[V0] RF response of thermal BF mixture with two-body interaction

HQB

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1 Context

In our experiment we begin with a thermal mixture of ^{23}Na in the hyperfine state $|F = 1, m_F = 1\rangle$ and ^{40}K in the hyperfine state $|F = 9/2, m_F = -9/2\rangle$ at around 100 G. A Blackman pulse of duration ~100 ms with Rabi frequency ~5 kHz is turned on. The frequency $\omega_{\rm rf}$ of the rf field is tuned across the resonance for the $m_F = -9/2 \rightarrow m_F = -7/2$ hyperfine transition in ^{40}K. There are two relevant Na-K scattering lengths which we denote $a_{-9/2}$ and $a_{-7/2}$. At 100 G, we have $a_{-9/2} = -1698a_0$ and $a_{-7/2} = 644a_0$, which means there is a two-body bound state of NaK with $|^{23}\text{Na}, F = 1, m_F = 1\rangle$ and $|^{40}\text{K}, F = 9/2, m_F = -9/2\rangle$ and no bound state of NaK with ^{40}K in $m_F = -9/2$. It is thus possible to create these bound states (a.k.a. Feshbach molecules) using the rf field when $\omega_{\rm rf}$ is an amount E_b that is the molecule binding energy from the bare hyperfine resonance $\omega_{\rm HF}$. The molecule association lineshape is known (see, for example, [1]).

What we're after is the lineshape of the ^{40}K $m_F = -9/2 \rightarrow m_F = -7/2$ transition in the presence of Na. In our experiment, we observed the lineshape to have a threshold behavior with a high-frequency tail. We know this has to do with the interaction with the Na bath, but have not found a satisfactory quantitative model for this rf response. The goal of this document is to put together what we know and what we need to know in order to find this lineshape. There are at least two ways to get the rf response for our system.

Notes: This calculation for now neglects any three-body effect and focuses on two-body interaction. We want to see why/how the free-to-free peak has the lineshape that we see in experiments. Also, the spectral function calculation alone should not be used as a model for experimental data: there's an extra step involving finding the occupied initial and unoccupied final spectral functions in order to get the rf response. This, besides checking the existing results, is still in progress.

2 Momentum conservation

We consider a single $|^{23}\text{Na}, F = 1, m_F = 1\rangle$ atom interacting with a $|^{40}\text{K}, F = 9/2, m_F = -9/2\rangle$ atom. We assume that the Na atom has momentum $\hbar k_{\rm Na}$ and the K atom has momentum $\hbar k_K$. Moreover, we assume that the rf field with detuning δ from the hyperfine resonance does not change the total momentum of the two-body system.

3 Two-body scattering T-matrix

We assume wo-body short-range contact interaction between the Na and K atoms. The bare interaction strength is given by

$$\frac{1}{g} = \frac{\mu}{4\pi a_s} - \sum_k^\Lambda \frac{1}{2\epsilon_{\bf k}} \tag{1}$$

where μ is the Na-K reduced mass and $\epsilon_{\bf k}$ is the kinetic energy associated with the relative motion of the atoms. Just for clarity, we give useful relations between the various momenta. These can be readily derived from the coordinate transformation, but they are nice to have them at our finger tips.

$$P_{\rm COM} = p_{\rm Na} + p_K \qquad P_{\rm rel} = \hbar k = \mu \left(\frac{p_{\rm Na}}{m_{\rm Na}} - \frac{p_K}{m_K} \right). \tag{2}$$

The two-body scattering T-matrix is given in terms of the relative momentum $\hbar k$. As a reminder, the T-matrix is directly related to the scattering amplitude from the initial relative momentum $\mathbf{k}$ to final relative momentum $\mathbf{k}'$ (see Eq. 7.2.19 of [2]):

$$f(\mathbf{k}', \mathbf{k}) = -\frac{1}{4\pi} \frac{2\mu}{\hbar^2} (2\pi)^3 \langle \mathbf{k}' | T | \mathbf{k} \rangle . \tag{3}$$

For the case of forward scattering, $\mathbf{k}' = \mathbf{k}$, and the amplitude is given by

$$f(\mathbf{k}' = \mathbf{k}, \mathbf{k}) = f(\theta = 0, k) = -\frac{1}{4\pi} \frac{2\mu}{\hbar^2} (2\pi)^3 T(k). \tag{4}$$

But we also know that for low-energy, s-wave scattering, the (forward) scattering amplitude is given by (see, for example, Eq. 7.6.16 of [2])

$$f_{\ell=0}(k) = \frac{1}{k \cot \delta_{\ell=0} - ik} = \frac{a}{1 - ika}. \tag{5}$$

We can now put together Eq. (4) and Eq. (5) to get the commonly quoted expression for the T-matrix

$$\boxed{T(\omega) = \frac{4\pi}{2\mu} \frac{1}{a^{-1} - \sqrt{-2\mu\omega}}} \tag{6}$$

where we have dropped certain factors of π and $\hbar$ to adhere to conventions in the literature.

In the case of scattering between particles of equal mass, the reduced mass is $\mu = m^2/2m = m/2$. The two-body T-matrix is then:

$$T(\omega) = \frac{4\pi}{m} \frac{1}{a^{-1} - \sqrt{-m\omega}}, \tag{7}$$

where we have made the replacement $ik \to \sqrt{-m\omega}$. This is the expression found in Parish's [3] and Leyronas's [4]. Reinstating $\hbar$, we find that the T-matrix has a pole at $\omega = \hbar^2/2\mu a^2$ whenever $a > 0$. This is precisely the statement that the two-body problem admits a bound state when the interaction is repulsive.

4 Self-energy in the virial expansion for interacting equal mass fermions

4.1 Virial expansion of the Green's function

Following [4] and [5], we begin with the propagator for a free fermion of mass m_F in imaginary time:

$$G^{(0)}(\mathbf{k}, \tau) = e^{-(\epsilon_{\mathbf{k}} - \mu)\tau} [n_F(\epsilon_{\mathbf{k}} - \mu) - \Theta(\tau)] \tag{8}$$

where μ is the chemical potential, $\epsilon_{\mathbf{k}} = \hbar^2 k^2/2m_F$, $n_F(x) = 1/(e^{\beta x} + 1)$ is the Fermi-Dirac distribution, $\Theta(x)$ is the Heaviside step function, and τ is the imaginary time. The derivation for the free-fermion propagator can be found in many textbooks/lecture notes (see, for example, this page), but we can reproduce it here:

A free particle of mass m has the Hamiltonian

$$H = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} a_{\mathbf{k}}^\dagger a_{\mathbf{k}} \tag{9}$$

with $\epsilon_{\mathbf{k}} = \hbar^2 k^2 / 2m$, and $a^\dagger(t)$, $a(t)$ the (time-dependent) creation and annihilation operators. The time independence comes in via $a_{\mathbf{k}}(t) = e^{-i\epsilon_{\mathbf{k}} t/\hbar} a_{\mathbf{k}}(0) = e^{-i\epsilon_{\mathbf{k}} t/\hbar} a_{\mathbf{k}}$. The Green's function/propagator for the free particle is given by

$$G(\mathbf{k}, t) = -\langle \mathcal{T}[a_{\mathbf{k}}(t) a_{\mathbf{k}}^\dagger] \rangle \tag{10}$$

This is nothing but the amplitude of annihilating a particle of momentum $\hbar\mathbf{k}$ at $t' = 0$ and creating a particle of momentum $\hbar\mathbf{k}$ at $t' = t$. Here, $\mathcal{T}[\cdot]$ denotes the time-ordering operator. For fermions, we have $\langle a_{\mathbf{k}}^\dagger a_{\mathbf{k}} \rangle = n_F(\mathbf{k})$ and $\mathcal{T}[\cdot] \to \mathcal{T}_F[\cdot]$ is the fermionic time-ordering operator. By applying the fermionic anti-commutation rule and plugging this into the definition for the Green's function, we find the result in Eq. (8) after some small simplifications.

In the high-temperature limit, the Fermi-Dirac distribution can be expanded in powers of the fugacity $z = e^{\beta\mu} \ll 1$ as:

$$n_F(\epsilon_{\mathbf{k}}, \mu) = \sum_{n \geq 1} (-1)^{n+1} z^n e^{-n\beta\epsilon_{\mathbf{k}}}. \tag{11}$$

The free fermion Green's function is then

$$G^{(0)}(\mathbf{k}, \tau) = e^{\mu\tau} \left[\sum_{n \geq 0} G^{(0,n)}(\mathbf{k}, \tau) z^n \right], \tag{12}$$

where

$$G^{(0,0)}(\mathbf{k}, \tau) = -\Theta(\tau) e^{-\epsilon_{\mathbf{k}}\tau} \tag{13}$$

$$G^{(0,n)}(\mathbf{k}, \tau) = (-1)^{n-1} e^{-\epsilon_{\mathbf{k}}\tau} e^{-n\beta\epsilon_{\mathbf{k}}}, \quad n \geq 1. \tag{14}$$

We see that $G^{(0,0)}$ is retarded, but not $G^{(0,n)}$ for $n \geq 1$. In the language of Feynman diagrams, $G^{(0,0)}$ is a line going from left to right in the direction of increasing time, while $G^{(0,n)}$ can go either way (see [6] for an example of such a Feynman diagram). The leading order in z is thus given by the diagram with the least number of advanced propagators. In this case it would be $G^{(0,1)}$.

4.2 Self-energy

The self-energy operator Σ relates the free and dressed fermion Green's functions via

$$G = G^{(0)} + G^{(0)} \Sigma G \implies \Sigma = [G^{(0)}]^{-1} - [G]^{-1}. \tag{15}$$

We see that the contribution to the self-energy with the lowest order in z is $G^{(0,1)}$.

For the case of interacting fermions of spins $\uparrow, \downarrow$ of equal mass, [7] shows that the self-energy, to lowest order of z, has the form of an integral over some degrees of freedom of the T-matrix multiplied by $G^{(0,1)}$. The result is Eq. (5) of [4]:

$$\Sigma^{(1)}(\mathbf{k}, \tau) = z \int \frac{d^3 P}{(2\pi)^3} e^{\mu\tau} e^{-(\beta-\tau)\epsilon_{\mathbf{P}-\mathbf{k}}} T(\mathbf{P}, \tau). \tag{16}$$

This formula seems to be "out of the blue", but Figure 1(b) of [7] provides a Feynman diagram which better elucidates its origins. Basically, we want to think of the contribution to the self-energy of a particle with

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momentum $\hbar k$ to lowest order of z, due to another particle, is a product of the T-matrix and the advanced Green's function of that other particle (which has momentum $\mathbf{P} - \mathbf{k}$, where $\mathbf{P}$ is the total momentum), summed over all the possible values for $\mathbf{P}$ [5]. So, in the case of two interacting fermions of the equal mass, the self-energy has the form

$$\Sigma_\uparrow^{(1)}(\mathbf{k}, \tau) \approx \int_P d\mathbf{P} \, G_\downarrow(\mathbf{P} - \mathbf{k}, -\tau) T(\mathbf{P}, \tau). \tag{17}$$

How does the T-matrix $T(\mathbf{P}, \tau)$ in the imaginary time domain relate to the T-matrix $T(\omega)$ in the frequency domain? The answer is that $T(\omega)$ is the Laplace transform of $T(\mathbf{P}, \tau)$, or equivalently, $T(\mathbf{P}, \tau)$ is the inverse Laplace transform of $T(\omega)$. In the case of two interacting particles of equal mass, the total mass is $M = 2m$, so that

$$T(\mathbf{P}, \tau) = \int_{C_\gamma} \frac{d\omega}{2\pi i} e^{-\tau\omega} T\left(\omega - \frac{P^2}{2M}\right) \tag{18}$$

$$= e^{-\frac{\tau P^2}{4m}} \int_{C_\gamma} \frac{d\omega}{2\pi i} e^{-\tau\omega} T(\omega), \tag{19}$$

where we have made the change of variables $\omega \to \omega - \mathbf{P}^2/2M$. This is the "Galilean invariance" mentioned in [4], which gives $T(\mathbf{P}, \tau) = e^{-\mathbf{P}^2/4m} T(0, \tau)$. The contour C_γ is called the Bromwich contour. We won't go into the details here, but since $T(\omega)$ is already known, we can compute this integral. The result is [4]

$$T(\mathbf{P}, \tau) = e^{-\frac{\tau P^2}{4m}} \left[\Theta(a^{-1}) Z_m e^{E_b \tau} + \int_0^\infty e^{-\tau x} \rho(x) \, dx\right]. \tag{20}$$

Here $Z_m = \pi/\mu^2 a = 4\pi/m^2 a$ is the molecular residue, and

$$\rho(x) = -\frac{1}{\pi} \text{Im}[T(x + i0^+)] = \frac{4}{\mu^{3/2}} \frac{\sqrt{x}}{x + E_b} \tag{21}$$

is the spectral density of the T-matrix. It is worthwhile to prove the second equality:

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Using our definition for the T-matrix, the derivation here will give a result that is different by a constant multiplicative factor compared to what is given by [4], but we will see why:

$$-\frac{1}{\pi} \text{Im}[T(x + i0^+)] = -\frac{1}{\pi} \lim_{\eta \to 0^+} \text{Im}[T(x + i\eta)] \tag{22}$$

$$= -\frac{1}{\pi} \lim_{\eta \to 0^+} \frac{2\sqrt{2}\pi}{\mu} \sqrt[4]{\mu^2\eta^2 + \mu^2 x^2} \sin\left(\frac{1}{2} \arg(-\mu(x + i\eta))\right) \tag{23}$$

$$\times \left\{ \left[\frac{1}{a} - \sqrt{2}\sqrt[4]{\mu^2\eta^2 + \mu^2 x^2} \cos\left(\frac{1}{2} \arg(-\mu(x + i\eta))\right)\right]^2 \tag{24}$$

$$+ 2\sqrt{\mu^2\eta^2 + \mu^2 x^2} \sin^2\left(\frac{1}{2} \arg(-\mu(x + i\eta))\right) \right\}^{-1} \tag{25}$$

$$= \frac{1}{\pi} \frac{2\sqrt{2}\pi}{\mu} \frac{\sqrt[4]{\mu^2 x^2}}{\frac{1}{a^2} + 2\sqrt{\mu^2 x^2}} \tag{26}$$

$$= \frac{1}{\pi} \frac{2\sqrt{2}\pi \sqrt{x}}{\sqrt{\mu} \left(\frac{1}{a^2} + 2\mu x\right)} \tag{27}$$

$$= \frac{2\sqrt{2}}{\mu^{3/2}} \frac{\sqrt{x}}{x + \frac{1}{2\mu a^2}} \tag{28}$$

$$= \frac{2\sqrt{2}}{\mu^{3/2}} \frac{\sqrt{x}}{x + E_b}. \tag{29}$$

The factor $2\sqrt{2}$ becomes 4 when $\mu = m/2$, so we're in agreement with [4]. In order to go from the first to the second line, we have used the function `ComplexExpand[]` in `Mathematica`.

Leyronas interprets the expression for $T(\mathbf{P}, \tau)$ as follows: the first term comes from the two-body bound state (which exists in the case where $a > 0$), while the second term comes from the two-particle scattering states continuum of energy x. Putting this expression back into the expression for the self-energy, we find to first order in z after Fourier-transforming (via Matsubara frequencies – I don't really understand this) and analytically-continuing:

$$\Sigma^{(1)}(\mathbf{k}, \omega) \approx z F(\mathbf{k}, \omega + \mu + i0^+), \tag{30}$$

where

$$F(\mathbf{k}, E) = \int \frac{d\mathbf{P}}{(2\pi)^3} e^{-\beta \frac{(\mathbf{P} - \mathbf{k})^2}{2m}} \left\{ \int_0^\infty dx \frac{\rho(x)}{E - \left[\frac{P^2}{4m} + x - \frac{(\mathbf{P} - \mathbf{k})^2}{2m}\right]} + \Theta(a^{-1}) \frac{Z_m}{E - \left[\frac{\mathbf{P}^2}{4m} - E_b - \frac{(\mathbf{P} - \mathbf{k})^2}{2m}\right]} \right\}. \tag{31}$$

The case of interacting fermions $(\uparrow, \downarrow)$ of equal masses is then done, at least to first order in z. From the self-energy, we can then compute the retarded Green's function via the Dyson's equation. The spectral function is directly related to the imaginary part of the Green's function. Following [8], one can then extract the rf response from the spectral function depending on the initial and final states.

4.3 Spectral function

The spectral function is computed from the identity

$$A(\mathbf{k}, \omega) = -\frac{1}{\pi} \text{Im}(G_R(\mathbf{k}, \omega)), \tag{32}$$

where the retarded Green's function $G_R(\mathbf{k}, \omega)$ is given by

$$G_R(\mathbf{k}, \omega) = \frac{1}{\omega + \mu + i0^+ - \epsilon_\mathbf{k} - \Sigma_R(\mathbf{k}, \omega)}. \tag{33}$$

In order to proceed with this calculation, we have to know the real and imaginary parts of the retarded self-energy. Due to Eq. (47) and subsequently Eq. (50), this comes down to finding the real and imaginary parts of the T-matrix for $\omega + i0^+$ in the frequency domain, which we fortuitously already found.

The resulting spectral function is given by

$$A(\mathbf{k}, \omega) \propto \frac{-2 \, \mathrm{Im}[\Sigma^{(1)}(\mathbf{k}, \omega + \mu)]}{(\omega + \mu - \epsilon_\mathbf{k} - \mathrm{Re}[\Sigma^{(1)}(\mathbf{k}, \omega + \mu)])^2 + \, \mathrm{Im}[\Sigma^{(1)}(\mathbf{k}, \omega + \mu)]^2} \tag{34}$$

We now need to evaluate the function F:

$$F(\mathbf{k}, E) = \int \frac{d\mathbf{P}}{(2\pi)^3} e^{-\beta \frac{(\mathbf{P}-\mathbf{k})^2}{2m}} T\left(E - \frac{\mathbf{P}^2}{4m} + \frac{(\mathbf{P}-\mathbf{k})^2}{2m}\right), \tag{35}$$

The imaginary part of F can be found by substituting in the expression for the imaginary part of the T-matrix. The real part of F can be found by using the full expression of the T-matrix and taking the real part of the result of the integration. The integration that is to follow is done using in `Python`'s package `scipy.integrate.quad`. The trick to not get weird results is actually to let Python know that the integrand is complex and to avoid hitting the pole on the real axis by shifting the argument E by a small imaginary part $E \to E + i\eta$.

In order to get some qualitative behavior of $F(\mathbf{k}, E)$ and eventually $A(\mathbf{k}, \omega)$, let us assume for simplicity that $\hbar = m = 1$. Moreover, assume that energies are in units of $1/\beta = k_B T = 1$ and that the scattering length is $a = 0.2$, so that the binding energy is $E_b = 1/(2 \times 0.2^2) = 12.5$. For the integral, we integrate over P from 0 to a momentum cutoff of 100.

Python code:

```
(*Code for the integrands*)
from scipy.integrate import quad

def imaginary_integrand(P, En, a_scat, beta):
    s = En + 0.0025j + P**2
    Eb = 1/(2 * a_scat**2)
    return -4*np.pi*(P**2)*np.exp(-beta * P**2) * np.sqrt(s)/ (s + Eb)

def real_integrand(P, En, a_scat, beta):
    s = En + 0.0025j + P**2
    return (P**2)*np.exp(-beta * P**2) / (1/a_scat - np.sqrt(-s))

(*Code for calculating real and imaginary parts*)
points = 300
momentum_cutoff = 20
En = np.linspace(-60,40,points)
a_scat = 0.13
beta = 0.1
z = 0.1
imaginary_results = []*points
real_results = []*points
for i in range(points):
    real_results.append(z*quad(real_integrand, 0, momentum_cutoff,
    args=(En[i], a_scat, beta), epsrel=1e-16, limit=200)[0])
    imaginary_results.append(z*quad(imaginary_integrand, 0,
    momentum_cutoff, args=(En[i], a_scat, beta), epsrel= 1e-16, limit=200)[0])

(*Plot the spectral function*)
A =  -2* np.array(imaginary_results)/( (En - np.array(real_results))**2 + np.array(imaginary_results)**2)
plt.plot(En,A, color = 'red')
plt.ylim([0,0.04])
plt.vlines(x = -1/(2 * a_scat**2), ymin = 0, ymax = np.max(A), color = 'black', linestyles='--')
plt.grid()
plt.xlabel('$\omega + \mu$ (arb)', fontsize = 16)
```

```
plt.ylabel('Spectral function', fontsize = 16)
plt.yticks(fontsize = 14)
plt.xticks(fontsize = 14)
plt.show()
```
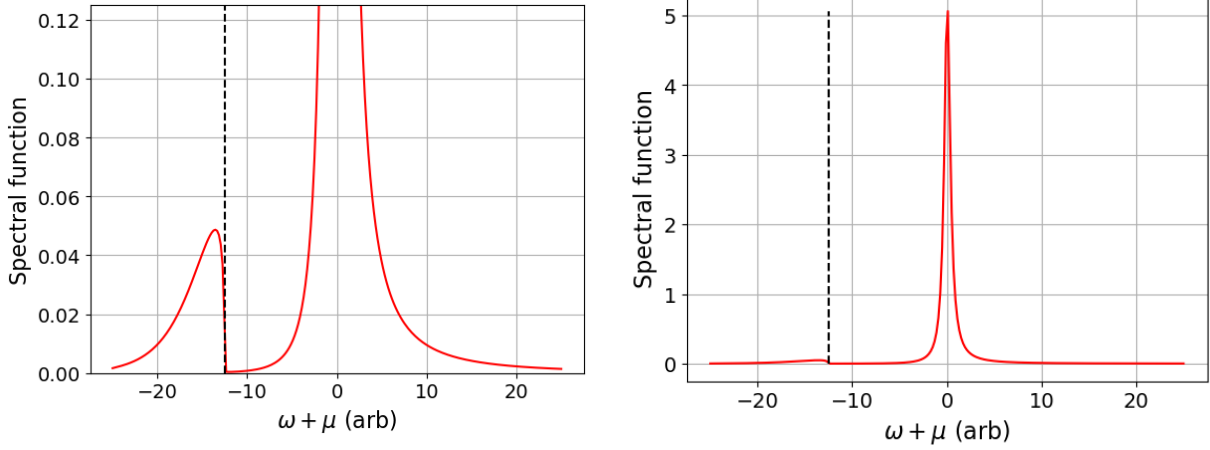

Figure 1: Spectral function $A(0, \omega)$. The dashed black line on the left figure denotes frequency $\omega + \mu = -E_b$, marking the onset for the molecule association lineshape. The feature on the right of the molecular feature is the free-to-free lineshape. It is the noninteracting free-particle spectrum, modified by two-body contact interaction. The figure on the right shows the full spectrum. The single-particle peak has much larger spectral weight compared to the molecular peak.

Figure 2 shows the result of the calculation for the case of $\mathbf{k} = 0$. This plot is similar to Figure 2a of [4]. and Figure 2 of [9]. For more detailed studies of how $A(\mathbf{k}, \omega)$ as a function of $\mathbf{k}$ and the scattering length a, refer to [4], for example. We're more interested in applying the formalism developed here to tackle our problem of a fermion impurity interacting with a boson bath.

5 Self-energy a fermion interacting with a boson of unequal mass

We would like to treat a slightly different scenario, with two main differences: the interacting particles have different quantum statistics and unequal mass. The self-energy for the fermion is now different: it is now the convolution of the T-matrix with the boson Green's function [10], [11]. The self-energy for the fermion looks like

$$\Sigma_F \sim \sum T \times G_B, \tag{36}$$

where T denotes the two-body T-matrix and G_B is the bosonic Green's function. To make the formalism consistent with what was done in the previous section, we should also find a virial expansion for this and obtain the self-energy to lowest order of the fugacity z.

5.1 Virial expansion of the Green's function

We now attempt to obtain the free boson Green's function in the virial expansion. First, we expand the Bose-Einstein distribution in powers of the fugacity $z_B = e^{\beta \mu_B}$:

$$n_B(\mathbf{k}, \mu) = \frac{1}{e^{\beta(\epsilon_\mathbf{k} - \mu_B)} - 1} = \sum_{n \geq 1} z^n e^{-n\beta\epsilon_\mathbf{k}}. \tag{37}$$

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Next, we find the free boson Green's function from the steps outlined in the beginning of the previous section:

$$G_B^{(0)}(\mathbf{k}, \tau) = -e^{-(\epsilon_{\mathbf{k}} - \mu_B)\tau} \{[1 + n_B(\epsilon_{\mathbf{k}} - \mu_B)]\Theta(\tau) + n_B(\epsilon_{\mathbf{k}} - \mu_B)\Theta(-\tau)\} \tag{38}$$

$$= -e^{-(\epsilon_{\mathbf{k}} - \mu_B)\tau}[n_B(\epsilon_{\mathbf{k}} - \mu_B) + \Theta(\tau)]. \tag{39}$$

In powers of the fugacity μ_B, we have

$$G_B^{(0)}(\mathbf{k}, \tau) = e^{\mu_B \tau} \sum_{n \geq 0} G_B^{(0,n)}(\mathbf{k}, \tau) z^n \tag{40}$$

where

$$G_B^{(0,0)}(\mathbf{k}, \tau) = -\Theta(\tau)e^{-\epsilon_{\mathbf{k}}\tau} \tag{41}$$

$$G_B^{(0,n)}(\mathbf{k}, \tau) = e^{-\epsilon_{\mathbf{k}}\tau}e^{-n\beta\epsilon_{\mathbf{k}}}, \quad n \geq 1. \tag{42}$$

5.2   Self-energy

The two-body T-matrix describing scattering between a fermion of mass m_F and a boson of mass m_B was already found. It is Eq. (6). Following the formalism by [4], the fermion self-energy to is gotten (approximately) from multiplying the T-matrix with the free bosonic Green's function, then integrating over all total momentum $\mathbf{P}$:

$$\Sigma_F(\mathbf{k}, \tau) \approx z e^{\mu_B \tau} \int \frac{d\mathbf{P}}{(2\pi)^3} G_B^{(0,1)}(\mathbf{P} - \mathbf{k}, -\tau) T(\mathbf{P}, \tau) \tag{43}$$

$$= z e^{\mu_B \tau} \int \frac{d\mathbf{P}}{(2\pi)^3} e^{-(\beta - \tau)\epsilon_{\mathbf{P}-\mathbf{k}}^B} T(\mathbf{P}, \tau), \tag{44}$$

The Feynman diagram for the fermionic self-energy for the case of a fermion interacting with a boson can be found in [10] and [11], for instance. Just to be explicit here: the momentum of the fermion is $\mathbf{k}$, and the momentum of the boson is $\mathbf{P} - \mathbf{k}$, with $\mathbf{P}$ being the total momentum. The expression for $T(\mathbf{P}, \tau)$ is found in the previous section:

$$T(\mathbf{P}, \tau) = e^{-\frac{\tau P^2}{2M}} \left[\Theta(a^{-1})Z_m e^{E_b \tau} + \int_0^\infty e^{-\tau x} \rho(x)\, dx\right], \tag{45}$$

but now the total mass is $M = m_{\mathrm{Na}} + m_{\mathrm{K}}$ and the molecular residue $Z_m = \pi/\mu^2 a$ is in terms of the reduced mass μ. The function $\rho(x)$ is also already found from the previous section:

$$\rho(x) = -\frac{1}{\pi} \mathrm{Im}[T(x + i0^+)] = \frac{2\sqrt{2}}{\mu^{3/2}} \frac{\sqrt{x}}{x + E_b}. \tag{46}$$

Converting $\Sigma_F(\mathbf{k}, \tau)$ into its frequency-domain counter part (via Fourier-transforming over the Matsubara frequencies???) and analytically continuing, we find

$$\Sigma_F(\mathbf{k}, \omega) = z F(\mathbf{k}, \omega + \mu_B + i0^+), \tag{47}$$

where

$$F(\mathbf{k}, E) = \int \frac{d\mathbf{P}}{(2\pi)^3} e^{-\beta \frac{(\mathbf{P}-\mathbf{k})^2}{2m_{\mathrm{Na}}}} \left\{\int_0^\infty dx \frac{\rho(x)}{E - \left[\frac{\mathbf{P}^2}{2M} + x - \frac{(\mathbf{P}-\mathbf{k})^2}{2m_{\mathrm{Na}}}\right]} + \Theta(a^{-1})\frac{Z_m}{E - \left[\frac{\mathbf{P}^2}{2M} - E_b - \frac{(\mathbf{P}-\mathbf{k})^2}{2m_{\mathrm{Na}}}\right]}\right\}. \tag{48}$$

I once again don't know how this Fourier transform is done exactly. I would expect a Lorentzian because the object being transformed is an exponential in the imaginary time variable, but apparently that's not the

case? In any case, Leyronas claims that this function $F(\mathbf{k}, E)$ can be further simplified by observing that the T-matrix can be put into the form

$$T(\omega) = \Theta(a^{-1})\frac{Z_m}{\omega + E_b} + \int_0^\infty dx \frac{\rho(x)}{\omega - x},$$

(49)

which we can verify directly by plugging it into Mathematica (or doing the integral by hand). From here, [4] is able to simplify the expression for the function F to:

$$F(\mathbf{k}, E) = \int \frac{d\mathbf{P}}{(2\pi)^3} e^{-\beta \frac{(\mathbf{P}-\mathbf{k})^2}{2m_{\text{Na}}}} T\left(E - \frac{\mathbf{P}^2}{2M} + \frac{(\mathbf{P}-\mathbf{k})^2}{2m_{\text{Na}}}\right).$$

(50)

5.3 Spectral function

The spectral function is computed from the identity

$$A(\mathbf{k}, \omega) = -\frac{1}{\pi}\text{Im}(G_R(\mathbf{k}, \omega)),$$

(51)

where the retarded Green's function $G_R(\mathbf{k}, \omega)$ is given by

$$G_R(\mathbf{k}, \omega) = \frac{1}{\omega + \mu + i0^+ - \epsilon_\mathbf{k} - \Sigma_R(\mathbf{k}, \omega)}.$$

(52)

In order to proceed with this calculation, we have to know the real and imaginary parts of the retarded self-energy. Due to Eq. (47) and subsequently Eq. (50), this comes down to finding the real and imaginary parts of the T-matrix for $\omega + i0^+$ in the frequency domain, which we fortuitously already found.

The resulting spectral function is given by

$$A(\mathbf{k}, \omega) \propto \frac{-2 \, \text{Im}[\Sigma^{(1)}(\mathbf{k}, \omega + \mu)]}{(\omega + \mu - \epsilon_\mathbf{k} - \text{Re}[\Sigma^{(1)}(\mathbf{k}, \omega + \mu)])^2 + \text{Im}[\Sigma^{(1)}(\mathbf{k}, \omega + \mu)]^2}$$

(53)

We now need to evaluate the function F:

$$F(\mathbf{k}, E) = \int \frac{d\mathbf{P}}{(2\pi)^3} e^{-\beta \frac{(\mathbf{P}-\mathbf{k})^2}{2m_{\text{Na}}}} T\left(E - \frac{\mathbf{P}^2}{2M} + \frac{(\mathbf{P}-\mathbf{k})^2}{2m_{\text{na}}}\right),$$

(54)

The imaginary part of F can be found by substituting in the expression for the imaginary part of the T-matrix. The real part of F can be found by using the full expression of the T-matrix and taking the real part of the result of the integration. The integration that is to follow is done using in `Python`'s package `scipy.integrate.quad`. The trick to not get weird results is actually to let Python know that the integrand is complex and to avoid hitting the pole on the real axis by shifting the argument E by a small imaginary part $E \rightarrow E + i\eta$.

We now want to evaluate the spectral function using physical values for the variables. IN PROGRESS. See Figure 2. I think I got sensible results using "real" lab values such as temperature and scattering length, but I need to check...

6 $O(z^2)$ contributions to $\Sigma(\mathbf{k}, \omega)$ and effects on $A(\mathbf{k}, \omega)$?

7 RF response

Here we follow the formalism in e.g. [8] to obtain the rf response from the spectral function. In experiments, the rf field transfers atoms from an occupied spin state into an empty final state. From the previous sections,
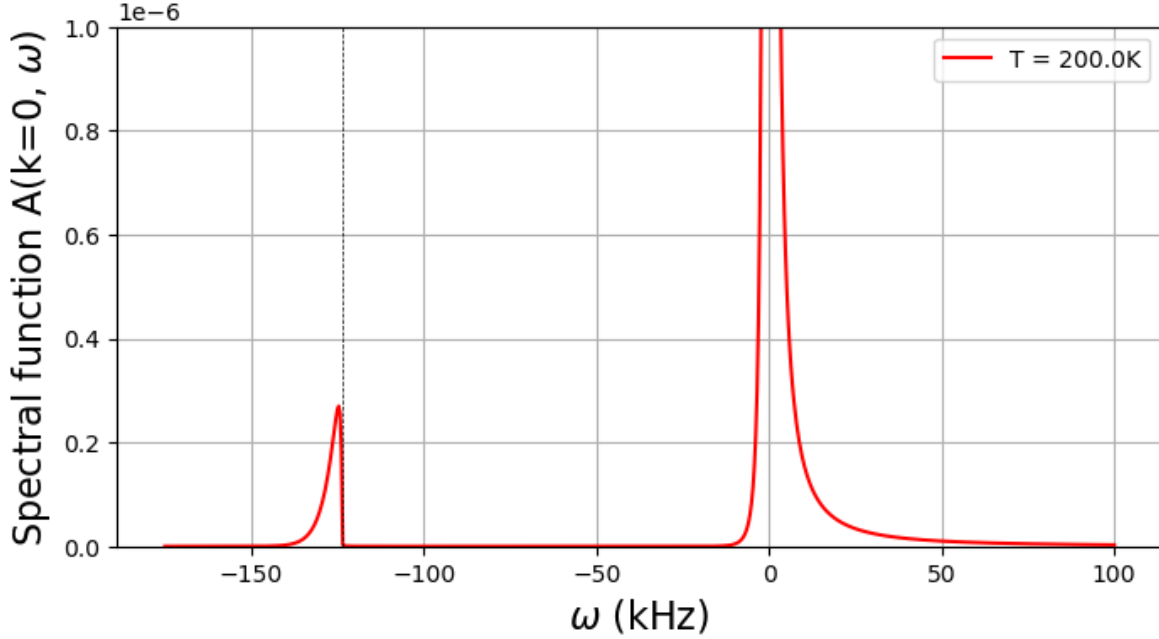
Figure 2: Spectral function $A(0, \omega)$ for a K atom interacting with an Na atom at $T = 500$ nK and scattering length $a = 1000\,a_0$, giving $E_b \approx 125$ kHz for the two-body bound-state. Need to check some details, but the numerics seem to work.

we have found the spectral functions for both. Let's assume that the rf field flips the spin $\uparrow$ to $\downarrow$. Within linear response, the rate of transitions out of the initial state induced by the rf field with frequency ω and wave vector $\mathbf{q}$ is given by the convolution

$$I(\mathbf{q}, \omega) \propto \int \frac{d^3k}{(2\pi)^3} \int d\epsilon \, A_\downarrow(\mathbf{k} + \mathbf{q}, \epsilon + \hbar\omega) A_\uparrow(\mathbf{k}, \epsilon) e^{-\beta\epsilon}. \tag{55}$$

Here, unwritten is a prefactor that depends on the coupling strength to the rf field. Since the momentum transfer due to the rf field is very small, we can simply set $\mathbf{q} = 0$. With this simplification, the rf spectrum is

$$I(\omega) \propto \int \frac{d^3k}{(2\pi)^3} \int d\epsilon \, A_\downarrow(\mathbf{k}, \epsilon + \hbar\omega) A_\uparrow(\mathbf{k}, \epsilon) \tag{56}$$

If the final state is non-interacting, its spectral function is a delta-function:

$$A_{\downarrow,\text{non-interacting}}(\mathbf{k}, \epsilon) \propto \delta(\epsilon - \epsilon_\mathbf{k}). \tag{57}$$

This gives the rf response function for this case:

$$I_{\downarrow\,\text{non-interacting}}(\omega) \propto \hbar \int \frac{d^3k}{(2\pi)^3} A_\uparrow(\mathbf{k}, \epsilon_\mathbf{k} - \hbar\omega). \tag{58}$$

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