A simple model of Feshbach molecules

Cheng Chin

James Franck Institute and Department of Physics, University of Chicago, Chicago, IL 60637
Institut für Experimentalphysik, Universität Innsbruck, Technikerstr. 25, 6020 Innsbruck, Austria

(Dated: March 23, 2022)

We present a two-channel model to describe the quantum state of two atoms with finite-range interaction near a Feshbach resonance. This model provides a simple picture to analytically derive the wave function and the binding energy of the molecular bound state. The results agree excellently with the measurements and multichannel calculations. For small binding energies, the system enters a threshold regime in which the Feshbach molecules are identical to long range atom pairs in single channel. According to their threshold behavior, we find Feshbach resonances can be classified into two types.

PACS numbers: 03.75.Hh, 05.30.Fk, 34.50.-s, 39.25.+k

I. INTRODUCTION

Formation and Bose-Einstein condensation (BEC) of molecules have recently been achieved based on ultracold atoms with magnetically-tuned Feshbach resonances. In these experiments, Feshbach coupling is induced by tuning a foreign molecular state near the scattering continuum, which allows for an efficient transfer of colliding atoms into molecules. This method works for virtually all alkali atoms, and can create ultracold molecules from various sources including Bose condensates, degenerate Fermi gases, or normal thermal gases.

Feshbach molecules have special and unique properties. They typically populate only one weakly-bound quantum state, and the bound state can strongly couple to the scattering continuum via Feshbach resonance. We may ask the following question: should Feshbach molecules rather be considered as molecules in a specific rovibrational state or as pairs of scattering atoms near the continuum? This distinction is particularly crucial in the studies of the BEC to BCS (Bardeen-Cooper-Schrieffer state) crossover in degenerate Fermi gases, which call for a clarification of the quantum nature of the Feshbach molecules.

Molecular states near Feshbach resonances have been recently investigated based on sophisticated and complete two-body or many-body theory and multichannel scattering calculations. All works suggest that the Feshbach molecule is generally a coherent mixture of the foreign molecule in the closed channel and long-range atom pair in the open scattering channel. Near resonances with large resonance widths, the molecules can be well approximated as pairs in the open channel. For narrow resonances, as suggested by numerical calculation, the closed channel dominates and a short-range molecule picture is appropriate.

In this paper, we use a simple two-channel model to describe two interacting atoms near a Feshbach resonance (Sec. II). To account for the finite interaction range of real atoms, we introduce a spherical box potential, which allows us to analytically calculate the molecular bound state in different regimes and their threshold behavior (Sec. III and Sec. IV). Finally, we apply our model to Feshbach molecules in recent Fermi gas experiments and to characterize the associated Feshbach resonances (Sec. V).

II. MODEL

We model the interaction of two identical, ultracold atoms with mass $m$ based on an open channel $|o\rangle$ that supports the scattering continuum and a closed channel $|c\rangle$ that supports the foreign bound state. The wave function of the atoms is generally expressed as $|\psi\rangle = \psi_o(r)|o\rangle + \psi_c(r)|c\rangle$, where $\psi_o(r)$ and $\psi_c(r)$ are the amplitudes in the open and closed channels, respectively, and $r$ is the inter-atomic separation. We assume the interaction $(\hbar^2/m)\hat{\sigma}$ is described by a spherical box potential with an interaction range of $r_0$, see Fig. (1). For $r > r_0$, the potential energy of the open channel is 0 and the closed channel $\propto \frac{1}{r}$. For $r < r_0$, the open (closed) channel has an attractive potential of $-\hbar^2 q^2_o/m$ ($-\hbar^2 q^2_c/m$), and a coupling term $\Omega = |\Omega|$ between the channels. The wave function satisfies the Schrödinger equation:

\[ E|\psi\rangle = \frac{\hbar^2}{m}(-\nabla^2 + \hat{\sigma})|\psi\rangle \]

\[ \hat{\sigma} = \begin{cases} -\left( \frac{q^2_o}{\Omega} \Omega \right) & \text{for } r < r_0 \\ \left( 0 \ 0 \ \infty \right) & \text{for } r > r_0. \end{cases} \]

The solution of the above equation for zero scattering energy $E = 0$ can be expressed as:

\[ \text{for } r > r_0 : |\psi\rangle \propto \frac{r-a}{r}|o\rangle, \]

\[ \text{for } r < r_0 : |\psi\rangle \propto \frac{\sin q_+r}{r}|+\rangle + \frac{A\sin q_-r}{r}|\rangle, \]

where the scattering length $a$ and $A$ are constants, $q_\pm$ are the “eigen wave numbers” for $r < r_0$ associated with the eigen states.
FIG. 1: A two-channel model for Feshbach resonances. We assume a spherical box potential between two atoms with an interaction range of $r_0$. A bound state with energy $E_c$ relative to the scattering continuum is supported by the closed channel.

\[ |+\rangle = \cos \theta |\alpha\rangle + \sin \theta |\beta\rangle \]
\[ |-\rangle = -\sin \theta |\alpha\rangle + \cos \theta |\beta\rangle, \]

and $\tan 2\theta = 2\Omega/(q_0^2 - q_0^2)$.

Based on the boundary conditions $\psi_c(r_0) = 0$ and $\psi_o(r_0)/\psi_o'(r_0) = r_0(r_0/a - 1)$, we get

\[ A = -\tan \theta \frac{\sin(q_+ r_0)}{\sin(q_- r_0)} \]
\[ \frac{1}{r_0 - a} = q_+ \cos^2 \theta \tan q_+ r_0 + q_- \sin^2 \theta \tan q_- r_0. \]

The latter equation shows how in general, each channel contributes to the scattering length.

In cold atom systems, Feshbach resonances are, in most cases, induced by hyperfine interactions or spin-spin interactions. Both interactions are many orders of magnitude weaker than the relevant short range exchange potential. It is an excellent approximation to assume $\Omega \ll q_0^2 - q_0^2$ and $|q_0^2 - q_0^2|$. Hence, we have $\theta \ll 1$, $q_+ \approx q_0$ and $q_- \approx q_c$.

In this limit, the closed channel contribution is significant only when the foreign state is close to the continuum, in which case the last term in Eq. (7) diverges. Given the energy of the closed channel state as $E_c = (\hbar^2/m)\epsilon_c$ and $\epsilon_c \ll q_0/r_0$, the boundary condition $\psi_o(r_0) = \sin \sqrt{q_0^2 + \epsilon_c} r_0 = 0$ allows us to expand the last term in Eq. (7) as $-\gamma/\epsilon_c$. Here $\gamma = 2q_0^2/\epsilon_c r_0$ characterizes the Feshbach coupling strength. To the same order of expansion, the middle term in Eq. (7) is a constant across the resonance and can be identified as $(r_0 - a_{bg})^{-1}$, where $a_{bg}$ is the background scattering length. Equation (7) reduces to

\[ \frac{1}{r_0 - a} = \frac{1}{r_0 - a_{bg}} - \frac{\gamma}{\epsilon_c}. \]

III. SCATTERING LENGTH AND THE MOLECULAR EIGEN STATE

Experimentally, the relative energy between the continuum and the bare state can be adjusted linearly by a magnetic field $B$-induced Zeeman shift $-\mu B$, where $\mu = \mu_o - \mu_c$ and $\mu_o(\mu_c)$ is the magnetic moment of the open(closed) channel. Replacing $E_c$ by $E_c + \mu B$, we can rewrite Eq. (8) in terms of the magnetic field as

\[ \frac{a - r_0}{a_{bg} - r_0} = 1 + \frac{\Delta B}{B - B_{res}}, \]

where the resonance width $\Delta B$ and the resonance position $B_{res}$ are given by

\[ \Delta B = -\mu^{-1}(\hbar^2/m)\gamma(a_{bg} - r_0) \]
\[ B_{res} = -\mu^{-1}E_c + \Delta B. \]

Several interesting features are shown here. First of all, we find the resonance position is offset by exactly $\Delta B$ relative to the crossing of the bare state and the continuum, $B = -\mu^{-1}E_c$, see Eq. (11). For a positive scattering length $a_{bg} > r_0$, this shift is negative $\Delta B < 0$. This feature leads to the “renormalization” of the Feshbach resonance location discussed in Ref. [4].

To understand the origin of the resonance shift, we should return to Eq. (8). The divergence of the scattering length occurs when the open channel contribution (middle term) is exactly canceled by the closed channel one (last term). For systems with large background scattering lengths $a_{bg} \gg r_0$ and strong Feshbach couplings $\gamma$, this cancellation can occur even when the bare state is far away from the continuum. A large resonance shift then results.

Now we turn to the binding energy of the molecules. Assuming a bound eigen state $|\psi_m\rangle$ exists near the continuum at $E = -E_m = -(\hbar^2/m)\epsilon_m$, where $E_m > 0$ is the binding energy, we can determine $E_m$ by following essentially the same calculation as Eq. (1)-(7). The equivalence of Eq. (7) gives

\[ -\sqrt{\epsilon_m} = \frac{\tilde{q}_+ \cos \theta^2}{\tan \tilde{q}_+ r_0} + \frac{\tilde{q}_- \sin \theta^2}{\tan \tilde{q}_- r_0}, \]

where $\tilde{q}_\pm = (q_0^2 - \epsilon_m)^{1/2}$.

Assuming $\theta \ll 1$ and the bound states in both channels are close to the continuum, namely, $|a_{bg}| \gg r_0$ and $|\epsilon_c| \ll\]
states in the closed channel and the open channel (for of Eq. (13) are 

$$\epsilon$$

the absence of the Feshbach coupling on a contact potential. We can immediately see that in 

$$\text{continuum (dotted lines), bare molecular states (dashed lines), and the dressed molecular state (c., solid lines). We assume (a) } a_{bg} - r_0 = l \text{ and } \gamma = l^{-3} \text{ and (b) } a_{bg} - r_0 = -3l \text{ and } \gamma = l^{-3}; \text{ where } l \gg r_0 \text{ can be any relevant length scale. Arrows mark the offset resonance positions. Insets show the threshold behavior of the bound state.}

$$q_0/r_0$$, we can expand the two terms on the right side of Eq. (12) to leading order as \((r_0 - a_{bg})^{-1}\) and \(-\gamma (\epsilon_c + \epsilon_m)^{-1}\), respectively. Equation (12) then reduces to

$$(\epsilon_m + \epsilon_c)(\sqrt{\epsilon_m - \frac{1}{a_{bg} - r_0}}) = \gamma.$$  \(13\)

This result shows the evolution of the eigen state near the resonance. Similar result is obtained in Ref. [2] based on a contact potential. We can immediately see that in the absence of the Feshbach coupling \(\gamma = 0\), the solutions of Eq. (13) are \(\epsilon_m = -\epsilon_c\) and \(\epsilon_m = (a_{bg} - r_0)^{-2}\) (for \(a_{bg} > r_0\)), which exactly correspond to the bare bound states in the closed channel and the open channel (for \(a_{bg} > r_0\), respectively.

In the presence of the Feshbach coupling \(\gamma > 0\), Eq. (13) suggests an “avoided level crossing”-like energy structure, see Fig. (2), which also illustrates the resonance position shifts. The level crossing, however, is not hyperbolic as it is in a two-level system. In particular, at small binding energies, the bound state energy approaches the continuum quadratically, see Fig. (2) inset. Far below the continuum, the bound state approaches the bare state in the closed channel.

To better quantify the role of the open and closed channel, we can write the wave function of the eigen state as

$$r > r_0 : |\psi_m\rangle \propto e^{-\sqrt{\epsilon_m}r}/r$$  \(14\)

$$r < r_0 : |\psi_m\rangle \propto \sin \frac{\sqrt{\epsilon_m}r}{r} |+\rangle + \frac{A_m \sin \sqrt{\epsilon_m}r}{r} |-\rangle,$$  \(15\)

and, with our approximations, \(A_m\) satisfies

$$A_m^2 = \frac{2\gamma r_0 (\epsilon_c + \epsilon_m)^{-2}}{(\epsilon_c + \epsilon_m)^2 + 2\sqrt{\epsilon_m}r_0}$$  \(16\)

and the mixing angle \(\phi\) is defined below.

We show in Eq. (15) that the eigen state generally occupies both the closed channel and open channel. We can introduce a mixing amplitude \(\sin \phi\) as the amplitude in the closed channel

$$|\psi_m\rangle = \sin \phi |c\rangle + \cos \phi |o\rangle.$$  \(17\)

The mixing fraction \(\sin^2 \phi\) can be evaluated by a direct integration of the closed channel wave function. Alternatively, noticing that the mixing also leads to a dependence of the eigen state on the bare state, we can also derive \(\sin^2 \phi\) from the dependence of \(E_m\) on \(E_c\), or from the magnetic moment of the Feshbach molecule \(\mu_m = \partial E_m/\partial B\). All methods lead to the same result

$$\sin^2 \phi = -\frac{\partial E_m}{\partial E_c} = \frac{\mu_a - \mu_m}{\mu}$$  \(18\)

$$= \frac{2\sqrt{\epsilon_m}r_0}{(\epsilon_c + \epsilon_m)^2 + 2\sqrt{\epsilon_m}r_0}.$$  \(19\)

**IV. THRESHOLD REGIME IN OPEN CHANNEL**

Despite the seemingly complex equations shown in previous sections, the Feshbach molecules are simple and universal near the scattering continuum. Expanding Eq. (13) with small \(E_m\) and using Eq. (9)-(11), we find the binding energy of the Feshbach molecules has a simple dependence on the scattering length and increases quadratically in magnetic field near the resonance, namely,

$$E_m = \frac{\hbar^2}{m(a - r_0)^2}$$  \(20\)

$$= \frac{\mu^2 (B - B_{\text{res}})^2}{4E^*},$$  \(21\)

where \(E^* = (\hbar/4m)\gamma^2(a_{bg} - r_0)^4\).

Equation (20) shows identical dependence on scattering length and interaction range as of single channel molecules in the threshold regime [12]. Furthermore,
the Feshbach molecules are identical to long-range atom pairs in the open channel. We note that this definition is purely based on the range of the single channel regime, so we find the closed channel fraction can be expressed as

$$\sin^2 \phi = \sqrt{\frac{E_m}{E^*} - (1 + \delta)} \frac{E_m}{E^*} + \ldots,$$

where \(\delta = \gamma(\alpha_{bg} - r_0)^3\).

From Eq. (22), we see that \(E^*\) provides the leading order estimation of the closed channel admixture. When \(E_m < E^*\) or \(E_m \ll E^*/|\delta|\) (this condition applies when \(\delta \ll 1\), the Feshbach molecule is purely in the open channel. As expected, the threshold regime is wider for resonances with larger \(\gamma\) and \(|\alpha_{bg} - r_0|\).

We can further determine the "open channel-dominated" regime by setting \(\sin^2 \phi < \frac{1}{2}\) in Eq. (19). For resonances with small \(|\delta| \ll 1\), this condition corresponds to \(E_m < E^*\), which, in terms of magnetic field, maps to only a small fraction of \(|\delta| \Delta B\) near the resonance \(B_{res}\). For resonances with large \(|\delta| \gg 1\), the open channel dominates when \(E_m < (\gamma/2)^2/3\), which covers the full resonance width when \(\alpha_{bg} - r_0 < 0\), and covers the entire upper branch of the bound state when \(\alpha_{bg} - r_0 > 0\).

Based on the range of the single channel regime, we suggest the broad(narrow) resonances be defined as those with \(|\delta| \gg 1\) \((|\delta| \ll 1)\). Within the width of the Feshbach resonance, the molecules associated with a broad (narrow) resonance are better described as long range pairs in the open channel (short range molecules in the closed channel). We note that this definition is purely based on two-body physics.

V. FESHBACH MOLECULES IN \(^6\text{Li}\) AND \(^{40}\text{K}\)

Finally, we apply our model to the \(^6\text{Li}\) and \(^{40}\text{K}\) Feshbach molecules created in recent BEC-BCS experiments. These molecules are stable near the resonance and both the molecular binding energies and the scattering lengths have been well measured and studied.

![FIG. 3: Binding energies \(E_m\) (dotted lines) and mixing fractions \(\sin^2 \phi\) (solid lines) of the molecules near the \(^6\text{Li}\) and \(^{40}\text{K}\) Feshbach resonances. The curves are calculated from Eq. (13), Eq. (19) and the parameters in Table 1. Binding energies from multi-channel calculation (dashed lines), from JILA group measurement (open square) and the mixing fractions measurement from Rice group (open circles) are shown for comparison. The shaded areas indicate the typical BEC-BCS crossover regimes, |\(a| > 3000a_0\).](image)

To model the interaction of atoms, we adopt \(B_{res}, \Delta B, B_{bg}\) and \(\mu\) from recent measurements and numerical calculations. To account for the finite range of the atomic interaction, which at low temperatures is determined by the van der Waals potential of \(|A| / r^6\), we choose the interaction range \(r_0\) in our model to be the mean scattering length \(\bar{a}\) defined in Ref. 12. This choice ensures the same behavior of the scattering length in the threshold regime 12. All parameters are given in Table I.
For the narrower Li resonance at \( \sim 543 \) G, we obtain \( \delta \sim 0.0005 \) and \( E^* = \hbar 31 \) Hz \( \ll E_F = \hbar 20 \) kHz. This indicates an extremely narrow open channel regime of less than 50 \( \mu \)G near the resonance, where the gas parameter is still over \( k_F a \sim 20 \). Crossover experiments based on these Feshbach molecules cannot be described by open channel atom pairs and may lead to qualitatively different physics. We attribute the large difference between the two Li resonances to their different couplings \( \gamma \) and very different background scattering length \( a_{bg} \), see Table I.

In the above discussions, we note that Fermi energy \( E_F \) is an external parameter which depends on the density of the sample. Whether the molecules in the crossover regime can be described by single channel strongly depends on the density. The \( \delta \) parameter, however, provides a better and independent measure to classify Feshbach resonances. We find that the two Feshbach resonances in \( ^6\)Li are the two extremes of broad and narrow resonances with \( \delta = -2900 \) and \( \delta = 0.0005 \).

In summary, the two-channel model provides a simple picture to understand the molecular state near the Feshbach resonances. The analytic results of the molecular binding energy and mixing fraction on \( ^6\)Li and \( ^{40}\)K agree with the measurements and other sophisticated calculations very well. Based on the threshold behavior of the bound state, we suggest a dimensionless parameter to assess the “broadness” of the Feshbach resonance.

**Acknowledgements**

We thank P.S. Julienne and N. Nygaard for stimulating discussions and R. Grimm’s lithium and cesium groups in Innsbruck for the support during our visit. The author is partially supported by the Lise-Meitner program of the Austrian Science Fund (FWF).

[1] S. Jochim, M. Bartenstein, A. Altmeyer, G. Hendl, S. Riedl, C. Chin, J. Hecker Denschlag and R. Grimm, Science 302, 2101 (2003); M. Greiner, C.A. Regal, D.S. Jin, Nature 426, 537 (2003); M. Zwierlein, C.A. Stan, C.H. Schunck, S.M.F. Raupach, S. Gupta, Z. Hadzibabic, and W. Ketterle, Phys. Rev. Lett. 91, 250401 (2003).

[2] E. Tiesinga, B.J. Verhaar, and H.T.C. Stoof, Phys. Rev. A 47, 4114 (1993); S. Inouye, M. Andrews, J. Stenger, H.-J. Miesner, S. Stamper-Kurn, and W. Ketterle, Nature 392, 151 (1998).

[3] J. Herbig, T. Kraemer, M. Mark, T. Weber, C. Chin, H.-C. Nägerl, and R. Grimm, Science 301, 1510 (2003); S. Dürr, T. Volz, A. Marte, and G. Rempe Phys. Rev. Lett. 92, 020406 (2004); K. Xu, T. Mukaiyama, J.R. Abo-Shaeer, J.K. Chin, D. Miller, and W. Ketterle, Phys. Rev. Lett. 91, 210402 (2003).

[4] M. Greiner, C. A. Regal, D. S. Jin, Nature 426, 537 (2003).

[5] C. Chin, V. Vuletić, A.J. Kerman, and S. Chu, Phys. Rev. Lett. 90, 033201 (2003).

[6] S. Jochim, M. Bartenstein, A. Altmeyer, G. Hendl, C. Chin, J. Hecker Denschlag, and R. Grimm, Phys. Rev. Lett. 91, 240402 (2003).

[7] S. Simonucci, P. Pieri and G.C. Strinati, Europhys. Lett. 69 713 (2005).

[8] R.A. Duine and H.T.C. Stoof, Phys. Rep. 396, 115 (2004).

[9] B. Marcelis, E.G.M. van Kempen, B.J. Verhaar, and S.J.J.M.F. Kokkelmans, Phys. Rev. A 70, 012701 (2004); S.J.J.M.F. Kokkelmans, J.N. Milstein, M.L. Chiofalo, R. Walser, and M.J. Holland, Phys. Rev. A 65, 053617 (2002).

[10] K. Goral, T. Koehler, S.A. Gardiner, E. Tiesinga, P.S. Julienne, J. Phys. B 37, 3457 (2004).

[11] M. Bartenstein, A. Altmeyer, S. Riedl, R. Geursen, S. Jochim, C. Chin, J. Hecker Denschlag, R. Grimm, A. Simoni, E. Tiesinga, C.J. Williams, and P.S. Julienne, Phys. Rev. Lett. 94, 103201 (2005).

[12] G.F. Gribakin and V.V. Flambaum, Phys. Rev. A 48, 546 (1993).

[13] A. Simoni, V. Venturi and P. S. Julienne, private communication.

[14] C.A. Regal and D.S. Jin, Phys. Rev. Lett. 90, 230404 (2003); C.A. Regal, C. Ticknor, J.L. Bohn, and D.S. Jin, Nature 424, 47 (2003).

[15] K.E. Strecker, G.B. Partridge and R.G. Hulet, Phys. Rev. Lett. 91, 080406 (2003).

[16] G.B. Partridge, K.E. Strecker, R.I. Kamar, M.W. Jack, R.G. Hulet, cond-mat/0505353