

The lineshape of RF association of Feshbach molecules

Huan Q. Bui

November 24, 2023

1 Context

We consider the free-to-bound transition: an rf photon associates two free atom into a (weakly-bound) Feshbach molecule. The lineshape can be obtained from Fermi's Golden rule: it is a product of the Franck-Condon overlap \mathcal{F} between the wavefunction of a bound Feshbach molecule and that of a pair of two free atoms and the probability p of finding two free atoms in phase space which, along with the RF photon, satisfy the required resonance condition.

2 Franck-Condon factor calculation

Here we follow the steps outlined by [1]. We first provide the bound and free wavefunctions. The normalized molecule wavefunction is assumed to have the typical asymptotic form:

$$\phi_m = \sqrt{\frac{2}{a}} \frac{\exp(-r/a)}{r} \quad (1)$$

where a is the scattering length which, along with the background scattering length a_{bg} , gives the binding energy $E_b = \hbar^2/2\mu(a - \bar{a})^2$, where \bar{a} is the mean scattering length. The free atom pair assumes a scattering wavefunction $\psi_k(r) \propto \sin(kr + \delta')/r$, where k is the wavevector associated with the kinetic energy $E_k = \hbar^2 k^2/2\mu$ of the incoming wave and δ' is the phase-shift associated with the scattering length $a' = a_{bg}$ of the free-atom pair. While wavefunctions of scattering states are not normalizable in the usual sense, they are δ -function normalizable. We first follow [1] and require that the scattering wavefunctions be energy-normalized:

$$\int \psi_k(r)^* \psi_{k'}(r) r^2 dr = \pi \delta(E_k - E_{k'}) = \delta(k - k') \frac{\pi \hbar^2 k}{2\mu}, \quad (2)$$

where the second equality comes from the composition rule for the δ -function. From here, we find the appropriate normalization:

$$\psi_k(r) = \sqrt{\frac{2\mu}{\pi \hbar^2 k}} \frac{\sin(kr + \delta')}{r}. \quad (3)$$

The Franck-Condon overlap can now be evaluated:

$$\mathcal{F}(k) = \left| \int_0^\infty \phi_m^*(r) \psi_k(r) r^2 dr \right|^2 = \frac{4a\mu(ak \cos \delta' + \sin \delta')^2}{\pi \hbar^2 k(1 + a^2 k^2)^2}. \quad (4)$$

The interaction range r_0 for the Van der Waals potential of ^{23}Na and ^{40}K is given by

$$r_0 = 2^{-3/2} \frac{\Gamma(3/4)}{\Gamma(5/4)} \left(\frac{2\mu C_6}{\hbar^2} \right)^{1/4} \approx 50a_0, \quad (5)$$

where $C_6 \approx 2322 E_{\text{Hartree}} a_0^6$ ¹. In the Fermi1 experiment, $T \approx 200$ nK, so $k \sim \sqrt{2\mu k_B T/\hbar^2} \approx 1/6000a_0 \ll 1/r_0 = 1/50a_0$. As a result, we may use the low-energy expansion of the scattering phase shift:

$$k \cot \delta' \approx -\frac{1}{a'} + \frac{r'_e}{2} k^2 + \mathcal{O}(k^4) \approx -\frac{1}{a'} = -\frac{1}{a_{bg}} \quad (6)$$

where $r'_e = \Gamma(1/4)^4 r_0 / 6\pi^2$. Substituting this into Eq. (4), we find

$$\mathcal{F}(k) = \frac{4a(a - a_{bg})^2 k \mu}{\pi \hbar^2 (1 + a^2 k^2)^2 (1 + a_{bg}^2 k^2)}.$$

¹need citation, see Tiecke 2010

3 Calculating the probability of finding a suitable pair of atoms for Feshbach RF association

Consider a particle in a 3D harmonic trap. The Hamiltonian is

$$\mathcal{H}(\mathbf{p}, \mathbf{r}) = \frac{\mathbf{p}^2}{2m} + \frac{1}{2} \sum_i^3 m \omega_i^2 \mathbf{r}_i^2. \quad (7)$$

The probability of finding the particle in some phase space cell $d^3\mathbf{p}d^3\mathbf{r}$ at temperature T is given by

$$\Pr(\mathbf{p}, \mathbf{r}) = \frac{1}{\mathcal{Z}} \exp(-\beta\mathcal{H}) = \frac{\exp(-\beta\mathcal{H})}{\int d^3p \int d^3r \exp(-\beta\mathcal{H})} = \frac{\bar{\omega}^3}{(2\pi k_B T)^3} \exp(\mathcal{H}/k_B T) \quad (8)$$

where $\beta = k_B T$ and $\bar{\omega}$ denotes the geometric mean of the three trapping frequencies.

Now let us introduce another particle. Let these two particles be an Na atom and a K atom and assume that they do not interact. The probability for finding them textitssomewhere in phase space is trivially the product $\Pr(\mathbf{p}_{\text{Na}}, \mathbf{r}_{\text{Na}}) \times \Pr(\mathbf{p}_{\text{K}}, \mathbf{r}_{\text{K}})$. For RF association, we are interested in the total probability of finding a pair of Na and K for which their *relative kinetic energy* and the RF photon energy satisfy the energy conservation condition for molecular association:

$$E_k = \frac{\hbar^2 k^2}{2\mu} = \hbar\omega - E_b, \quad (9)$$

where μ is the reduced mass $m_{\text{Na}}m_{\text{K}}/(m_{\text{Na}} + m_{\text{K}})$. In order to define E_k and evaluate the total probability of finding an Na and a K atom that satisfy this condition, we must first transform to the COM and reduced mass coordinates. The COM and relative coordinates are given by

$$\mathbf{r}_{\text{COM}} = \frac{m_{\text{Na}}\mathbf{r}_{\text{Na}} + m_{\text{K}}\mathbf{r}_{\text{K}}}{m_{\text{Na}} + m_{\text{K}}}, \quad \mathbf{r}_{\text{rel}} = \mathbf{r}_{\text{K}} - \mathbf{r}_{\text{Na}}, \quad M = m_{\text{Na}} + m_{\text{K}}, \quad \mu = \frac{m_{\text{Na}}m_{\text{K}}}{m_{\text{Na}} + m_{\text{K}}} \quad (10)$$

from which it follows that

$$\mathcal{H} = \frac{\mathbf{p}_{\text{Na}}^2}{2m_{\text{Na}}} + \frac{\mathbf{p}_{\text{K}}^2}{2m_{\text{K}}} + \underbrace{\frac{1}{2} \sum_i^3 m_{\text{Na}} \omega_{i,\text{Na}}^2 \mathbf{r}_{i,\text{Na}}^2 + \frac{1}{2} \sum_i^3 m_{\text{K}} \omega_{i,\text{K}}^2 \mathbf{r}_{i,\text{K}}^2}_{\text{relative term}} \quad (11)$$

$$= \frac{\mathbf{p}_{\text{COM}}^2}{2M} + \frac{\mathbf{p}_{\text{rel}}^2}{2\mu} + V(\mathbf{r}_{\text{Na}}, \mathbf{r}_{\text{K}}) \quad (12)$$

where the relative term is simply the sum of the kinetic energies calculated relative to the COM:

$$\frac{1}{2} m_{\text{Na}} (\dot{\mathbf{r}}_{\text{Na}} - \dot{\mathbf{r}}_{\text{COM}})^2 + \frac{1}{2} m_{\text{K}} (\dot{\mathbf{r}}_{\text{K}} - \dot{\mathbf{r}}_{\text{COM}})^2 = \frac{1}{2} \frac{m_{\text{Na}}m_{\text{K}}}{m_{\text{Na}} + m_{\text{K}}} (\dot{\mathbf{r}}_{\text{K}} - \dot{\mathbf{r}}_{\text{Na}})^2 \equiv \frac{\mathbf{p}_{\text{rel}}^2}{2\mu}. \quad (13)$$

Here, we have defined $\mathbf{p}_{\text{rel}} \equiv \mu \dot{\mathbf{r}}_{\text{rel}}$. Additionally, we have assumed that $\omega_{i,\text{Na}} = \omega_{i,\text{K}} = \omega_i$ for all $i = x, y, z$. We note that is a fairly safe assumption to make, since $\omega_{\text{K}}/\omega_{\text{Na}} \approx 1.16$ in reality.

The probability of finding a pair of Na and K atoms with $E_k = \hbar\omega - E_b$ is a product of the spatial and momentum integrals. These are uncoupled, so we can evaluate them separately. With overall normalization factor, the spatial integrals give the contribution

$$S = \frac{(2\pi k_B T)^3}{(m_{\text{Na}}m_{\text{K}})^3 \bar{\omega}^6} \times \left(\frac{\bar{\omega}}{2\pi k_B T} \right)^6 = \frac{1}{(2\pi k_B T)^3} \frac{1}{(m_{\text{Na}}m_{\text{K}})^3}. \quad (14)$$

The momentum integral has two uncoupled parts: the COM integral and relative integral. The Jacobian for the $(\mathbf{p}_{\text{Na}}, \mathbf{p}_{\text{K}}) \rightarrow (\mathbf{p}_{\text{COM}}, \mathbf{p}_{\text{rel}})$ is unity. The COM integral reads:

$$M_{\text{COM}} = (2\pi M k_B T)^{3/2}. \quad (15)$$

The integral involving the relative kinetic energy is a convolution of the "bare" relative kinetic energy and a δ -function for picking out the correct kinetic energy:

$$M_{\text{rel}} = \int d^3 p_{\text{rel}} \exp\left(-p_{\text{rel}}^2/2\mu\right) \delta\left(p_{\text{rel}}^2/2\mu = E_k\right) \quad (16)$$

$$= \int d^3 p_{\text{rel}} \exp\left(-p_{\text{rel}}^2/2\mu\right) \delta\left(p_{\text{rel}}^2/2\mu = E_k\right) \quad (17)$$

$$= \int d^3 p_{\text{rel}} \exp\left(-p_{\text{rel}}^2/2\mu\right) \frac{\mu}{\hbar k} \delta(p_{\text{rel}} = \hbar k) \quad (18)$$

$$= \frac{4\pi\mu}{\hbar k} (\hbar k)^2 \exp\left(\frac{-E_k}{k_B T}\right) \quad (19)$$

$$= 4\pi\mu\hbar k \exp\left(\frac{-\hbar^2 k^2}{2\mu k_B T}\right). \quad (20)$$

Putting everything together, we find the desired expression for the probability of finding an Na-K pair satisfying the energy conservation condition:

$$\text{Pr}(k) \propto \frac{k}{(2\pi k_B T)^{3/2}} \exp\left(\frac{-\hbar^2 k^2}{2\mu k_B T}\right), \quad (21)$$

where we have left out the irrelevant multiplicative constants and kept only factors that depend on the temperature T and wavevector k .

4 The ideal lineshape

From the previous two sections, we readily find the RF lineshape:

$$\Gamma(k) \propto \frac{k}{(2\pi k_B T)^{3/2}} \exp\left(\frac{-\hbar^2 k^2}{2\mu k_B T}\right) \times \frac{4a(a - a_{bg})^2 k \mu}{\pi \hbar^2 (1 + a^2 k^2)^2 (1 + a_{bg}^2 k^2)}. \quad (22)$$

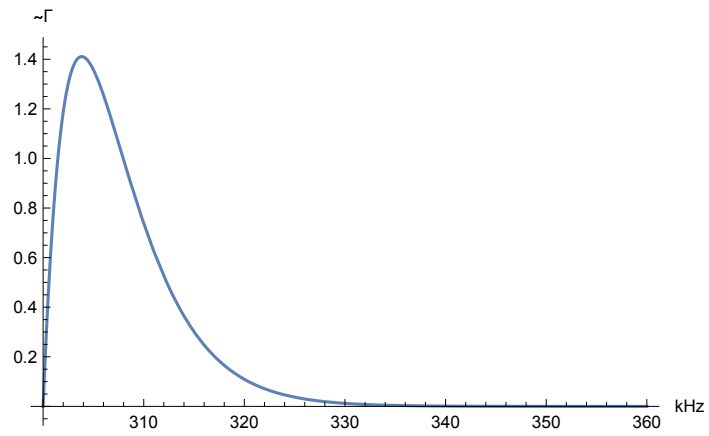
With $k = \sqrt{2\mu(\hbar\omega - E_b)/\hbar^2}$, we find

$$\Gamma(\omega) \propto \frac{\hbar\omega - E_b}{(k_B T)^{3/2}} \frac{1}{\left[1 + \frac{2\mu a^2}{\hbar^2}(\hbar\omega - E_b)\right]^2 \left[1 + \frac{2\mu a_{bg}^2}{\hbar^2}(\hbar\omega - E_b)\right]} \exp\left[\frac{-(\hbar\omega - E_b)}{k_B T}\right]. \quad (23)$$

For the purpose of fitting to RF lines, we care about the lineshape, which includes the "resonance" feature and its width. As a result, a more practical expression for the lineshape is as follows:

$$\Gamma(\omega) \propto \frac{\omega - \omega_b}{\left(1 + \frac{\omega - \omega_b}{\omega_a}\right)^2 \left(1 + \frac{\omega - \omega_b}{\omega_{a_{bg}}}\right)} \exp\left(-\frac{\omega - \omega_b}{k_B T/\hbar}\right). \quad (24)$$

What does this lineshape look like for some practical cases? Suppose we have $\omega_b = 2\pi \times 300$ kHz, $\omega_a = 2\pi \times 287$ kHz, $\omega_{a_{bg}} = 2\pi \times 259$ kHz and $T = 200$ nK $\implies k_B T/\hbar =$. Then the lineshape looks something like the following.



5 Thermal equilibrium

6 Others

References

- [1] Cheng Chin and Paul S. Julienne. Radio-frequency transitions on weakly bound ultracold molecules. *Phys. Rev. A*, 71:012713, Jan 2005.