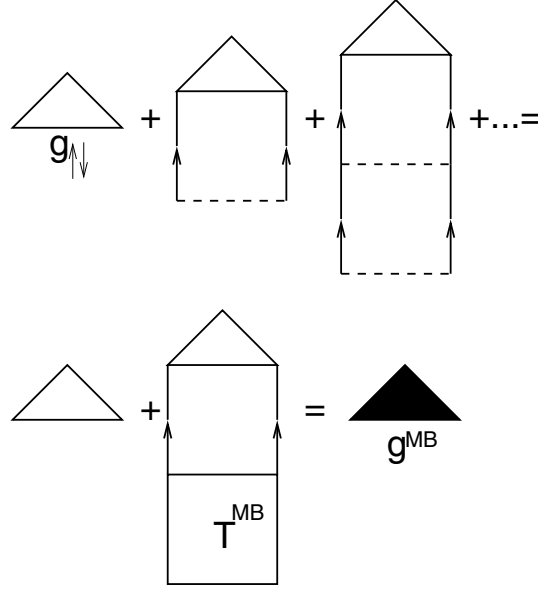

Figure 2. Diagrammatic representation of renormalization of the bare atom–molecule coupling $g_{\uparrow\downarrow}$.
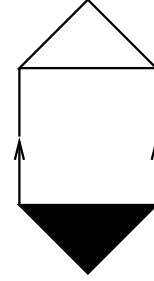

Figure 3. Diagrammatic representation of the self-energy of the molecules.

where the detuning is defined by $\delta(B) = \Delta\mu(B - B_0)$ and $T_{\rm bg}^{2B} = 4\pi a_{\rm bg}\hbar^2/m$. This is the most important result of our work. Note that the time derivative and gradient terms appear exactly, such that both equations of motion are manifestly Galilean invariant. Note also that an external trapping potential can just be added to the right-hand sides of these equations if required. It is interesting to mention that the above equations can immediately be generalized to a Fermi gas near a Feshbach resonance. Moreover, a simple Hartree–Fock approximation to the resulting theory reproduces exactly the interesting crossover physics recently discussed by Ohashi and Griffin [14] on the basis of the Nozières and Schmitt-Rink formalism for the normal phase of the gas. Having made this observation, it is now clear how the same crossover phenomena can be studied in the superfluid phase of the gas. Work in this direction is in progress and will be reported elsewhere.

From (19) we determine the retarded Green function of the molecules $G_{\rm m}^{(+)}(\mathbf{x}, t; \mathbf{x}', t')$. For fixed detuning, the poles of its Fourier transform determine the bound-state energy. This Fourier transform is given by

$$G_{\rm m}^{(+)}(\mathbf{k}, \omega)$$
$$= \frac{\hbar}{\hbar\omega^+ - \epsilon_k/2 - \delta(B) + (g^2 m^{3/2}/2\pi\hbar^3){\rm i}\sqrt{\hbar\omega - \epsilon_k/2}}, \qquad (20)$$
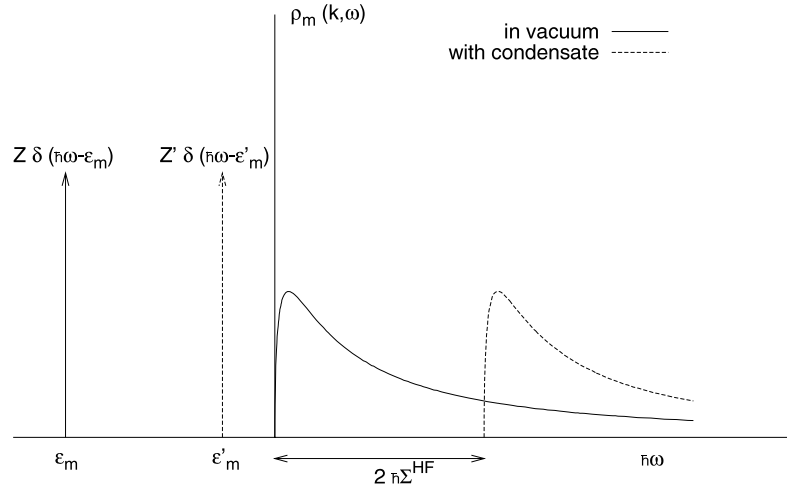
Figure 4. Molecular density of states.

with $\epsilon_k/2 = \hbar^2 k^2/4m$ the kinetic energy of a molecule. For positive detuning the propagator has a pole with non-zero imaginary part, which shows that the molecule has a finite lifetime in this case. To a first approximation the energy of the molecule is $\epsilon_{\mathrm{m}}(B) + \epsilon_k/2$ with $\epsilon_{\mathrm{m}}(B) = \delta(B)$ and its rate of decay equals $\Gamma_{\mathrm{m}}(B) = (g^2 m^{3/2}/\pi\hbar^4)\sqrt{\delta(B)}$. For negative detuning the molecular propagator has a real pole at $\hbar\omega = \epsilon_{\mathrm{m}} + \epsilon_k/2$, where the bound-state energy of the molecule is given by

$$\epsilon_{\mathrm{m}}(B) = \delta(B) + \frac{g^4 m^3}{8\pi^2\hbar^6}\left[\sqrt{1 - \frac{16\pi^2\hbar^6}{g^4 m^3}\delta(B)} - 1\right]. \quad (21)$$

Close to the resonance the bound-state energy is, using (10), found to be equal to

$$\epsilon_{\mathrm{m}}(B) = -\frac{\hbar^2}{m[a(B)]^2}. \quad (22)$$

It is important to realize that this last equation, which is well-known to be true for a weakly bound state in a single-channel scattering problem [22], has now thus been proven to also be valid for the case of a multichannel Feshbach resonance.

The physics of (20) is best understood by considering the molecular density of states, related to the retarded propagator by

$$\rho_{\mathrm{m}}(\mathbf{k}, \omega) = -\frac{1}{\pi}\operatorname{Im}[G_{\mathrm{m}}^{(+)}(\mathbf{k}, \omega)]. \quad (23)$$

For negative detuning, it has two contributions as shown in figure 4. The first comes from the bound state, i.e. the dressed molecule, the second comes from the two-atom continuum. It is the latter part of the density of states that incorporates into our theory the rogue dissociation process put forward recently by Mackie *et al* [6]. More explicitly, the density of states is found to be equal to

$$\rho_{\mathrm{m}}(\mathbf{k}, \omega) = \frac{1}{1 + g^2 m^{3/2}/(4\pi\hbar^3\sqrt{|\epsilon_{\mathrm{m}}|})}$$

$$\times \delta(\hbar\omega - \epsilon_k/2 - \epsilon_{\mathrm{m}}) + \frac{1}{\pi}\theta(\hbar\omega - \epsilon_k/2)$$

$$\times \frac{(g^2 m^{3/2}/2\pi\hbar^3)\sqrt{\hbar\omega - \epsilon_k/2}}{[\hbar\omega - \epsilon_k/2 - \delta(B)]^2 + (g^4 m^3/4\pi^2\hbar^6)(\hbar\omega - \epsilon_k/2)},$$
$$(24)$$

and can be shown to obey the sum rule

$$\int \mathrm{d}(\hbar\omega)\,\rho_{\mathrm{m}}(\mathbf{k}, \omega) = 1. \quad (25)$$

We thus conclude that the wavefunction renormalization factor of the molecules is given by $Z = 1/[1 + g^2 m^{3/2}/(4\pi\hbar^3\sqrt{|\epsilon_{\mathrm{m}}|})]$, which close to resonance is much smaller than one. Physically, this implies that in this case the wavefunction of the molecule is strongly affected by the interaction with the continuum in the incoming channel and contains only the wavefunction $\chi_{\mathrm{m}}(\mathbf{x})$ of the bound state in the closed channel with an amplitude $\sqrt{Z}$.

The molecular density of states changes when an atomic BEC is present, due to the mean-field interactions with the condensate. In particular, in this case we expect that the two-atom continuum part of the density of states is less important because of the mean-field barrier that the two colliding condensate atoms have to overcome. Mathematically this comes about because to include the Hartree–Fock mean-field shift of the energy of the atoms we have to replace in (20) $\sqrt{\hbar\omega - \epsilon_k/2}$ by $\sqrt{\hbar\omega - 2\hbar\Sigma^{\mathrm{HF}} - \epsilon_k/2}$, where $\hbar\Sigma^{\mathrm{HF}}$ denotes the Hartree–Fock self-energy of the non-condensed atoms due to their interaction with the condensate.

The mean-field shift of the thermal atoms leads to a change of the bound-state energy as well. In equilibrium we estimate the magnitude of this shift by approximately calculating the self-energy $\hbar\Sigma^{\mathrm{HF}}$ from

$$\hbar\Sigma^{\mathrm{HF}} \simeq 2n_0\left[T_{\mathrm{bg}}^{2\mathrm{B}} + \frac{2g^2}{2\hbar\Sigma^{\mathrm{HF}} - \delta(B)}\right], \quad (26)$$

for a given condensate density n_0. In this manner we have calculated the mean-field shift of the bound-state energy as a function of the magnetic field for the Feshbach resonance at $B_0 \simeq 154.9$ G in the $|f = 2; m_f = -2\rangle$ state of ^{85}Rb. In figure 5 the results of this calculation are presented for two experimentally relevant condensate densities, namely $n_0 = 1.1 \times 10^{13}$ and 5.4×10^{13} cm^{-3} [1, 21]. As expected, the shift of the bound-state energy is largest for the highest condensate density and decreases away from the resonance. Although (26) is only a first approximation to calculate the Hartree–Fock mean-field energy, figure 5 shows that the shift
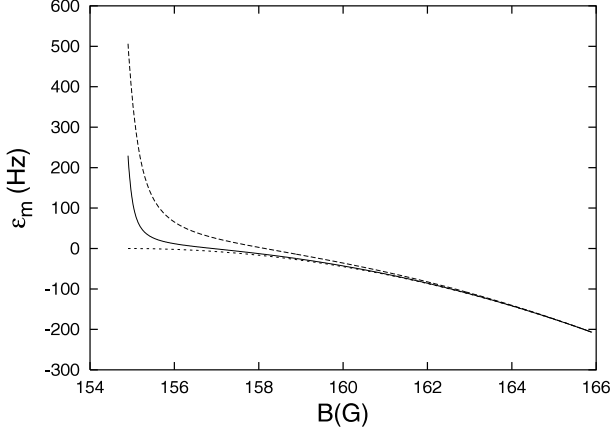
Figure 5. Mean-field shift of the bound-state energy as a function of the magnetic field. The solid curve corresponds to an atomic condensate density of $n_0 = 1.1 \times 10^{13}$ cm^{-3} and the dashed curve corresponds to $n_0 = 5.4 \times 10^{13}$ cm^{-3}. The dotted curve corresponds to the molecular binding energy in a vacuum. The calculations are performed for the resonance at $B_0 \simeq 154.9$ G in the $|f = 2; m_f = -2\rangle$ state of ^{85}Rb [1, 21].

in the bound-state energy is significant. A more thorough calculation of the mean-field effect on the bound-state energy and also on the position of the resonance is postponed to future work. With respect to this remark, it should be noted that, since the retardation time of the interaction is only of the order of $\hbar/\epsilon_m(B)$, the mean-field effects are not instantaneous. Therefore, the relevance of the mean-field shifts to non-equilibrium situations, such as in the recent experiments with time-dependent detuning [1, 21], is also subject to further research.

5. Mean-field theory

The mean-field theory for the coupled atomic and molecular condensates is found by taking the expectation value of (19). We assume for simplicity that the temperatures are so low that the thermal cloud of the Bose gas can be neglected. It is, however, straightforward to include the mean-field effects of the thermal cloud in the same manner as in the by now standard Popov theory for weakly interacting Bose gases. Furthermore, we neglect for simplicity the effect of the Hartree–Fock energy shift on the two-atom continuum and the molecular binding energy. The resulting mean-field equations are then given by

$$i\hbar \frac{\partial \psi_a(t)}{\partial t} = T_{bg}^{2B} |\psi_a(t)|^2 \psi_a(t) + 2g\psi_a^*(t)\psi_m(t),$$

$$i\hbar \frac{\partial \psi_m(t)}{\partial t} = \left[\delta(B(t)) - g^2 \frac{m^{3/2}}{2\pi\hbar^3} i\sqrt{i\hbar\frac{\partial}{\partial t}} \right] \psi_m(t) + g\psi_a^2(t). \tag{27}$$

Note that the time dependence is determined by the Hamiltonian $\hat{H}$ and not by the grand-canonical Hamiltonian $\hat{H} - \mu\hat{N}$. In equilibrium the atomic and bare molecular condensate wavefunctions are therefore not time independent but behave as as $\psi_a(t) = \psi_a e^{-i\mu t/\hbar}$ and $\psi_m(t) = \psi_m e^{-i2\mu t/\hbar}$ respectively, where ψ_a and ψ_m obey the time-independent version of (27) at chemical potential μ. In agreement with our remarks in the introduction the above equations contain no anomalous density or pairing field. One way to understand

the reason for this is that the effects of the anomalous density are already included by using the renormalized couplings and including the molecular self-energy. Including these effects again would lead to double counting problems and, therefore, to a theory that is not gapless. Another way to understand it is that equation (27) is explicitly $U(1)$ invariant and the gaplessness of the theory is thus automatically guaranteed.

A crucial ingredient in our formulation is the (non-local) term[1] proportional to $\sqrt{i\hbar\partial/\partial t}$. It is this term that incorporates the correct binding energy of the molecules for negative detuning, and their lifetime if the detuning is positive. In principle this term must be treated as follows. Using the Green function in (20) we find that the wavefunction of the molecular condensate is, for time-independent detuning, given by

$$\psi_m(t) = \frac{g}{\hbar} \int_0^t dt'\, G_m^{(+)}(t - t')\psi_a^2(t') + \psi_m(0), \tag{28}$$

where the Fourier transform of $G_m^{(+)}(\mathbf{0}, \omega)$ is given by

$$G_m^{(+)}(t - t') = -i\theta(t - t')Z/\hbar$$
$$\times \exp\left[-\frac{i}{\hbar}\epsilon_m(t - t') \right] - \frac{i\theta(t - t')g^2 m^{3/2}}{\pi\hbar^3}$$
$$\times \int_0^\infty \frac{d\omega}{2\pi} \frac{\sqrt{\hbar\omega}e^{-i\omega(t-t')}}{[\hbar\omega - \delta(B)]^2 + (g^4 m^3/4\pi^2\hbar^6)\hbar\omega}. \tag{29}$$

This result can then be substituted in the equation for the atomic condensate wavefunction, which can now be easily solved numerically, as we will show in future work.

6. Conclusions and outlook

We have derived from first principles an effective quantum field theory for Feshbach resonant interactions in atomic Bose gases. In future work we intend to apply this quantum field theory to study various equilibrium and non-equilibrium properties of ultracold atomic gases near a Feshbach resonance. This will include a further study of the mean-field shifts of the bound-state energy and the position of the resonance, as well as the study of the BEC/BCS crossover in the superfluid phase of a two-component Fermi gas [14]. Moreover, we are now in a position to also study the normal phase for both bosonic and fermionic gases. In order to apply the theory also to the recent pulse experiments with BECs of ^{85}Rb [1, 21], we need to include a detuning that varies rapidly with time. This leads to some technical complications with the proper treatment of our non-local term that remain to be resolved. With respect to the latter experiments we also want to further study the importance of the quantum evaporation process, which previous work has shown to be non-negligible [11].

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[1] Note that this term can be interpreted as a fractional derivative. See, for instance [23].

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