Formation of Feshbach molecules in the presence of artificial spin-orbit coupling and Zeeman fields

Doga Murat Kurkcuoglu and C. A. R. Sá de Melo
School of Physics, Georgia Institute of Technology, Atlanta, 30332, USA
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We derive general conditions for the emergence of singlet Feshbach molecules in the presence of artificial Zeeman fields for arbitrary mixtures of Rashba and Dresselhaus spin-orbit orbit coupling in two or three dimensions. We focus on the formation of two-particle bound states resulting from interactions between ultra-cold spin-1/2 fermions, under the assumption that interactions are short-ranged and occur only in the s-wave channel. In this case, we calculate explicitly binding energies of Feshbach molecules and analyze their dependence on spin-orbit couplings, Zeeman fields, interactions and center of mass momentum, paying particular attention to the experimentally relevant case of spin-orbit couplings with equal Rashba and Dresselhaus (ERD) amplitudes.

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The effects of spin-orbit interactions is ubiquitous in nature, from the macroscopic scale of the Earth-Moon complex in astronomy and astrophysics, to the microscopic scale of the electron in the hydrogen atom in atomic physics. The interest in spin-orbit coupled systems has been revived in condensed matter physics due to the emergence of non-trivial topological properties of insulators and superconductors subject to Rashba spin-orbit fields [1, 2], and in atomic physics due to the creation of artificial spin-orbit coupling in ultra-cold atoms [3], which made possible the study of special quantum phase transitions in bosonic systems.

This new tool in the toolbox of atomic physics was experimentally developed first to study interacting bosonic atoms where an equal Rashba-Dresselhaus (ERD) artificial spin-orbit coupling was created [3]. It was suggested that interacting fermions could be studied using the same technique [3, 4]. Estimulated by the dense literature of the effects of Rashba spin-orbit coupling (SOC) encountered in condensed matter physics [1, 2], several theoretical groups investigated the effects of Rashba SOC for interacting ultra-cold fermions using mean field theories [4, 5] or for interacting bosons [6, 7]. Unfortunately, the experimental study of Rashba SOC requires more laser and further developments are necessary to overcome several difficulties [11]. Thus, presently, artificial Rashba SOC has not yet been created in the context of ultra-cold atoms. However, simultaneous theoretical studies of superfluidity for the experimentally relevant ERD spin-orbit coupling were performed for ultra-cold bosons by others [12, 13] and for ultra-cold fermions by our group [14, 15].

One of the benchmarks of experimental studies of Fermi superfluidity of cold atoms without artificial spin-orbit coupling was the emergence of molecular bound states via the use of Feshbach resonances [11], which lead to the formation of molecules [13] and their posterior Bose-Einstein condensation in $^{40}$K$_2$ [19] and $^6$Li$_2$ [20]. In the present published literature of ultra-cold fermions with spin-orbit coupling, only non-interacting systems have been investigated [21, 22]. However, very recently, the NIST group [23] has demonstrated experimentally the formation of Feshbach molecules of ultra-cold fermions (40K) in the presence of artificial SOC. Our theoretical results, described next, are in excellent agreement with the NIST experiment.

To address the important issue of the emergence of Feshbach molecules for interacting fermions in the presence of artificial SOC and Zeeman fields, we start from the Hamiltonian for two non-interacting fermions

$$H_0 = H_1 + H_2,$$  

written as the sum of two contributions, which have the generic form (with $\hbar = 1$)

$$H_j = \frac{k^2}{2m} - \left[ (\mathbf{h}_R + \mathbf{h}_D) \cdot \sigma_j \right] - \mathbf{h} \cdot \sigma_j.$$  

The term containing $\mathbf{h}_R = v_R \left( \hat{k}_x \mathbf{e}_y - \hat{k}_y \mathbf{e}_x \right)$ represents the Rashba spin-orbit field, the term containing $\mathbf{h}_D = v_D \left( \hat{k}_x \mathbf{e}_y + \hat{k}_y \mathbf{e}_x \right)$ represents the Dresselhaus spin-orbit field and $\mathbf{h} = h_x \mathbf{e}_y + h_z \mathbf{e}_z$ is the Zeeman field with $h_y = -\delta/2$ representing the detuning $\delta$ and $h_z = -\Omega R/2$ representing the Raman intensity $\Omega_R$. All these fields are described in energy units. In addition, $\hat{k}_j = -i \nabla_j$ is the momentum operator of the j-th particle, and $\sigma_j = \sigma_{x,j} \mathbf{e}_x + \sigma_{y,j} \mathbf{e}_y + \sigma_{z,j} \mathbf{e}_z$ is the vector Pauli matrix.

The interaction Hamiltonian $H_I(\mathbf{r}_1, \mathbf{r}_2) = -g \delta(\mathbf{r}_1 - \mathbf{r}_2) \delta_{s_1+s_2,0}$ describes zero-ranged attractive s-wave interactions between fermions with opposite spins $s_1 = -s_2$. The bare coupling constant $g$ is renormalized through the use of the Lippman-Schwinger relation $L^3/g = -m/4 \pi a_s + \sum_k 1/(2 \varepsilon_k)$, where $L^3$ is the volume, $a_s = a_{bg} \left[ 1 + \Delta B/(B - B_0) \right]$ is the three-dimensional scattering length expressed in terms of the background scattering length $a_{bg}$, the real magnetic field $B$, the width $\Delta B$ of the Feshbach resonance, and the field $B_0$, where the...
resonance is located. While in the two-dimensional case, the bare coupling constant $g$ is eliminated in favor of the bare binding energy $E_{bs}$ via $L^2/g = \sum_k 1/(2\epsilon_k - E_{bs})$.

Writing our Hamiltonian in relative momentum $k = (k_x - k_y)/2$, and center of mass (CM) momentum $K = k_x + k_y$ coordinates and performing a global SU(2) spin rotation into singlet and triplet channels of the initial spin basis leads to the non-interacting Hamiltonian matrix

$$ H_0 = \begin{pmatrix} \epsilon_{12} - 2h_z & -h_{12s} & 0 & -h_{12d} \\ -h_{12s} & \epsilon_{12} - h_{12s} & 0 & 0 \\ 0 & -h_{12s} & \epsilon_{12} + 2h_z & h_{21d} \\ -h_{12d} & 0 & -h_{21d} & \epsilon_{12} \end{pmatrix}, $$

where $\epsilon_{12} = \epsilon_{12}(k, K) = \epsilon_{k_1} + \epsilon_{k_2}$ is the sum of the kinetic energy of the two particles, $h_{12s} = h_{12s}(k, K) = [(h_{x_1} + h_{x_2}) + i(h_{y_1} + h_{y_2})]/\sqrt{2}$ is the scaled sum of the transverse fields felt by both particles, $h_{12d} = h_{12d}(k, K) = [(h_{x_1} - h_{x_2}) + i(h_{y_1} - h_{y_2})]/\sqrt{2}$ is the scaled sum of the transverse fields felt by the particles, while $h_{21d} = -h_{21d}$. More explicitly $\epsilon_{12}(k, K) = k^2/m + K^2/(4m)$; the matrix element from total spin projection $m_s = 0 \rightarrow m_s = 1$ or $m_s = -1 \rightarrow m_s = 0$ in the triplet sector is $h_{12s} = [\beta K_y + i(2h_x + \gamma K_x)]/\sqrt{2}$; and the matrix element that couples the singlet ($S = 0$) and triplet ($S = 1$) sectors with changes in total spin projection from $m_s = 0 \rightarrow m_s = 1$ is $h_{12d} = -\sqrt{2}\beta k_x - iv\sqrt{2}k_x$, while the one with changes from $m_s = 0 \rightarrow m_s = -1$ is $h_{21d} = \sqrt{2}\beta k_y + iv\sqrt{2}k_x$. The variables $\gamma$ and $\beta$ are defined in terms of the Rashba ($v_R$) and Dresselhaus ($v_D$) coefficients as $\gamma = v_D + v_R$ and $\beta = v_D - v_R$. Notice that $H_0$ is not Galilean invariant, and that $h_{12s}$ depends only on the CM momentum $K$, while $h_{12d}$ and $h_{21d}$ depend only on the relative momentum $k$, however the CM and relative coordinates remain coupled. Furthermore, in the experimentally relevant ERD case $v_D = v_R = v/2$ leading to $\beta = 0$ and $\gamma = v$.

Conditions for the emergence of Feshbach molecules are obtained from the Schrödinger equation

$$ (H_0 + H_I) \Lambda_{k, k'} = E \Lambda_{k, k'}, $$

where the four-dimensional spinor $\Lambda_{k, k'} = [\Lambda_{1,1}(k, K), \Lambda_{1,0}(k, K), \Lambda_{1,-1}(k, K), \Lambda_{0,0}(k, K)]$ that includes both the triplet wavefunctions $\Lambda_{1,1}(k, K) = \psi_{↑↑}(k, K)$ corresponding to ($S = 1, m_s = 1$); $\Lambda_{1,0}(k, K) = [\psi_{↑1}(k, K) + \psi_{↓1}(k, K)]/\sqrt{2}$ corresponding to ($S = 1, m_s = 0$); $\Lambda_{1,-1}(k, K) = \psi_{↓↑}(k, K)$ corresponding to ($S = 1, m_s = -1$); and the singlet wavefunction $\Lambda_{0,0}(k, K) = [\psi_{↑1}(k, K) - \psi_{↓1}(k, K)]/\sqrt{2}$ corresponding to ($S = 0, m_s = 0$). In this basis, the action of the interaction Hamiltonian on the four-dimensional spinor leads to the vector $H_I \Lambda_{k, k'} = [0, 0, 0, -g\Sigma_k \Lambda_{0,0}(k, K)]$. The equation above can be formally solved in any dimension by rearranging the Hamiltonian as $[E I - H_0] \Lambda_{k, k'} = H_I \Lambda_{k, k'}$ to obtain the relation

$$ \Lambda_{k, k'} = \frac{\text{Adj}[E I - H_0]}{\text{Det}[E I - H_0]} H_I \Lambda_{k, k'}, $$

where $\text{Adj}[M]$ is the adjugate matrix and $\text{Det}[M]$ is the determinant of $M$. Integration over the relative momentum $k$ leads to the integral equation

$$ \frac{L^d}{g} = -\sum_k \frac{(E - \epsilon_{12})(E - \epsilon_{12} + |h_t|)(E - \epsilon_{12} - |h_t|)}{(E - E_1)(E - E_2)(E - E_3)(E - E_4)}. $$

Here, the function $|h_t| = \sqrt{4h_x^2 + |h_{12s}(k, K)|^2}$ is the amplitude of the total field $h_t = h_1 + h_2$, $d$ is the dimension of the system, and $E_{1,2}(k, K)$ are the eigenvalues of $H_0$, corresponding to the two-particle generalized helicity bands $E_{a\beta}(k, K)$. We identify the right-hand-side of Eq. 5 with the function $G_s(E, K) = \sum_{k, \alpha, \beta} |U_{a\alpha s}(k, K)|^2/(E - E_{a\beta}(k, K))$, which corresponds to the spectral representation of the two-body Green’s function for non-interacting fermions in the singlet channel of the original spin states ($\uparrow, \downarrow$). Here, $|U_{a\alpha s}(k, K)|^2$ represents the spectral weight in the singlet channel ($s$) associated with the spinor eigenvector $U_{a\beta}(k, K)$ of $H_0$ with eigenvalue $E_{a\beta}(k, K)$. Only, the singlet channel contributes to $G_s(k, K)$, as the interactions between fermions are non-zero only between the original $\uparrow$ and $\downarrow$ spins.
By ordering the eigenvalues $E_1 \geq E_2 \geq E_3 \geq E_4$, a simple inspection of Eq. (4) shows that a necessary condition for the formation of singlet Feshbach molecules occurs when $E(K) \leq \min_k \{E_4(k, K)\}$, provided that there is spectral weight in the singlet interaction channel for the lowest energy of two free fermions. The energies $E_{\alpha\beta}(k, K)$ can be written in terms of the two-particle kinetic energy $\epsilon_{12}(k, K)$ and the effective fields $h_\alpha(k, K) = |h(k_1)| + |h(k_2)|$, and $h_{d}(k, K) = |h(k_1)| - |h(k_2)|$, where $|h(k_1)| = \sqrt{h_y^2(k_1) + h_z^2(k_1) + h_{d}^2(k_1)}$ is the magnitude of the total field (spin-orbit and Zeeman) felt by the $i^{th}$ particle. The momenta are $k_1 = k + K/2$ and $k_2 = -k + K/2$. The eigenenergies for two free fermions are $E_{\uparrow\downarrow}(k, K) = \epsilon_{12}(k, K) - h_y(k, K)$; $E_{\uparrow\downarrow}(k, K) = \epsilon_{12}(k, K) - h_d(k, K)$; $E_{\downarrow\uparrow}(k, K) = \epsilon_{12}(k, K) + h_d(k, K)$ and $E_{\downarrow\downarrow}(k, K) = \epsilon_{12}(k, K) + h_y(k, K)$.

From Eq. (5), we obtained Feshbach molecule energies $E = E_B(K)$ for an arbitrary mixture of Rashba and Dresselhaus terms at any value of $K$ in 2D and 3D. We also calculated the effective mass tensor and the corresponding Bose-Einstein condensation temperature $T_c$. However, we will show here results only for the ERD case, because of its experimental relevance for ultra-cold fermions $[6]$. Respectively, we use as units of energy and momentum, the recoil energy $E_R = h^2_k/(2m)$ and the recoil momentum $k_R = 2\pi/\lambda$, where $\lambda$ is the wavelength of the light used in the Raman beams $[3]$. We parametrize the ERD coupling parameter as $v = [1 - \cos(\theta)]k_R/(2m)$ for Raman beams that cross at an arbitrary angle $\theta$. Current experiments correspond to $\theta = \pi$ and $v = k_R/m$.

To gain insight in the ERD case, first we solve the problem for zero CM momentum $K = 0$ and zero detuning $h_y = 0$, but finite $h_z$. In this case, the eigenvalues take the simple form $E_{\uparrow\downarrow}(k, 0) = k^2/m + 2|h_{\text{eff}}(k)|$ for the highest energy, $E_{\uparrow\downarrow}(k, 0) = E_{\uparrow\downarrow}(k, 0) = k^2/m$, for the intermediate energies, and $E_{\downarrow\downarrow}(k, 0) = k^2/m - 2|h_{\text{eff}}(k)|$ for the lowest energy, where the magnitude of the effective field is $|h_{\text{eff}}(k)| = \sqrt{(vk_x)^2 + h_z^2}$. The condition for the emergence of zero CM momentum Feshbach molecules is then $E(K = 0) \leq \min_k \{E_{\uparrow\downarrow}(k, 0)\}$. See Fig. 1 for examples of $E_{\alpha\beta}(k, K)$ in various regimes.

In Fig. 2, we show the bound-state energy $E = E_B$ of Feshbach molecules (in units of $E_R$) versus the scattering parameter $1/(k_Ra_s)$ at zero CM momentum $(K = 0)$ and zero detuning $(h_y = 0)$ in two situations. In the limit of $h_z \to 0$, the Feshbach molecule energy can be obtained analytically as $E_{B,0} = -1/(ma_z^2) - m\omega^2$, which means that the existence of spin-orbit coupling lowers the energy of the bound state from the standard value $E_{B,0} = -1/(ma_z^2)$ by an amount equal to twice the kinetic energy transferred to individual atoms. However, the threshold scattering length for the emergence of bound states remains at $a_s = \infty$ or $1/(k_Ra_s) = 0$. The binding energy at $K = 0$ is defined as $E_{\text{Bin}} = E_B - \min_k E_4(k, K = 0)$ is a better indicator of the effects of spin-orbit coupling since the minimum energy of two free fermions also changes with $v$, where $E_1 \to E_{\uparrow\uparrow}$ when $h_z \neq 0$, but $E_1 \to E_{\uparrow\uparrow}$ when $h_z \to 0$ due to zero spectral weight in $\uparrow\uparrow$ channel. An example of $E_{\text{Bin}}$ is shown in Fig. 2b, where we plot $E_{\text{Bin}}/E_R$ versus $1/(k_Ra_s)$ for fixed $v = k_R/m$ and increasing Zeeman field $h_z$. As $h_z$ increases, the threshold for the formation of Feshbach molecules is shifted from infinite to finite and positive scattering lengths, indicating that stronger attraction between fermions is necessary to overcome the depairing effects of $h_z$.

In Fig. 2c, we show the threshold bound-state energy $E_{B,th}$ for $K = 0$ and $h_y = 0$ as a function of $h_z$ and varying $v$, obtained from the threshold condition $E(K) \leq \min_k \{E_{\uparrow\downarrow}(k, K)\}$. For $(K = 0)$, $E_B \leq E_{B,th} = m\omega^2 - h_z^2/(m\omega^2)$, having the dimensionless form $E_{B,th} = \bar{E}_{B,th} = 2\bar{p}^2 - \bar{h}_z^2/(2\bar{p}^2)$, where $\bar{E}_{B,th}$ and $\bar{h}_z = h_z/E_R$, where $\bar{h}_z = h_z/E_R$, and $\bar{p} = p/k_R$ with $p = mv$. In Fig. 2d, we show the threshold scattering length $a_{s,th}$ as a function of $h_z$, which behaves differently as $h_z$ reaches the critical value $h_{z,c} = m\omega^2$. This condition is expressed in dimensionless units as $\bar{h}_z,c = 2\bar{p}^2$. It is at this critical value that $E_{\uparrow\downarrow}(k, K)$ changes from a double minimum when $h_z \leq h_{z,c}$ to a single minimum when $h_z \geq h_{z,c}$. For fixed SOC $v$, the threshold $a_{s,th}$ progressivly grows with increasing $h_z$ first quadratically for $h_z < h_{z,c}$ and then linearly for $h_z \geq h_{z,c}$, as stronger attractive s-wave (singlet) interactions are necessary to overcome the de-
pairing effect of $h_z$ that tends to align the original spins.

![Graphs](image.png)

**FIG. 3:** (color online) a) Plots of $E_B/E_R$ versus $1/(k_R a_s)$ with $K = 0$, $h_y = 0.25E_R$, and $h_z = 0.5E_R$ for $v = 0.05k_R/m$ (blue dotted), $v = 0.25k_R/m$ (red dotted), $v = 0.75k_R/m$ (green dashed), $v = k_R/m$ (black solid). b) Plots of $E_{Bin}/E_R$ versus $1/(k_R a_s)$ with $K = 0$, $h_z = E_R$, and $v = k_R/m$ for $h_y = 0$ (blue dotted), $h_y = E_R$ (green dashed), $h_y = 2E_R$ (red dotted), $h_y = 3E_R$ (black solid). Plots of $E_{B,th}/E_R$ and $1/(k_R a_s,th)$ versus $h_y/E_R$ with $K = 0$, and $v = k_R/m$ are shown respectively in c) and d) for $h_z = 0$ (black solid); $h_z = E_R$ (red dotted); $h_z = 2E_R$ (green dashed); $h_z = 3E_R$ (blue dotted).

In Fig. 3 we show some results for finite $h_y$ and ERD spin-orbit coupling $v$, but zero CM momentum ($K = 0$). Fig. 3a contains plots of the Feshbach molecule energy $E_B/E_R$ versus interaction parameter $1/(k_R a_s)$ for $h_y = 0.25E_R$ and $h_z = 0.5E_R$ and changing ERD spin-orbit coupling $v$. The threshold interaction parameter decreases with increasing $v$ showing that larger SOC facilitates the formation of molecules when Zeeman fields are present. In Fig. 3b, we show $E_{Bin}/E_R$ versus $1/(k_R a_s)$ for $v = k_R/m$, $h_z = E_R$, and $K = 0$, but changing $h_y$. The scattering parameter threshold increases with $h_y$ as a stronger attractive interaction is necessary to form singlet Feshbach molecules in the original spin basis ($\uparrow, \downarrow$). The bound state energy threshold $E_{B,th}/E_R$ and the scattering parameter threshold $1/(k_R a_{s,th})$ versus $h_y/E_R$ are shown respectively in Figs. 3c and 3d for $K = 0$, and $v = k_R/m$, but changing $h_z$.

In Fig. 4 we show the energy dispersions $E(K)$ of Feshbach molecules and the threshold energy $E_{B,th} = \min_{k} E_{\uparrow \uparrow}(k, K)$ along CM momentum $K = (K_x, 0, 0)$ for four different cases with fixed scattering parameter $1/(k_R a_s) = 0.75$, spin-orbit coupling $v = k_R/m$, and Raman intensity $h_z = 0.5E_R$. In Fig. 4a, $h_y = 0$, while in b, c and d, the values are $h_y = 0.5E_R$, $1.5E_R$, and $2.5E_R$, respectively. Only in Fig. 4b the dispersions are even in $K_x$ since $h_y = 0$, otherwise, for $h_y \neq 0$, parity is lost. In particular, Feshbach molecules are stable only in a range of CM momenta, outside this region they decay into the two-particle continuum due to Landau damping. It is important to notice that for $h_y$ positive and increasing, the region of stable Feshbach molecules shifts towards negative CM momenta, and that beyond a critical value $h_y, _c$ no Feshbach molecules with zero CM momentum are stable. This unusual effect is a direct consequence of the absence of Galilean invariance and the loss of parity.

We have investigated the emergence of Feshbach molecules in the presence of spin-orbit coupling and Zeeman fields for any mixture of Rashba and Dresselhaus terms, but focused on the experimentally relevant equal Rashba and Dresselhaus (ERD) spin-orbit coupling. For zero detuning ($h_y = 0$) and fixed ERD spin-orbit coupling, we have found that the threshold scattering parameter $[1/(k_{F a_s,th})]$ required to form Feshbach molecules with zero center-of-mass (CM) momentum is shifted to larger positive values when the Raman coupling ($h_z$) is increased. Furthermore, for fixed scattering parameter $[1/(k_{F a_s})]$ these molecules are stable only for a symmetric range of CM momenta, outside which they decay into the two-particle continuum. However, for finite detuning ($h_y \neq 0$) and fixed Raman intensity, ERD spin-orbit coupling and scattering parameter, Feshbach molecules are stable only in an asymmetric range of CM momenta, and if the detuning is sufficiently large Feshbach molecules with zero CM momentum are not possible. These effects are a manifestation of the absence of Galilean invariance and the loss of parity.

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