



THE STUDY AND EVALUATION OF THE ATOM MOLECULE MIXTURE AT THE FIXED TOTAL ATOMIC DENSITY

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Abstract

One can show that the effective field theory correctly contains the two-atom physics of a Feshbach resonance. Firstly, one shows that the correct Feshbach-resonant atomic scattering length is obtained after the elimination of the molecular field. Secondly, one calculates the bound energy and shows that it has the correct threshold behaviour near the resonance. To get more insight in the nature of the molecular state near the resonance, one also investigates the molecular density of states. To calculate the effective interatomic scattering length, one has to eliminate the molecular field from the Heisenberg equation of motion. Since the scattering length is related to the scattering amplitude at zero energy and zero momentum, one is allowed to put all the time and spatial derivatives in the equation of motion for the molecular field operator equal to zero.

Introduction

Higher order are straight forwardly included. The leading order energy dependence of the self-energy is after Wick rotation is the real energies. For the positive energy E , this result is in agreement with Wigner-threshold law. This law gives the rate for a static well a well defined positive energy to decay into three dimensional continuum. In order to study

the properties of the gas in the normal state, one considers the two-atom properties of many-body theory.

In order to evaluate the critical temperature for Bose- Einstein Condensation of the atom molecule mixture at the fixed total atomic density, one studies the effective atom-molecular theory. In this study one considers the real-time dynamics of the system by driving the Heisenberg equation of motion for the field operators that annihilate an atom and a molecule at a given space and time. To determine the Heisenberg equation of motion for these field operators, one first have to perform an analytical continuation from the Matsusara frequencies to real frequencies. For simplicity, one assumes that one is close to the resonance and one is allowed to neglect the energy dependence of the effective atomic interactions and the effective atom-molecule coupling. Moreover, one takes only the leading order energy dependence of the molecular self-energy into account. The energy of the molecular state is determined by the poles of the retarded molecular propagator. For positive detuning δ (B) there only exists a pole with a non-zero and negative imaginary part. This is in agreement with the fact that the molecule decays when its energy is above the two atom continuum threshold. The imaginary part of the energy is related to the lifetime of the molecular state. For negative detuning the molecular propagator has a real and negative pole corresponding to the bound state energy.

The molecular density of state is obtained by taking the imaginary part of the retarded molecular propagator. One can discuss only the situation when one is close to resonance and therefore approximate the retarded molecular self-energy by the square root term resulting from Wigner threshold law. For the case of negative detuning, the molecular density of states has two contributions. One arising from the pole at the bound state energy and the second from the two atom continuum. Then one defines the wave function renormalization factor $Z(B)$. This factor goes to zero as one approaches the resonance and it becomes equal to one far off resonance. Far off resonances, the bound state of the coupled channels ie. the dressed molecules is almost equal to the bound state of the closed channel potential and has zero amplitude in the open channel. This corresponds to the situation. A the resonances is approached, the dressed molecule contain only with an amplitude. The closed channel bound state i.e. bare molecule.

Accordingly, the contribution of the open channel becomes larger and gives rise to the threshold behaviour of the bound state energy. For positive detuning the molecular density of states has only a contribution for positive energy.

Theory

Density Of Atoms And Molecules

The density of the gas is most easily calculated. One reports all our results as a function of the detuning in units of the energy $g^2/m/n 2n^\circ$. The temperature is given in units of the critical temperature for Bose-Einstein condensation of an ideal gas of atoms with a total density.

The total number of atoms is, of course, also constant throughout the sweep. As one has seen, for sufficiently large absolute values of the detuning, the gas is well-described by an ideal-gas approximation. For simplicity, one will therefore treat the gas here as an ideal-gas mixture since one is mostly interested in the final density of atoms and molecules and the final temperature of the gas after the sweep, for which an ideal-gas treatment is sufficient.

Mathematical Formulae Used In The Evaluation

The equilibrium properties of the gas are determined by the equation of state, which relates the total density of the gas to the chemical potential. This equation can be calculated in two ways, either by calculating the thermodynamic potential and differentiating with respect to the chemical potential, or by directly calculating the expectation value of the operator for the total density.

The so-called ring diagrams that contribute to the thermodynamic potential in this approximation. The full molecular propagator is denoted by the thick dashed line and the non-interacting molecular propagator are indicated by the thin solid lines.

After performing the summation over the Matsubara frequencies in this expression the first term corresponds to the density of an ideal gas of bosons. The second term is more complicated and should, in principle, be dealt with numerically. For negative

detuning one can gain physical insight, however, by within the approximations, in first instance it is given by the first, one calculates the thermodynamic potential expression atomic propagator of the atoms. The full molecular propagator is given here, we recall that $G_0(\mathbf{k}, i\omega)$ is the noninteracting where AE is the molecule self energy. The so-called ring diagrams that contribute to the thermodynamic potential in this approximation are given in Fig. 4A. The full molecular propagator is denoted by the thick dashed line and the noninteracting molecular propagator are indicated by the thin solid lines. The total atomic density is calculated by using the thermodynamic identity $N = -\partial \Omega / \partial \mu$, which results in (4.3) After performing the summation over the Matsubara frequencies in this expression the first term corresponds to the density of an ideal gas of bosons. The second term in Eq. (4.3) is more complicated and should, in principle, be dealt with numerically. For negative detuning one can gain physical insight, however, by

An important difference between directly calculating the density in this manner and calculating it indirectly from the thermodynamic potential is that one should not use the noninteracting atomic propagator. Instead, one should use an approximation to the atomic propagator that contains the same self-energy diagrams. Conversely, in calculating the thermodynamic potential, one should not use the full atomic propagator. The reason for this is that if one calculates ring diagrams with this propagator one finds diagrams which are already contained in the ring diagram of the full molecular propagator.

If one uses for the atomic propagator the approximation given diagrammatically. The ring diagram that contributes to the thermodynamic potential. On the other hand, if one uses for the molecular propagator the approximation given in Fig. 4B(c) the resulting ring diagram. Clearly to avoid double counting problems in the calculation of the thermodynamic potential, one should take only one of these diagrams into account. However, if one calculates the density directly from the atomic and molecular propagator one should use both the diagrams. One now argues that the direct calculation of the density, again for negative detuning, one indeed recovers the result. One first calculates the contribution arising from the molecular propagator. It is found to be equal to Adv XP Taking into account only the pole in the density of states leads to the result. At first sight this result seems a factor $Z(B)$ too small to agree with the result. However, one has, in fact,

that the contribution from the atoms to the density results in a term proportional. Taking this into account, the result from the direct calculation agrees with the result obtained previously. A different way for obtaining the factor $(2 - 2z(B))$ in the atomic density is to include the self-energy diagram. The corresponding mathematical expression in first instance is given by the physics of this expression, one notes $(k+4, i.)G$, that if one neglects the energy and momentum dependence or the molecular propagator one has that $G(k, i_0) = A/5(B)$. With this approximation the self-energy is given by $8 n n, ares(B)A^2/m$, which corresponds precisely to the Feshbach-resonant part of the self-consistent Hartree-Fock self-energy of the atoms, as expected from the diagram. The full calculation of the expression for the self-energy is complicated due to the fact that one has to use the full atomic and molecular propagators, which makes the calculation self-consistent. To illustrate in perturbation theory that one is able to reproduce the result let us simply take the noninteracting atomic and molecular propagators. The self-energy is then given by To compare with the two-atom calculation for negative detuning performed, one must take only one other atom present A_k , and no molecules. The self-energy is then with momentum.

Discussion of Results

We have given the result of evaluation of fraction of atoms as a function of the detuning for an adiabatic sweep through the resonance. The total density is again kept equal to $(n-10^{13} \text{cm}^{-3})$. The calculations have been performed for two initial temperatures $T = 2 T_0$ and $4 T_0$. In table 4T4, we have presented the result of evaluation of twice the fraction of molecules as a function of the detuning for an adiabatic sweep through the resonance. The other parameters are the same as shown in table 4T3. There are some recent calculations [5-20] which also reveal the same behavior.

For positive detuning and far from the resonance, one is essentially dealing with an atomic gas. Hence one has in this regime $T_{BEC} = T_0$. For sufficiently negative detuning, one is dealing with a gas of molecules with twice the atomic traps and one has $T_{BEC} = (2/ST_0)$. The feature in the critical temperature at zero detuning turns out to be a signature of a true thermodynamic phase transition between a phase with a single Bose-Einstein Condensate of molecules and a phase containing two Bose-Einstein Condensates,

one of atoms and one of molecules. This was first pointed out by Sachdev. This should be contrasted with the situation of atomic Fermi gas near a Feshbach resonance, where only a BCS-BEC cross-over exists.

we have evaluated the critical temperature for Bose-Einstein Condensation (BEC) for the atom-molecule mixture at the fixed total atomic density. In table 4T1, we have shown the temperature of the gas as a function of the detuning for a sweep through the resonance from positive to negative detuning for two initial temperature $T-2 T_0$ and $4 T_0$. The total density is equal to $n = 10^{13} \text{ cm}^{-3}$, The gas is heated as the detuning is changed from positive to negative. This is easily understood, since molecules form as the detuning is changed from positive to negative values, and their binding energy is released as kinetic energy into the gas. In table 4Ta, we have given the evaluated result of critical temperature for Bose-Einstein Condensation of the atom-molecule mixture at a fixed total atomic density $n = 10^{13} \text{ cm}^{-3}$, Two results are given one for the exact calculation and other of treating the gas as an ideal gas mixture.

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