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Theory for p -Wave Feshbach Molecules

K. B. Gubbels* and H. T. C. Stoof

*Institute for Theoretical Physics, Utrecht University,
Leuvenlaan 4, 3584 CE Utrecht, The Netherlands*

We determine the physical properties of p -wave Feshbach molecules in doubly spin-polarized ^{40}K and find excellent agreement with recent experiments. We show that these molecules have a large probability Z to be in the closed channel or bare molecular state responsible for the Feshbach resonance. In the superfluid state this allows for observation of Rabi oscillations between the molecular and atomic components of the Bose-Einstein condensed pairs, which contains a characteristic signature of the quantum phase transition that occurs as a function of applied magnetic field.

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Introduction. — The continuous excitement in the field of ultracold atoms is to a large extent caused by the ever increasing experimental control over the creation and manipulation of degenerate quantum gases. Arguably the most important example of such control is the use of Feshbach resonances with which the interaction between the atoms can be manipulated by simply varying the magnetic field. The so-called s -wave Feshbach resonance occurs when atoms collide with zero orbital angular momentum ($\ell = 0$) and is experimentally most easily accessible. It has been widely used in the study of degenerate Fermi gases, especially for the crossover between a Bardeen-Cooper-Schrieffer (BCS) superfluid and a Bose-Einstein condensate (BEC) of diatomic molecules [1, 2, 3, 4, 5, 6].

A novel challenge is to obtain superfluidity also with pairs in nonzero orbital angular momentum states by using p -wave ($\ell = 1$), or maybe even d -wave ($\ell = 2$) Feshbach resonances. Up to now, p -wave resonances have been seen in Fermi gases of ^{40}K [7] and ^6Li atoms [8]. Most recently, Gaebler *et al.* have been able to create and detect p -wave Feshbach molecules in a gas of ^{40}K with lifetimes on the order of milliseconds on both the BEC and the BCS side of the resonance [9]. The lifetime on the BEC side, where the energy of the Feshbach molecule lies below the open-channel continuum, is presumably limited by collisional losses, whereas the lifetime on the BCS side is determined by the decay of the molecular state into the open-channel continuum. However, upon entering the superfluid regime on the BCS side, the Bose-Einstein condensed pairs are stabilized by the presence of a Fermi sea [10]. Now that their dominant decay mechanism is absent, the lifetime of the pairs on the BCS side is expected to become significantly enhanced, giving hope that p -wave superfluidity is indeed within reach.

There are many exciting aspects about p -wave superfluidity. First of all, a p -wave superfluid has a more complex order parameter than a s -wave superfluid, due to the various possible projections of its angular momentum ($m=0,\pm 1$), which can give rise to anisotropic superfluids. Second, a p -wave superfluid undergoes various classical and quantum phase transitions as a function of temper-

ature and magnetic field [11, 12, 13, 14, 15, 16]. As an example, the evolution from the BEC to the BCS side of the Feshbach resonance at zero temperature contains a topological quantum phase transition [17], rather than the crossover known from the s -wave case. Third, the p -wave resonances are intrinsically narrow. As a result, the two-channel nature of the Feshbach resonance becomes very prominent. This can be quantified as follows.

The superfluid phase near a Feshbach resonance arises from the Bose-Einstein condensation of pairs or so-called dressed molecules [18], which are characterized by the linear superposition $|\psi_{\text{dressed}}\rangle = \sqrt{Z}|\psi_{\text{m}}\rangle + \sqrt{1-Z}|\psi_{\text{aa}}\rangle$, where $|\psi_{\text{m}}\rangle$ is the wave function of the bare molecular state in the closed channel, and $|\psi_{\text{aa}}\rangle$ describes the atom pairs in the open channel. In the case of an s -wave resonance, the magnitude of the probability Z can be estimated at resonance (unitarity) by $Z \simeq 2\sqrt{2\Delta}/\pi\eta$ [10], where Δ is the universal BCS gap parameter at unitarity and η^2 is a measure for the energy width of the resonance. For the extremely broad s -wave resonance of ^6Li at 834 G, this leads at a Fermi energy of $\varepsilon_{\text{F}} = 380$ nK to $Z \simeq 4 \cdot 10^{-5}$. For the s -wave resonance of ^{40}K at 202 G, we obtain at the same Fermi energy $Z \simeq 5 \cdot 10^{-3}$, which is much larger but still a rather small number. However, we will show below that for a p -wave resonance the value of Z at unitarity can become as large as 0.7.

This shows that for typical p -wave Feshbach resonances the two-channel nature of the dressed molecules is very important. Whereas p -wave Feshbach molecules have recently been carefully studied experimentally, theoretically the physical properties of these molecules have not received much attention, even though they are very interesting in their own right. In particular, important quantities such as the probability Z , the binding energy and the lifetime have not been determined yet in terms of the experimentally known Feshbach parameters, i.e., the background p -wave scattering length a_{bg} , the width of the resonance ΔB , and the magnetic moment difference between the closed and the open channel $\Delta\mu$. In this Letter, we show that given these parameters, all two-body properties can be computed exactly and in excellent agreement with experiment. Moreover, we per-

form a two-channel many-body calculation to compute the frequency of coherent Rabi or Josephson oscillations between the closed and open channel components of the Bose-Einstein condensed pairs.

Two-body physics. — The two-body problem near a p -wave Feshbach resonance can be treated along the same lines as the corresponding problem for the s -wave resonance [18]. We consider two fermionic particles that are in the same hyperfine spin state and that interact with each other through a coupling with a closed molecular channel and through a p -wave background interaction in the open channel, both with angular momentum projection m . The scattering due to the background interaction generates a ladder sum, which can be conveniently incorporated into the atom-molecule coupling [18], and gives rise to a dressed coupling $g_m(\mathbf{k}) = \langle \psi_m | V_{\text{ma}} | \psi_{\mathbf{k}}^{(+)} \rangle / \sqrt{2} = g_m k_m / [1 + i(k a_{\text{bg}})^3]$, where $|\psi_{\mathbf{k}}^{(+)}\rangle$ is the scattering state with momentum \mathbf{k} in the open channel, V_{ma} the coupling potential between open and closed channels, and a_{bg} is directly related to the effective hard-core radius a_{hc} of the background potential by $a_{\text{bg}} = a_{\text{hc}}/3^{1/3}$. The subscript m refers to the projection of the angular momentum $m = 0, \pm 1$, such that $k_0 = k_z$ and $k_{\pm 1} = \mp(k_x \pm ik_y)/\sqrt{2}$, while the coupling constant g_m characterizes the strength of atom-molecule interactions. Note that the dressed or renormalized coupling $g_m(\mathbf{k})$ is exact at low energies.

With this dressed atom-molecule coupling we can calculate the two-body molecular self-energy analytically,

$$\begin{aligned} \hbar\Sigma_m(z) &= \frac{2}{V} \sum_{\mathbf{k}} |g_m(\mathbf{k})|^2 \left(\frac{1}{z - 2\varepsilon_{\mathbf{k}}} + \frac{1}{2\varepsilon_{\mathbf{k}}} \right) \\ &= \frac{m_a g_m^2}{18\pi\hbar^2 |a_{\text{bg}}|^3} \frac{-\zeta(2 + \sqrt{-\zeta})}{1 + 2\sqrt{-\zeta} - \zeta(2 + \sqrt{-\zeta})}, \end{aligned} \quad (1)$$

where $\varepsilon_{\mathbf{k}} = \hbar^2 k^2 / 2m_a$ is the kinetic energy with m_a the mass of a single atom. The dimensionless energy ζ is given by $\zeta = m_a a_{\text{bg}}^2 z / \hbar^2$. To obtain this result we have renormalized the bare self-energy $\hbar\Sigma_m^{\text{B}}(z)$ by subtracting $\hbar\Sigma_m^{\text{B}}(0)$. This is convenient because in the equation for the bound state energy of the dressed molecule [18], namely $E - \delta_m^{\text{B}} = \hbar\Sigma_m^{\text{B}}(E)$, we can subtract $\hbar\Sigma_m^{\text{B}}(0)$ on both sides, which also renormalizes the bare detuning δ_m^{B} to the renormalized detuning δ_m and leads to $E - \delta_m = \hbar\Sigma_m(E)$. The two-body resonance now indeed occurs when the bound-state energy reaches the atomic continuum, i.e., at $E = 0$ and $\delta_m = 0$. Therefore, the renormalized detuning is the experimentally relevant quantity and given by $\delta_m = \Delta\mu(B - B_m)$, with B the applied magnetic field and B_m the location of the Feshbach resonance. Note that in general the Feshbach resonances with different values of m need not be located at the same magnetic field [19]. This is because only the projection of the total angular momentum is conserved in the collision of two alkali atoms. Also note that by using the dressed atom-molecule coupling, the right-hand side of Eq. (1) is

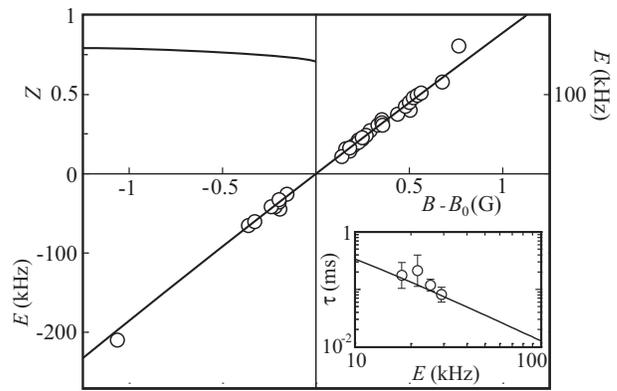


FIG. 1: Two-body physics near the $m = 0$ p -wave resonance of ^{40}K located at $B_0 = 198$ G. The upper left panel shows the probability Z to be in the closed Feshbach channel as a function of the magnetic field B . In the lower left and the upper right panel the black line shows the binding energy E as a function of magnetic field. For positive detuning the molecules are not stable, resulting in a finite lifetime τ , shown in the lower right panel. The open circles are data from the experiments of Gaebler *et al.*

finite, so no arbitrary, undetermined cutoff needs to be introduced. For small energy we obtain that $\hbar\Sigma_m(z) \simeq (g_m^2 m_a / \hbar^2) [-m_a z / 9\pi\hbar^2 |a_{\text{bg}}| - (-m_a z / \hbar^2)^{3/2} / 6\pi]$. The ‘universal’ coefficient of $(-m_a z / \hbar^2)^{3/2}$ is in agreement with Refs. [16, 20].

The binding energy of p -wave Feshbach molecules in a gas of spin-polarized ^{40}K atoms near the $m = 0$ Feshbach resonance at 198 G has been accurately measured as a function of magnetic field by Gaebler *et al.* [9], where they find an almost perfectly linear behavior. From the slope, which is given by $Z\Delta\mu$, we obtain $\Delta\mu = 0.175\mu_B$ with μ_B the Bohr magneton. However, for small detuning they report tiny deviations in this linear behavior. In Fig. 1 we have calculated the binding energy with the use of Eq. (1), where we extract the relevant Feshbach parameters a_{bg} and g_0 from the collisional phase shift of the considered p -wave resonance obtained in Ref. [19]. This results in $a_{\text{bg}} = 98a_0$ and $g_0 = 33a_0^{1/2}\hbar^2/m_a$, with a_0 the Bohr radius. We see that the agreement with our two-body calculation is excellent. The nonlinearities arise from the slight variation of Z with magnetic field.

Having obtained the self-energy and the equation for the binding energy of the molecules, we can also determine the two-body wave function renormalization factor Z , given by $Z = [1 - \partial\hbar\Sigma_m(E)/\partial E]^{-1}$ with E the solution of the equation for the binding energy. The behavior of Z as a function of magnetic field is shown in Fig. 1. We indeed observe that for the considered p -wave resonance Z is very large at unitarity, namely $Z \simeq 0.7$, which proves the two-channel nature of the p -wave molecules near this resonance. Since the difference in magnetic moment between a dressed molecule and two atoms is $Z\Delta\mu$, we see that this difference does not go to zero at a p -wave res-

onance. As a result, the binding energy of the dressed molecule vanishes only as $(B - B_m)$ and not as $(B - B_m)^2$, which is the well-known behavior from the s -wave case [14, 20].

In the two-body case, there are only stable molecules for negative detuning and strictly speaking Z ceases to have meaning for positive detuning. In the many-body case the Feshbach molecules are also stable at the BCS side, due to the presence of a Fermi sea, preventing decay into the atomic continuum [10]. It is then possible to determine Z at the BCS side using many-body techniques, which has been done for the s -wave case both theoretically [10] and experimentally [6]. In the two-body case the p -wave molecules are not stabilized by a Fermi sea and the decay rate Γ_m is readily calculated from the self-energy by $\Gamma_m = -2\text{Im}[\Sigma_m(E + i0)]$. The lifetime is thus $\tau_m = 1/\Gamma_m$. The calculated lifetimes are shown in Fig. 1, leading to very good agreement with the experimentally observed lifetimes without any adjustable parameters.

Internal Josephson oscillations.— Having obtained the analytic solution to the two-body p -wave Feshbach problem, the next step is to incorporate this two-body physics into the many-body physics. To this end we use the following effective grand-canonical Hamiltonian with chemical potential μ_a for the atoms and μ_m for the molecules,

$$H = \sum_{\mathbf{k}} (\varepsilon_{\mathbf{k}} - \mu_a) a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + \sum_{\mathbf{k}} \left(\frac{\varepsilon_{\mathbf{k}}}{2} + \delta_m - \mu_m \right) b_{m,\mathbf{k}}^\dagger b_{m,\mathbf{k}} + \frac{1}{\sqrt{V}} \sum_{\mathbf{p},\mathbf{k}} \left(g_m(\mathbf{k}) b_{m,\mathbf{p}}^\dagger a_{\mathbf{p}/2+\mathbf{k}} a_{\mathbf{p}/2-\mathbf{k}} + \text{h.c.} \right), \quad (2)$$

where $a_{\mathbf{k}}^\dagger$ creates an atom with momentum \mathbf{k} , $b_{m,\mathbf{k}}^\dagger$ creates a bare p -wave molecule with angular momentum projection m and momentum \mathbf{k} , and V is the volume of the gas. This Hamiltonian is valid when different values of m lead to resonances at well-separated magnetic fields B_m , as is experimentally the case for the $m = 0$ resonance of ^{40}K . If this is not true, then on the right-hand side of Eq. (2) we also have to perform a sum over m . Furthermore, in equilibrium we have that $\mu_m = 2\mu_a$, but for reasons that become clear shortly, we enforce this relation only at the end of the calculations. For p -wave resonances the total scattering length satisfies $a^3 = a_{\text{bg}}^3 - m_a g_m^2 / 6\pi \hbar^2 \delta_m$. If we parametrize this in analogy with the s -wave case as $a^3 = a_{\text{bg}}^3 [1 - \Delta B_m / (B - B_m)]$, we see that the atom-molecule coupling obeys $g_m = \hbar (6\pi \Delta \mu \Delta B_m a_{\text{bg}}^3 / m_a)^{1/2}$, with ΔB_m the magnetic field width of the Feshbach resonance. Near resonance the background interaction may be safely neglected in the Hamiltonian, except for its effect on the atom-molecule coupling $g_m(\mathbf{k})$. The reason for the latter is that, although the effective Hamiltonian above is designed to be accurate for low energies, we still need high-energy states to properly describe the two-body physics near a Feshbach resonance. As we have seen, the effect of these states is to renormalize the atom-molecule coupling and therefore it is essential to use the

dressed coupling $g_m(\mathbf{k})$ in the effective Hamiltonian [10].

In order to discuss internal Josephson oscillations [21, 22], we turn to the functional-integral formalism [18] in which the creation and annihilation operators become complex fields that not only depend on momentum, but also on time t . A sketch of the derivation goes as follows. First, we rewrite the atomic and molecular fields as $a_{\mathbf{k}}(t) \rightarrow a_{\mathbf{k}}(t) e^{i\theta_a(t)}$, $b_{m,\mathbf{k}}(t) \rightarrow b_{m,\mathbf{k}}(t) e^{i\theta_m(t)}$ to explicitly consider the atomic and molecular phase fluctuations $\theta_a(t)$ and $\theta_m(t)$, respectively. Substituting these expressions in the action, it changes in the following way: $g_m(\mathbf{k}) \rightarrow g_m(\mathbf{k}) e^{i[2\theta_a(t) - \theta_m(t)]}$ and $\mu_j \rightarrow \mu_j - \hbar \dot{\theta}_j(t)$, where the last substitution is due to the time-derivatives in the action and the index j runs over two possible subscripts, namely atomic and molecular. Next, we separate the action into the part S_{ph} containing the phase fluctuations, and the part S that doesn't contain these fluctuations. This allows us to do perturbation theory in the phase fluctuations by expanding the exponential containing S_{ph} . Expanding in the fluctuations up to second order, we see that the coefficients in front of the phase fluctuations get averaged over the original action S . For example, the term linear in $\dot{\theta}_m(t)$ becomes $\int dt \dot{\theta}_m(t) \sum_{\mathbf{k}} \langle b_{m,\mathbf{k}}^*(t) b_{m,\mathbf{k}}(t) \rangle$, where the average $\sum_{\mathbf{k}} \langle b_{m,\mathbf{k}}^*(t) b_{m,\mathbf{k}}(t) \rangle$ equals the total number of bare molecules and is conveniently expressed as $-\partial\Omega(\mu_a, \mu_m)/\partial\mu_m$ with $\Omega(\mu_a, \mu_m)$ the thermodynamic potential of the gas. By re-exponentiating all terms up to quadratic order, we obtain the effective action for the phase fluctuations,

$$S^{\text{eff}}[\theta_j] = \int dt \left\{ \sum_j \hbar \dot{\theta}_j \frac{\partial\Omega}{\partial\mu_j} - \sum_{j,j'} \frac{\hbar^2}{2} \dot{\theta}_j \dot{\theta}_{j'} \frac{\partial^2\Omega}{\partial\mu_j \partial\mu_{j'}} + J \cos(2\theta_a - \theta_m) \right\}, \quad (3)$$

where the Josephson coupling is given by the expression $J = 2 \sum_{\mathbf{k}} g_m(\mathbf{k}) \langle b_{\mathbf{0}}^*(t) a_{\mathbf{k}}(t) a_{-\mathbf{k}}(t) \rangle / \sqrt{V}$.

In deriving the quadratic action for the phase fluctuations we made one approximation, namely a gradient expansion of the fluctuations that takes into account static number correlations. To calculate the coefficients in Eq. (3) we make another approximation, namely mean-field theory. The mean-field thermodynamic potential for a Fermi gas near a p -wave resonance at zero temperature is the direct generalization of the s -wave case, giving

$$\Omega = \frac{1}{2} \sum_{\mathbf{k}} \left\{ \varepsilon_{\mathbf{k}} - \mu_a - \hbar\omega_{\mathbf{k}} + \frac{2|g_m(\mathbf{k})|^2 n_{\text{mc}}}{\varepsilon_{\mathbf{k}}} \right\} + (\delta_m - \mu_m) n_{\text{mc}} V, \quad (4)$$

with $\hbar\omega_{\mathbf{k}} = \sqrt{(\varepsilon_{\mathbf{k}} - \mu_a)^2 + 4|g_m(\mathbf{k})|^2 n_{\text{mc}}}$ and n_{mc} the bare molecular condensate density. The gap equation

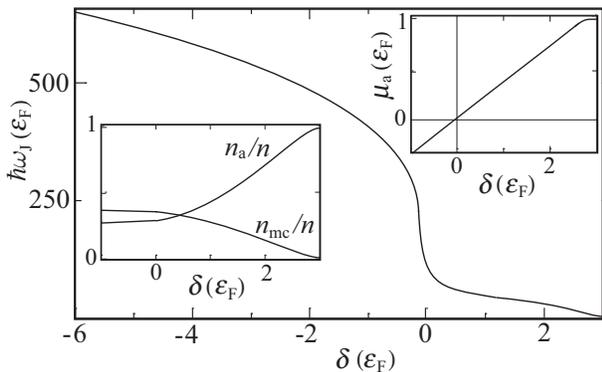


FIG. 2: Josephson frequency ω_J as a function of the detuning δ . Energies are expressed in terms of the Fermi energy $\epsilon_F = \hbar^2(6\pi^2n)^{2/3}/2m_a$, with $n = 2n_{mc} + n_a$ the total density of atoms, which is kept fixed during the calculation at $n = 3 \times 10^{18} \text{ m}^{-3}$, so that $\epsilon_F/\hbar \simeq 2\pi \times 4 \text{ kHz}$. In the left inset, the number of bare molecules n_{mc} and open-channel atoms n_a are given as a function of the detuning. In the right inset we have the atomic chemical potential vs. detuning.

follows from differentiation with respect to n_{mc} , yielding

$$\delta_m - \mu_m = \frac{1}{V} \sum_{\mathbf{k}} |g_m(\mathbf{k})|^2 \left(\frac{1}{\hbar\omega_{\mathbf{k}}} - \frac{1}{\epsilon_{\mathbf{k}}} \right), \quad (5)$$

which can be seen as the many-body generalization of the two-body bound state equation $E - \delta_m = \hbar\Sigma_m(E)$, with $E = \mu_m$. Within mean-field theory, the coefficients in Eq. (3) are readily determined. For example, $-\partial\Omega/\partial\mu_m = n_{mc}V$, where n_{mc} is obtained from the gap equation. Also, we have that $-\partial\Omega/\partial\mu_a = n_aV = \sum_{\mathbf{k}} [1 - (\epsilon_{\mathbf{k}} - \mu_a)/\hbar\omega_{\mathbf{k}}]/2$, with n_a the atomic density. Even the second derivatives are given by simple analytic expressions in terms of momentum integrals. Finally, the Josephson coupling is given by $J = 2n_{mc} \sum_{\mathbf{k}} |g_m(\mathbf{k})|^2/\hbar\omega_{\mathbf{k}}$. These expressions all depend quantitatively on a_{bg} , showing that the background interaction is important.

From the effective action we can then derive the equations of motion by writing down the Euler-Lagrange equations. The remaining second-order differential equations can be solved analytically, and gives rise to two types of modes. One has frequency zero and is recognized as the Goldstone mode due to the spontaneous broken $U(1)$ symmetry associated with the conservation of the total number of atoms in the gas. The other mode has a nonzero frequency ω_J and is recognized as the collective mode corresponding to internal Josephson or Rabi oscillations between the molecular and the atomic components of the Bose-Einstein condensed pairs. In Fig. 2, we show the Josephson oscillation frequency, the atomic chemical potential, the atomic density and the bare molecular density as a function of the detuning with the parameters for the $m = 0$ Feshbach resonance of ^{40}K . Far below resonance, not visible on the scale of the figure, we find that $\omega_J \simeq \delta$. However, near resonance, where

the detuning is no longer the dominant energy scale, we observe completely different behavior. In particular, on approach of the quantum critical point at $\mu_a = 0$ [17], we find that the slope of the Josephson frequency develops a logarithmic divergence. Since internal Josephson oscillations can be accessed experimentally by performing a Ramsey-type experiment [23], this characteristic feature in the Josephson frequency is an observable signature for the occurrence of the quantum phase transition. Although the Josephson oscillations are damped by pair breaking, we expect this effect to be suppressed since the single-atom continuum is Pauli-blocked by the Fermi sea and the Bose-Einstein condensed pairs are protected by the (mostly) gapped atomic spectrum. Also note that the collective mode of Josephson oscillations is intrinsically connected to the two-channel nature of p -wave resonances and is absent in a single-channel treatment of the interactions. Finally, we hope that our calculation will inspire further research towards p -wave superfluidity.

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* Electronic address: K.Gubbels@phys.uu.nl

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