Calculation of the thermal RF spectrum

We are interested in the RF spectrum on an impurity, say potassium, embedded in a thermal (Boltzmann) gas say of sodium.

The initial and final relative wavefunctions of a given pair of Na and K can be written as

$$\psi_{i,k}(r) = \langle r|k\rangle_i = \sqrt{\frac{2\mu}{\pi\hbar^2 k}}\sin(kr+\delta_i)$$

$$\psi_{f,k}(r) = \langle r|k\rangle_f = \sqrt{\frac{2\mu}{\pi\hbar^2 k}}\sin(kr+\delta_f)$$

These wavefunctions are energy-normalized, that is

$_i\langle k|p\rangle_i = \int \mathrm{dr}\,\psi_{i,k}(r)^*\psi_{i,p}(r) = \delta(E_k - E_p)$

with $E_k = \frac{\hbar^2 k^2}{2\mu}$.

We can verify this normalization using an artificial large box with radius R. The allowed k -states that fit in the box are quantized, with $kR = \pi n$ with $n = 1, 2, \ldots$ (in principle, it is rather $kR + \delta = \pi n$, but for fixed phase shift and large R, the difference to this vanishes).

For a very large box, the integral $\int \mathrm{d}r\ \sin(kr+\delta)\sin(pr+\delta)$ over the product of the two sines will vanish (on the scale of R itself) unless $k = p$, in which case we get $\frac{R}{2}$. So say the wavefunction is $\psi_k(r) = \mathcal{N}_k \sin(kr+\delta)$.

We have

$$1 = \int \mathrm{d}E_k\,\delta(E_p - E_k) = \frac{\hbar^2}{\mu}\int \mathrm{d}k\,k\,\langle k|p\rangle$$

The integral is now really a sum as $\int \mathrm{d}k = \frac{\pi}{R}\int \mathrm{d}n = \frac{\pi}{R}\sum_n$.

and we said only one state will give a non-zero result, the one with $k = p$. So we have

$$1 = \frac{\hbar^2 \pi p}{\mu R}{\mathcal{N}_p}^2\frac{R}{2} = \frac{\hbar^2\pi p}{2\mu}{\mathcal{N}_p}^2$$

So

$$\mathcal{N}_k = \sqrt{\frac{2\mu}{\pi\hbar^2 k}}$$

Now the RF spectrum in the limit of long, weak pulses is given by Fermi's Golden Rule:

$$I_{i\to f}(\omega) = \frac{2\pi}{\hbar}\sum_f |\langle i|V_{\mathrm{RF}}|f\rangle|^2\,\delta(E_i - E_f)$$

Here, $|i\rangle$ is an initial momentum state $|k\rangle_i$ (in the presence of an RF photon), $|f\rangle$ describes a state in the final state with momentum p (in the absence of an RF photon), $|p\rangle_f$, and $E_i - E_f = \hbar\omega + E_k + \Delta_k - E_p - \Delta_p$ in this process where an RF photon is absorbed. V_{RF} is the RF operator, which flips the spin, and Δ_k are the mean-field energy shifts of the atoms propagating in in the medium with initial and final scattering length, respectively.

So the RF photon, while it does not transfer momentum to the atoms, can connect states that differ in relative momentum.

Now superficially, it would look like this is a δ-function, but it is of course crucial that the states in the final state have a different phase shift from those in the initial state.

Let's calculate

$${}_i\langle k|p\rangle_f = \mathcal{N}_k\mathcal{N}_p\int_0^R \sin(kr+\delta_i)\sin(pr+\delta_f)$$

$$= \frac{1}{2}\mathcal{N}_k\mathcal{N}_p\int_0^R (\cos((k-p)r+\delta_i-\delta_f) - \cos((k+p)r+\delta_i+\delta_f))$$

$$= \frac{1}{2}\mathcal{N}_k\mathcal{N}_p\left(\frac{1}{k-p}\sin((k-p)r+\delta_i-\delta_f) - \frac{1}{k+p}\sin((k+p)r+\delta_i+\delta_f)\right)\Bigg|_0^R$$

Now thanks to the boundary conditions that $kR+\delta_i = n\pi$ and $pR+\delta_f = m\pi$ with n, m integer, we are left with

$$= \frac{1}{2}\mathcal{N}_k\mathcal{N}_p\left(\frac{1}{k+p}\sin(\delta_i+\delta_f) - \frac{1}{k-p}\sin(\delta_i-\delta_f)\right)$$

$$= \frac{1}{2}\mathcal{N}_k\mathcal{N}_p\frac{1}{k^2-p^2}\left((k-p)\sin(\delta_i+\delta_f) - (k+p)\sin(\delta_i-\delta_f)\right)$$

$$= \frac{1}{2}\mathcal{N}_k\mathcal{N}_p\frac{1}{k^2-p^2}\left(\sin\delta_i\cos\delta_f(k-p-k-p) + \sin\delta_f\cos\delta_i(k-p+k+p)\right)$$

$$= \mathcal{N}_k\mathcal{N}_p\frac{1}{k^2-p^2}\left(k\sin\delta_f\cos\delta_i - p\sin\delta_i\cos\delta_f\right)$$

$$= \mathcal{N}_k\mathcal{N}_p\cos\delta_i\cos\delta_f\frac{1}{k^2-p^2}\left(k\tan\delta_f - p\tan\delta_i\right)$$

$$= \mathcal{N}_k\mathcal{N}_p\cos\delta_i\cos\delta_f\frac{1}{k^2-p^2}\left(k(-pa_f) - p(-ka_i)\right)$$

$$= \mathcal{N}_k\mathcal{N}_p\cos\delta_i\cos\delta_f\frac{kp}{k^2-p^2}\left(a_i - a_f\right)$$

$$= \frac{2\mu}{\pi\hbar^2}\cos\delta_i\cos\delta_f\frac{\sqrt{kp}}{k^2-p^2}\left(a_i - a_f\right)$$

$$= \frac{1}{\pi}\cos\delta_i\cos\delta_f\frac{\sqrt{kp}}{E_k-E_p}\left(a_i - a_f\right)$$

Note also $\cos^2\delta_i = \frac{1}{1+k^2a_i^2}$ etc.

It's interesting to check whether we find, in the limit of $a_f = a_i$, that we retrieve again the delta-function, since ${}_i\langle k|p\rangle_i = \delta(E_k - E_p) = \frac{2\mu}{\hbar^2}\delta(k^2-p^2) = \frac{\mu}{\hbar^2 k}\delta(k-p)$

When $E_k \neq E_p$, of course we get zero overlap thanks to the $(a_i - a_f)$ term. If then $E_k \to E_p$, we get a large contribution from the term $\frac{1}{2}\frac{1}{k-p}\sin(\delta_i - \delta_f)$, where we replace $k - p = (\delta_f - \delta_i)/R$ and retrieve $R/2$, the correct magnitude of the "delta"-function at $E_k = E_p$ (the integral of $\sin^2(kr + \delta)$).

Maybe it's also interesting to tease out whether the integral over this expression, integrating over p, exists and makes sense. Mathematica knows

$$\mathcal{P}\int \mathrm{d}p \frac{\sqrt{p}}{k^2 - p^2}\frac{1}{\sqrt{1 + p^2 a_f^2}} = \frac{\pi}{2\sqrt{k}\sqrt{1 + k^2 a_f^2}} - \frac{2}{\sqrt{\pi}}\sqrt{a_f}\left(\Gamma\left(\frac{3}{4}\right)\right)^2 \left({}_2F_1\left(-\frac{1}{4}, 1; \frac{1}{4}\right.\right.$$

where $\mathcal{P}$ means take the principal value, and ${}_2F_1(a, b; c; x)$ is a hypergeometric function.

Now let's plug it into the formula for the RF spectrum:

$$I_{i\to f}(\omega) = \frac{2\pi}{\hbar}\sum_f |\langle i|V_{\mathrm{RF}}|f\rangle|^2\, \delta(E_i - E_f)$$

$$= \frac{2\pi}{\hbar}V_{\mathrm{RF}}^2 \sum_p \frac{1}{\pi^2}\frac{1}{1 + k^2 a_i^2}\frac{1}{1 + p^2 a_f^2}\frac{kp}{(E_k - E_p)^2}\,(a_i - a_f)^2\, \delta(E_p - E_k - \hbar\omega)$$

$$= \frac{2}{\pi\hbar}V_{\mathrm{RF}}^2 \frac{\sqrt{E_k}}{1 + E_k/E_{a_i}}\frac{1}{1 + (\hbar\omega + E_k)/E_{a_f}}\frac{\sqrt{\hbar\omega + E_k}}{\hbar^2\omega^2}\frac{2\mu}{\hbar^2}\,(a_i - a_f)^2$$

Assume $a_f = 0$:

$$= \frac{2}{\pi\hbar}V_{\mathrm{RF}}^2 \frac{\sqrt{E_k}}{1 + E_k/E_{a_i}}\frac{\sqrt{\hbar\omega + E_k}}{\hbar^2\omega^2}E_{a_i}$$

Now have to sum over the occupation probability of initial states of momentum k: $\sum_k e^{-\beta E_k}$ (can include proper normalization given by phase space density etc...)

If instead $a_i = 0$:

- $$= \frac{2}{\pi\hbar} V_{\mathrm{RF}}^2 \sqrt{E_k} \frac{1}{1 + (\hbar\omega + E_k)/E_{a_f}} \frac{\sqrt{\hbar\omega + E_k}}{\hbar^2\omega^2} \frac{2\mu}{\hbar^2} a_f^2$$

Now have to sum that as above: $\sum_k e^{-\beta E_k}$. The outcome will be different due to the extra frequency dependence in the case of final state interactions, which roll off the spectrum as $\omega^{-5/2}$ instead of $\omega^{-3/2}$.