I. DENSITY OF STATES: TO BE, OR NOT TO BE

To calculate the rf transition rate to the final scattering states, in our essentially 1d problem, it turns out one does not need to worry about the density of states. Michael Stone shows in his book, *Mathematics for Physics*, from Page 123 to Page 130 that given one normalizes the scattering states outside the potential rage as

$$v_k(r) = \sin[kr + \delta(k)], \tag{1}$$

the completeness of $v_k(r)$ is given by the expression

$$\frac{2}{\pi}\int_0^\infty dk v_k(r) v_k(r') = \delta(r - r') = \langle r|r'\rangle \tag{2}$$

$$\frac{2}{\pi}\int_0^\infty dk |v_k\rangle\langle v_k| = I, \tag{3}$$

(one can add on bound states if there're any).

The rf transition rate is the same as the decay rate of the initial state $|i(r)\rangle = u_i(r)|12\rangle$, which is an eigenstate of

$$H_0 = \left[-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} + V_{12}(r) + E_{z,12}\right]|12\rangle\langle 12| + \left[-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} + V_{13}(r) + E_{z,13}\right]|13\rangle\langle 13|, \tag{4}$$

under the perturbation Hamiltonian (after the rotating wave approximation)

$$H_{\rm rf} = M e^{-i\omega t}|13\rangle\langle 12| + M^* e^{i\omega t}|12\rangle\langle 13|. \tag{5}$$

After transforming to the rotating frame, we have

$$\tilde{H}_0 = \left[-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} + V_{12}(r) + E_{z,12}\right]|12\rangle\langle 12| + \left[-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} + V_{13}(r) + E_{z,13} - \omega\right]|13\rangle\langle 13|, \tag{6}$$

$$\tilde{H}_{\rm rf} = M|13\rangle\langle 12| + M^*|12\rangle\langle 13|. \tag{7}$$

Note

$$\tilde{H}_0 u_i(r)|12\rangle = (E_i + E_{z,12}) u_i(r)|12\rangle \tag{8}$$

$$\tilde{H}_0 v_k(r)|13\rangle = (\hbar^2 k^2/2\mu + E_{z,13} - \omega) v_k(r)|13\rangle. \tag{9}$$

The decay rate of the initial state to second order of $M_{\rm rf}$ is given by

$$\Gamma = 2\mathrm{Im}\left[\langle i|\tilde{H}_{\rm rf}\frac{1}{z - \tilde{H}_0}\tilde{H}_{\rm rf}|i\rangle|_{z=E_i+E_{z,12}-i0}\right]. \tag{10}$$

We have

$$\langle i|\tilde{H}_{\rm rf}\frac{1}{z - \tilde{H}_0}\tilde{H}_{\rm rf}|i\rangle = \langle i|M^*|12\rangle\langle 13|\frac{1}{z - \tilde{H}_0}M|13\rangle\langle 12|i\rangle \tag{11}$$

$$= |M|^2\langle i|12\rangle\langle 13|\frac{1}{z - \tilde{H}_0}\left(\frac{2}{\pi}\int_0^\infty dk|v_k\rangle\langle v_k| \otimes |13\rangle\langle 13|\right)|13\rangle\langle 12|i\rangle \tag{12}$$

$$= |M|^2\frac{2}{\pi}\int_0^\infty dk\frac{\langle u_i|v_k\rangle\langle v_k|u_i\rangle}{z - (\hbar^2k^2/2\mu + E_{z,13} - \omega)}. \tag{13}$$

Thus

$$\Gamma = |M|^2\frac{2}{\pi}\int_0^\infty \frac{dk^2}{k}|\langle u_i|v_k\rangle|^2\pi\delta[E_i + E_{z,12} - (\hbar^2k^2/2\mu + E_{z,13} - \omega)] \tag{14}$$

$$= |M|^2\frac{2}{\pi}\pi\frac{2\mu}{\hbar^2}\frac{|\langle u_i|v_k\rangle|^2}{k}|_{\hbar k=\sqrt{2\mu(E_i+E_{z,12}-E_{z,13}+\omega)}}. \tag{15}$$

A. Multi-channels?

It's straight forward to show that Eq. (14) holds when $|v_k\rangle$ is a multi-channel vector. For simplicity, let us assume $|v_k\rangle$ involves a single closed channel $|c\rangle$ and an open one $|o\rangle$. Our first step is from the Fermi golden rule

$$\Gamma = 2\pi \sum_n |\langle \chi_n|\tilde{H}_{\rm rf}|u_i\rangle|^2 \delta(\tilde{E}_i + \omega - \tilde{E}_n) \tag{16}$$

with the final states

$$\langle r|\chi_n\rangle = \chi_{n,o}(r)|o\rangle + \chi_{n,c}(r)|c\rangle \tag{17}$$

normalized in a sphere of radius R as Stone did. The states satisfy

$$\left\{-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} + \begin{bmatrix} V_{oo}(r) & V_{oc}(r) \\ V_{co}(r) & V_{cc}(r)\end{bmatrix}\right\}\begin{bmatrix}\chi_{n,o}(r)\\ \chi_{n,c}(r)\end{bmatrix} = \tilde{E}_n \begin{bmatrix}\chi_{n,o}(r)\\ \chi_{n,c}(r)\end{bmatrix} \tag{18}$$

and the boundary conditions $\chi_{n,o}(0) = \chi_{n,c}(0) = 0$ and $\chi_{n,o}(R) = \chi_{n,c}(R) = 0$. Outside the range of the potentials

$$-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}\chi_{n,o}(r) = [\tilde{E}_n - V_{oo}(\infty)]\chi_{n,o}(r), \tag{19}$$

and correspondingly

$$\chi_{n,o}(r) = A_n \sin(k_n r + \delta(k_n)) \tag{20}$$

$$k_n R + \delta(k_n) = n\pi \tag{21}$$

$$\tilde{E}_n = V_{oo}(\infty) + \hbar^2 k_n^2/2\mu. \tag{22}$$

In the closed channel

$$-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}\chi_{n,c}(r) = [V_{oo}(\infty) + \hbar^2 k_n^2/2\mu - V_{cc}(\infty)]\chi_{n,o}(r), \tag{23}$$

since we consider the energy scale $\hbar^2 k_n^2/2\mu < V_{cc}(\infty) - V_{oo}(\infty)$, $\chi_{n,c}(r)$ shall exponentially decays with r. We choose R so big (eventually we will take $R \to \infty$) that $\chi_{n,c}(R) = 0$ is automatically satisfied ($10^{-10} = 0$).

As Stone did, to convert the sum over n in Eq. (16) to an integral, by Eq. (21), we have

$$\sum_{n=0}^{\infty} = \sum_{n=0}^{\infty} \Delta n \to \int_0^\infty dk \frac{\Delta n}{dk} = \int_0^\infty dk \frac{1}{\pi}\left(R + \frac{d\delta(k)}{dk}\right). \tag{24}$$

We also introduce the scattering states satisfying Eq. (18) (first without applying the boundary condition at $r = R$)

$$\langle r|v_k\rangle = v_{k,o}(r)|o\rangle + v_{k,c}(r)|c\rangle \tag{25}$$

whose normalization is by setting $v_{k,o}(r) = \sin(kr + \delta(k))$ outside the potential range. We can calculate the norm of $\langle r|v_k\rangle$ in the radius domain $[0, R]$ as

$$\int_0^R dr\,(\langle v_{k'}|r\rangle H\langle r|v_k\rangle - \langle v_k|r\rangle H\langle r|v_{k'}\rangle) = [\hbar^2(k^2 - k'^2)/2\mu]\int_0^R dr\langle v_{k'}|r\rangle\langle r|v_k\rangle \tag{26}$$

$$\int_0^R dr\left(\langle v_{k'}|r\rangle(-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2})\langle r|v_k\rangle - \langle v_k|r\rangle(-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2})\langle r|v_{k'}\rangle\right) = [\hbar^2(k^2 - k'^2)/2\mu]\int_0^R dr\langle v_{k'}|r\rangle\langle r|v_k\rangle \tag{27}$$

$$[v_{k,o}(r)dv_{k',o}(r)/dr - v_{k',o}(r)dv_{k,o}(r)/dr]_{r=R} = (k^2 - k'^2)\int_0^R dr\langle v_{k'}|r\rangle\langle r|v_k\rangle \tag{28}$$

$$k'\sin(kR + \delta_k)\cos(k'R + \delta_{k'}) - k\sin(k'R + \delta_{k'})\cos(kR + \delta_k) = (k^2 - k'^2)\int_0^R dr\langle v_{k'}|r\rangle\langle r|v_k\rangle \tag{29}$$

Differentiating k and taking $k = k'$ of the above line and applying the condition $kR + \delta(k) = n\pi$, we have

$$\int_0^R dr\langle v_{k'}|r\rangle\langle r|v_k\rangle = \frac{1}{2}\left(R + \frac{d\delta(k)}{dk}\right). \tag{30}$$

In the end, in the limit $R \to \infty$

$$\Gamma = 2\pi \sum_n |\langle \chi_n | \tilde{H}_{\rm rf} | u_i \rangle|^2 \delta(\tilde{E}_i + \omega - \tilde{E}_n) \tag{31}$$

$$\to 2\pi \int_0^\infty dk \frac{1}{\pi} \left(R + \frac{d\delta(k)}{dk} \right) 2 \left(R + \frac{d\delta(k)}{dk} \right)^{-1} |\langle v_k | \tilde{H}_{\rm rf} | u_i \rangle|^2 \delta(\tilde{E}_i + \omega - V_{oo}(\infty) - \hbar^2 k^2/2\mu) \tag{32}$$

$$= 2\pi \frac{2}{\pi} \int_0^\infty dk |\langle v_k | \tilde{H}_{\rm rf} | u_i \rangle|^2 \delta(\tilde{E}_i + \omega - V_{oo}(\infty) - \hbar^2 k^2/2\mu) \tag{33}$$

II. FROM HARMONIC TO SCATTERING STATES

Paul's coupled channel calculation is carried out in a 3d isotropic harmonic trap as

$$\left[-\frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} + V(r) + \frac{1}{2}\mu\omega_0^2 r^2 \right] u(r) = E u(r), \tag{34}$$

with $u(r) = r\psi(r)$. In the coupled channel formulation, $V(r)$ is a matrix and $u(r)$ is a vector in terms of the basis of relevant channels. The boundary condition is $u(r = 0) = 0$ and $\lim_{r\to\infty} u(r) \to 0$. Of course the harmonic length $a_h \equiv \sqrt{\hbar/\mu\omega_0}$ is chosen to be much larger than the van de Waals length r_{vdW} [which we assume to be about the range r_0 of $V(r)$].

For simplicity, let's first consider the single channel case. If $u(r)$ is a highly excited state, namely having a lot of nodes and $E/\hbar\omega_0 \gg 1$, there exists a spatial range $r_{vdW} \ll r \ll a_h$ where $u(r)$ can be well approximated by the WKB approximation, i.e.,

$$u_E(r) \approx \frac{A_E}{\sqrt{|p(r)|}} \sin\left[\frac{1}{\hbar} \int_{r_0}^r p(r')dr' + \theta_E \right], \tag{35}$$

$$p(r) \equiv \frac{\hbar}{a_h} \sqrt{2E/\hbar\omega_0 - r^2/a_h^2}. \tag{36}$$

The phase θ_E accumulates the contribution where $V(r) \neq 0$, and the normalization factor A_E is determined by matching the full form of the normalized $u_E(r)$. When we flatten the trap, i.e., $\omega_0 \to 0$, for fixed E and sticking in the range $r_{vdW} \ll r \ll a_h$

$$u_E(r) \to \tilde{A}_E \sin\left\{ \frac{1}{\hbar}(2\mu E)^{1/2} r + \left[\theta_E - \frac{1}{\hbar}(2\mu E)^{1/2} r_0 \right] \right\}, \tag{37}$$

as expected matching spatial form of the scattering wave-function $v_k(r)$ apart from the normalization factor $\tilde{A}_E = \frac{A_E}{(2\mu E)^{1/4}}$. Thus each normalized $u_E(r)$ calculated by Paul corresponds to the scattering wave-function $v_k(r)$ with $E = \hbar^2 k^2/2\mu$, which is normalized in the range $r > r_0$ as

$$v_k(r) = \sin[kr + \delta(k)]. \tag{38}$$

Thus, the inter product in Eq. (15) shall be replaced as

$$\langle u_i | v_k \rangle \to \langle u_i | u_E \rangle / \tilde{A}_E |_{E = \hbar^2 k^2/2\mu}. \tag{39}$$

Note $\tilde{A}_E$ has to be determined from $u_E(r)$ in the range $r_0 \ll r \ll a_h$