Problem Set 9

Due: Friday 11:59pm, April 21st
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Office hour: TBA

Non-perturbative calculation of the radiofrequency response of a Feshbach molecule

In this problem we will treat the response of a Feshbach molecule to an applied radiofrequency drive non-perturbatively. It has an unusual amount of prose and explanations, as the goal here is understanding of the method and not getting lost in integrals (although that still might happen).

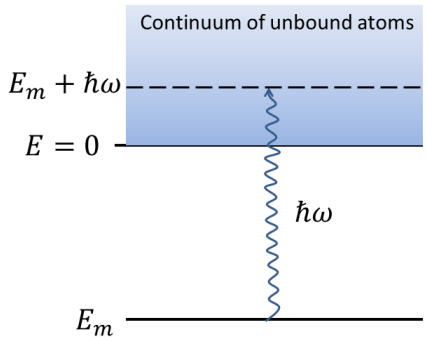

Figure 1: The molecular state at E_m is dressed by a radiofrequency photon of energy $\hbar\omega$ to lie near the continuum of free atom states at energy $E_m + \hbar\omega$. Shown is the situation $\hbar\omega > |E_m|$, but we can choose ω freely.

We start with a diatomic molecular state $|m\rangle$ of energy E_m that is coupled via a radiofrequency (rf) drive (frequency ω) to a continuum of final states corresponding to unbound atoms $\left|\vec{k}\right\rangle$ of energy $E_k = \frac{\hbar^2 k^2}{2\mu}$, where μ is the effective mass of the two-atom system. Instead of dealing with the time-dependent oscillatory terms in the original hamiltonian, we consider the molecule dressed by the radiofrequency light in the rotating wave approximation, which thus simply lifts its energy to $E_m + \hbar\omega$ (typically there is a large Zeeman energy to bridge between the molecular level and the free-atom threshold (10s or 100s of MHz), so one does not have to worry at all about the counter-rotating term). The setup is thus formally equivalent to calling the molecule energy $\hbar\delta = \hbar\omega - |E_m|$ as in last week's homework. We here are interested in varying the photon frequency at fixed magnetic field. As before, the coupling exclusively connects $|m\rangle$ to $|k\rangle$ and vice versa, but here the coupling is not an intrinsic hyperfine interaction (that we assume has already acted to make the molecular state be at E_m), but the coupling is under experimental control: It is the Rabi frequency of the rf drive Ω_R. This problem follows closely the spirit of API $C_{\rm III}$ (pp. 239), but with a concrete example of high relevance to quantum gas experiments. If you get lost, $C_{\rm III}$ is a great place to gain understanding.
Different from last week's problem, we will here consider the proper momentum-dependent coupling of a molecule of size $\sim a$, given by a wavefunction $\psi_m(r) = \sqrt{\frac{2}{a}} e^{-r/a}$, to a free wave of unbound atoms $\psi_k(r) = \sqrt{\frac{2}{R}} \sin(kr)$. Here, R is the radius of a large fictitious quantization box. Allowed

k-values are $k_n = n\pi/R$. Note that this problem is effectively 1D, as we deal with s-waves: The molecule has spherical symmetry, so it only couples to modes with angular momentum quantum numbers $l = 0$, $m = 0$. When replacing sums with integrals, use therefore $\sum_k \to \frac{R}{\pi}\int \mathrm{d}k$.
The goal is to find the full time evolution $U_m(\tau) = \langle m\,|U(\tau)|\,m\rangle$ giving the probability amplitude for the molecule to still be present after a time τ. We expect that for weak coupling, Fermi's Golden Rule should apply, giving the rate of exponential decay. However, we will find corrections at short and long times even in the weak coupling case. For strong coupling (we will have to see what "strong" means) we may expect Rabi oscillations between the molecule and the continuum: Those continuum states that are significantly coupled to the molecule form a "band" of finite width (to be specified), so for times short compared to the inverse width of the band, or for coupling strengths larger than the width, the molecule-atom pair system will first behave as a two-level system and display Rabi oscillations.

a) First, we calculate the coupling strength. Physically, the RF photon spin-flips one of the atoms in the molecule into another atomic hyperfine state where it is free. The coupling strength is given by $\hbar\Omega_R/2$ times the Franck-Condon overlap of the bound molecular wavefunction and the free two-atom wave (consisting of the transferred atom and the "left-over" partner). Calculate $V_{mk} = \frac{\hbar\Omega_R}{2}\int_0^\infty \mathrm{d}r\psi_k^*(r)\psi_m(r)$. Which k gives maximum coupling? What is the characteristic range of k that gives significant coupling? At low and high k, V_{mk} behaves like a power law on k. Give the powers in the two limits.

b) In this special case where the coupling V is only between the state of interest $|m\rangle$ and the continuum states, but not between two continuum states, the series for the level shift operator $R_m(z)$ (API, III.B.1, equation (B.4)) only contains one piece, the one that is quadratic in V. Near the real axis $z = E \pm i\eta$ we can write $R_m(E \pm i\eta) = \hbar\Delta_m(E) \mp i\hbar\frac{\Gamma_m(E)}{2}$. Write down the expressions for $\Delta_m(E)$ and $\Gamma_m(E)$ in terms of V_{mk}. Of the two, $\Gamma_m(E)$ is easier to calculate (we like delta-functions). Calculate $\Gamma_m(E)$ for $E < 0$ and $E > 0$. The answer can be written entirely in terms of E and $E_m = -\frac{\hbar^2}{2\mu a^2}$, the energy of the molecular state. Make a plot of $\Gamma_m(E)$. Evaluated at $E = \hbar\omega + E_m$ this is just the rf spectrum one obtains in linear response from Fermi's Golden Rule, assuming a weak and long drive. It is clearly not a Lorentzian. With what power law E^β does $\Gamma_m(E)$ behave near $E = 0$?

c) At large energies $E \gg E_m$, you should find that $\Gamma_m(E)$ can be written as

$$\Gamma_m(E) = \frac{C}{8\pi}\sqrt{\frac{1}{2\mu}}\hbar^2\Omega_R^2\frac{1}{E^{3/2}}.$$

Find C. This is the *contact* of a molecule. One can show that it is directly related to the change in the molecular energy with a: $C = -\frac{8\pi\mu}{\hbar^2}\frac{\partial E_m}{\partial a^{-1}}$, which can serve you as a check. Calculate also the integral

$$\Omega_1^2 = \frac{2}{\pi\hbar}\int_{-\infty}^{\infty}\mathrm{d}E\,\Gamma_m(E)$$

(Ω_1 thus defined differs by a factor of 2 from that defined in (22) in API C_{III}, for good reasons).

d) Calculate $\Delta_m(E)$ for $E < 0$ and $E > 0$. You can do this directly or by using the relation

$$\Delta_m(E) = \frac{1}{2\pi}\mathcal{P}\int \mathrm{d}E'\frac{\Gamma_m(E)}{E - E'} \tag{1}$$

A useful integral is

$$\int \mathrm{d}x \frac{\sqrt{x}}{(1+x)^2(y-x)} = -\frac{\pi}{2}\begin{cases}\frac{1}{(1+\sqrt{-y})^2}, & \text{for } E \le 0\\ \frac{1-y}{(1+y)^2}, & \text{for } E > 0\end{cases}$$

Find the limit of $\Delta_m(E)$ for $|E| \gg |E_m|$, and write it in terms of Ω_R and E. With $E \to \hbar\omega$ in this limit you see that this is the typical behavior of an AC Stark shift due to a far off-resonant drive.

Make a plot of $\Delta_m(E)$ and $\Gamma_m(E)$.

We now have all the ingredients to calculate the full time evolution:

$$U_m(\tau) = \int_{-\infty}^{\infty} \mathrm{d}E\, \mathcal{U}_m(E) e^{-iE\tau/\hbar}$$

where

$$\mathcal{U}(E) = \frac{1}{2\pi i}\left[(G_{m-}(E) - G_{m+}(E)\right] \quad (2)$$

$$= \lim_{\eta\to 0_+} \frac{1}{\pi} \frac{\hbar\Gamma_m(E)/2 + \eta}{\left[E - E_m - \hbar\omega - \hbar\Delta_m(E)\right]^2 + \left[\hbar\Gamma_m(E)/2 + \eta\right]^2} \quad (3)$$

e) Let's visualize what we are dealing with. Get Mathematica or equivalent to produce density plots of $\mathcal{U}_m(E)$, where E is the y-axis, and $\delta = \omega - |E_m|/\hbar$, the detuning from resonance, is the x-axis. Pick $|E_m|$ as your unit of energy and set $\eta = 0.01|E_m|$ (to be able to visualize delta-peaks). Produce plots for $\Omega_R/|E_m| = 2$, 8 and 20. Show a range in $\delta/|E_m|$ and in $E/|E_m|$ from -10 to 20.

Another educational plot you should make is $4\Delta_m(E)|E_m|/\hbar\Omega_R^2$ (which is independent of Ω_R) and the line $(E-\hbar\delta)|E_m|/\hbar^2\Omega_R^2$, together with $\mathcal{U}_m(E)$. Do this for $\delta = 5|E_m|$ and $\Omega_R/|E_m| = 2$, 10 and 30.

f) For weak coupling, $\mathcal{U}_m(E)$ is a δ-function for $\delta < 0$, centered at $E = \hbar\delta$ (so $|U_m(\tau)|^2 = 1$) and approximately a Lorentzian of full width half maximum $\Gamma_m(\delta)$ for $E > 0$. The probability to stay in state $|m\rangle$, $|U_m(\tau)|^2$ will thus exponentially decay at rate $\Gamma_m(\hbar\delta)$. This is the usual regime in which rf spectroscopy is performed. However, both at short and long times, the exponential decay cannot be correct. First, at long times, the Fourier transform singles out only the portion of $\mathcal{U}_m(E)$ for E close to zero. Find the power law $\mathcal{U}_m(E) \propto E^\beta$ and deduce the dependence on τ of $U_m(\tau)$ at long times (note that the energy integral is essentially cut off at $E = \hbar/\tau$ due to dephasing of $e^{-iE\tau}$.)

g) We now consider intermediate coupling strengths. For $\delta > 0$, i.e. when the bare molecular state is lifted into the continuum, one might think that the probability to stay in the molecular state should eventually decay. However, there is a critical coupling strength $\Omega_{R,c}^2$ for a given detuning δ where a portion of the function $\mathcal{U}(E)$ acquires a δ-function peak at $E < 0$, i.e. below the continuum. Find $\Omega_{R,c}^2$ in terms of δ and $|E_m|$. For larger coupling, find an expression for the energy of this discrete feature in terms of Ω_R^2, $\Omega_{R,c}^2$ and $|E_m|$. We thus see that, under rf dressing beyond the critical coupling strength, a portion of the molecular state is still discrete, split off from the continuum. The probability amplitude in this discrete portion does not decay. $|U_m(\tau)|^2$ will thus have a non-zero plateau at long times. See Eq. (46) in API C_{III} on how to obtain the magnitude of the plateau (you do not have to find this).

h) Finally, for strong coupling $\Omega_R >> \Omega_{R,c}$, inspection of $\mathcal{U}_m(E)$ or the graphs you created show that there will be basically two features in $\mathcal{U}_m(E)$, which both contribute to $U_m(\tau)$: A discrete portion as discussed above, and a broad Lorentzian feature at positive energies. Give the energies E where these two features are located, in the limit of strong coupling. How much weight is in either feature? Describe the evolution of the probability $|U_m(\tau)|^2$ to stay in the molecular state, for times short and long compared to the inverse width of the broad Lorentzian at $E > 0$.

Radiofrequency spectroscopy is a powerful tool to study the behavior of strongly interacting quantum gases. See for example:

1. Gupta, S., et al., Radio-Frequency Spectroscopy of Ultracold Fermions, Science 300, 1723 (2003)

2. Regal, C.A., et al., Creation of ultracold molecules from a Fermi gas of atoms, Nature 424, 47 (2003)

3. Cheng Chin, Paul S. Julienne, Phys. Rev. A 71, 012713 (2005), arXiv:cond-mat/0408254. Very useful to understand the radiofrequency spectrum of molecules in the presence of final state interactions.

4. Mukherjee, B. et al., Spectral response and contact of the unitary Fermi gas, arXiv: 1902.08548

5. Yan, Z., et al., Boiling a Unitary Fermi Liquid, PRL 122, 093401 (2019), arXiv:1811.00481 and many further references therein.

6. Review on resonant Fermi gases: W. Ketterle, M. Zwierlein, Ultracold Fermi Gases, Proceedings of the International School of Physics "Enrico Fermi", Course CLXIV, Varenna, 20 - 30 June 2006, edited by M. Inguscio, W. Ketterle, and C. Salomon (IOS Press, Amsterdam) 2008, arXiv:0801.2500