Multimode Renormalized Effective Theory for Cavity Rydberg Polaritons

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Part I
New Version

THINGS TO TRY IN THE FUTURE:

- can dominant balance enable you to provide some justification for this result? or learn something about it in vairous limits?

I. DERIVING THE FORM OF THE TWO-EXCITATION COLLECTIVE MODES

To ensure that I understand everything that I am doing here (and everything that I did previously), I'm going to re-do the key portions of this work.

In second order of non-Hermitian perturbation theory (see NHPT_unmodified.lyx), we write the state in the two-photon manifold as:

$$|\psi_2\rangle = \left(\sum_{n}^{N_{cav}} B_{cc}^{nn}\frac{\left(a_n^\dagger\right)^2}{\sqrt{2}} + \sum_{p>n}^{N_{cav}} B_{cc}^{np} a_n^\dagger a_p^\dagger + \sum_{n}^{N_{cav}}\sum_{j}^{N_{at}} B_{ce}^{nj} a_n^\dagger \sigma_j^{eg} + B_{cr}^{nj} a_n^\dagger \sigma_j^{rg} + \sum_{j\neq k}^{N_{at}} B_{er}^{jk}\sigma_j^{eg}\sigma_k^{rg} + \sum_{j>k}^{N_{at}} B_{rr}^{jk}\sigma_j^{rg}\sigma_k^{rg} + B_{ee}^{jk}\sigma_j^{eg}\sigma_k^{eg}\right)|0\rangle$$

The linear equations describing the rydberg-rydberg terms given the rydberg-excited terms are:

$$(2\delta_2 + U(|x_j - x_k|))B_{rr}^{jk} + \Omega_j^b B_{er}^{jk} + \Omega_k^b B_{er}^{kj} = 0$$

where $j > k$ are indices labeling unique atoms.

We will make the assumption that the relevant collective states outside of the rydberg-rydberg manifold are unmodified by the interactions. Indeed, until one considers the two-Rydberg manifold, the system is linear and collective modes can be calculated exactly. Here, the Hamiltonian separates exactly into Hamiltonians for each cavity mode along with its collective P-state excitation and collective Rydberg state excitation. For the k'th cavity mode, the collective p-state is created by the operator,

$$p_m^\dagger \equiv \frac{1}{G_m}\sum_{k}^{N_{at}} g_{km}\sigma_k^{eg},$$

and similarly the non-renormalized collective Rydberg-state is created by the operator,

$$r_m^\dagger \equiv \frac{1}{G_m}\sum_{k}^{N_{at}} g_{km}\sigma_k^{rg},$$

where the total squared atom-photon interaction in each mode is given by,

$$G_m^2 \equiv \sum_{k}^{N_{at}} |g_{km}|^2 .$$

Therefore, the rydberg-excited collective states can be written:

$$|R_\alpha E_\beta\rangle = r_\alpha^\dagger p_\beta^\dagger |0\rangle$$

$$|R_\alpha E_\beta\rangle = \frac{1}{G_\alpha G_\beta}\sum_{j\neq k} g_{j\alpha}g_{k\beta}\sigma_j^{rg}\sigma_k^{eg}|0\rangle$$

which, by comparison to $|\psi_2\rangle$ above, yields (for the collective state $|R_\alpha E_\beta\rangle$)

$$B_{er}^{kj} = \frac{g_{j\alpha}g_{k\beta}}{G_\alpha G_\beta}.$$

Noting again that the following step is not rigorously justified but is simply the approximation that we have chosen at the moment, we can write the the corresponding collective $|R_\alpha R_\beta\rangle$ state as:

$$|R_\alpha R_\beta\rangle = \sum_{j>k}^{N_{at}} B_{rr}^{jk}\sigma_j^{rg}\sigma_k^{rg}$$

where the coefficients satisfy the equation derived from NHPT:

$$(2\delta_2 + U(|x_j - x_k|))B_{rr}^{jk} + \Omega_j^b B_{er}^{jk} + \Omega_k^b B_{er}^{kj} = 0$$

$$B_{rr}^{jk} = -\frac{\Omega_j^b B_{er}^{jk} + \Omega_k^b B_{er}^{kj}}{2\delta_2 + U(|x_j - x_k|)}$$

The form of the RE states is only rigorously justified if Ω is homogeneous, so let's set $\Omega_j^b \equiv \Omega$ assuming it's homogeneous from here on out. Moreover, substituting the form of B_{er}^{kj},

$$B_{rr}^{jk} = -\Omega\frac{\frac{g_{k\alpha}g_{j\beta}}{G_\alpha G_\beta} + \frac{g_{j\alpha}g_{k\beta}}{G_\alpha G_\beta}}{2\delta_2 + U(|x_j - x_k|)}$$

$$B_{rr}^{jk} = -\frac{\Omega}{G_\alpha G_\beta}\frac{g_{k\alpha}g_{j\beta} + g_{j\alpha}g_{k\beta}}{2\delta_2 + U(|x_j - x_k|)}$$

Finally, normalize the overall state to arrive at the desired two-Rydberg collective state:

$$|R_\alpha R_\beta\rangle = i\frac{\sum_{j>k}^{N_{at}}\left(\frac{g_{k\alpha}g_{j\beta}+g_{j\alpha}g_{k\beta}}{2\delta_2+U(|x_j-x_k|)}\right)\sigma_j^{rg}\sigma_k^{rg}}{\sqrt{\sum_{j>k}^{N_{at}}\left|\frac{g_{k\alpha}g_{j\beta}+g_{j\alpha}g_{k\beta}}{2\delta_2+U(|x_j-x_k|)}\right|^2}}.$$

Under the chosen approximation, that is the only non-trivial collective state to derive. The others, for completeness, are:

$$|E_\alpha\rangle = p_\alpha^\dagger|0\rangle$$

$$|R_\alpha\rangle = r_\alpha^\dagger|0\rangle$$

$$|E_\alpha E_\beta\rangle = \frac{1}{\sqrt{1+\delta_{\alpha\beta}}}p_\alpha^\dagger p_\beta^\dagger|0\rangle$$

II. DERIVING THE EFFECTIVE HAMILTONIAN

The form of the effective Hamiltonian can now be derived as follows.

Given the form of the complete free Hamiltonian

$$H_0 = \sum_n^{N_{cav}} \delta_c^n a_n^\dagger a_n + \sum_n^{N_{cav}} \sum_m^{N_{at}} (g_{mn}\sigma_m^{eg} a_n + g_{mn}^* \sigma_m^{ge} a_n^\dagger) + \delta_e \sum_m^{N_{at}} \sigma_m^{ee} + \delta_2 \sum_m^{N_{at}} \sigma_m^{rr} + \sum_m^{N_{at}} (\Omega\sigma_m^{re} + \Omega^* \sigma_m^{er}) + \frac{1}{2}\sum_{p\neq q} \sigma_q^{rr}\sigma_p^{rr} U(|x_p - x_q|).$$

First, define a renormalized collective Rydberg operator $\tilde{r}_\alpha$ which satisfies the following:

$$|R_\alpha\rangle = \tilde{r}_\alpha^\dagger |0\rangle = r_\alpha^\dagger |0\rangle$$

$$|R_\alpha R_\beta\rangle = \frac{1}{\sqrt{1+\delta_{\alpha\beta}}} \tilde{r}_\alpha^\dagger \tilde{r}_\beta^\dagger |0\rangle = i \frac{\sum_{j>k}^{N_{at}} \left(\frac{g_{k\alpha}g_{j\beta} + g_{j\alpha}g_{k\beta}}{2\delta_2 + U(|x_j - x_k|)}\right) \sigma_j^{rg}\sigma_k^{rg}}{\sqrt{\sum_{j>k}^{N_{at}} \left|\frac{g_{k\alpha}g_{j\beta} + g_{j\alpha}g_{k\beta}}{2\delta_2 + U(|x_j - x_k|)}\right|^2}} |0\rangle$$

for the collective states given above. Our goal is to find an effective Hamiltonian $H_E(\{a_\alpha\}, \{p_\alpha\}, \{\tilde{r}_\alpha\})$ in terms of the collective operators across the set of modes which satisfies:

$$\langle\psi_y| H_E |\psi_x\rangle = \langle\psi_y| H_0 |\psi_x\rangle$$

for any normalized states constructed as

$$|\psi_x\rangle = N_x \prod_\alpha^{N_{cav}} \left(a_\alpha^\dagger\right)^{n_{a\alpha}} \left(p_\alpha^\dagger\right)^{n_{p\alpha}} \left(\tilde{r}_\alpha^\dagger\right)^{n_{r\alpha}} |0\rangle$$

for up to two excitations, that is

$$\sum_\alpha^{N_{cav}} (n_{a\alpha} + n_{p\alpha} + n_{r\alpha}) \leq 2.$$

We can then extrapolate the effective Hamiltonian to whatever excitation number we like, of course, but we will derive it using this relationship in the less-than-two excitation manifolds.

The number of states to consider is sufficiently limited that we can go state by state. The vacuum state is completely trivial, $H_E^{(0)} = 0$. The single-excitation manifolds are nearly as trivial (here I've gone ahead and assumed Ω is real; see LyX note for G term confirmation),

$$\boxed{H_E^{(1)} = \sum_\alpha^{n_{cav}} \left(\delta_c^\alpha a_\alpha^\dagger a_\alpha + \delta_e p_\alpha^\dagger p_\alpha + \delta_2 \tilde{r}_\alpha^\dagger \tilde{r}_\alpha + G_\alpha \left(p_\alpha^\dagger a_\alpha + a_\alpha^\dagger p_\alpha\right) + \Omega\left(\tilde{r}_\alpha^\dagger p_\alpha + p_\alpha^\dagger \tilde{r}_\alpha\right)\right)}$$

Everything is easy at up to the single excitation manifold, as it should be. At the two excitation manifold things get more interesting, specifically in the Ω coupling term and the interaction term. Keep in mind that our condition is now:

$$\langle\psi_y| H_E^{(1)} + H_E^{(2)} |\psi_x\rangle = \langle\psi_y| H_0 |\psi_x\rangle$$

and we don't want to change anything in the single-excitation manifold, so we're only going to add terms which are fourth order in creation/annihilation operators. That is, we take the ansatz:

where

$$\boxed{H_E^{(2)} \equiv \sum_{\alpha\geq\beta,\gamma\geq\xi}^{N_{cav}} U_{\alpha\beta\gamma\xi}\tilde{r}_\alpha^\dagger\tilde{r}_\beta^\dagger\tilde{r}_\gamma\tilde{r}_\xi + \sum_{\alpha\geq\beta,\gamma,\xi}^{N_{cav}}\left(\delta\Omega_{\alpha\beta\gamma\xi}\tilde{r}_\alpha^\dagger\tilde{r}_\beta^\dagger\tilde{r}_\gamma p_\xi + \delta\Omega^*_{\alpha\beta\gamma\xi}p_\xi^\dagger\tilde{r}_\gamma^\dagger\tilde{r}_\beta\tilde{r}_\alpha\right)}$$

we have additionally noted that only terms with some coupling to the two-Rydberg manifold will be significantly affected by the renormalized form of the Rydberg operator OR the presence of the interaction term itself.

**** WE SHOULD ALSO INCLUDE A LINDBLAD OPERATOR, BECAUSE I THINK IT WILL NOT BE ENTIRELY POSSIBLE TO SATISFY MY CONDITION IN THE TWO PHOTON MANIFOLD WITH THE LIMITED SET OF COLLECTIVE OPERATORS... BUT LET'S SEE WHERE THIS ALL GOES FIRST :) ****

A. Interaction Coefficient

Now let's derive the coefficients $U_{\alpha\beta\gamma\xi}$, which are easier because $\langle 0|\,\tilde{r}_\alpha\tilde{r}_\beta H_E^{(1)}\tilde{r}_\gamma^\dagger\tilde{r}_\xi^\dagger\,|0\rangle$ simply captures the δ_2 contribution and matches that component of H_0. Therefore, we need:

$$\frac{1}{\sqrt{1+\delta_{\alpha\beta}}\sqrt{1+\delta_{\gamma\xi}}}\langle 0|\,\tilde{r}_\alpha\tilde{r}_\beta H_E^{(2)}\tilde{r}_\gamma^\dagger\tilde{r}_\xi^\dagger\,|0\rangle = \frac{1}{\sqrt{1+\delta_{\alpha\beta}}\sqrt{1+\delta_{\gamma\xi}}}\langle 0|\,\tilde{r}_\alpha\tilde{r}_\beta\left(\sum_{p>q}^{N_{at}}\sigma_p^{rr}\sigma_q^{rr}U(|x_p-x_q|)\right)\tilde{r}_\gamma^\dagger\tilde{r}_\xi^\dagger\,|0\rangle\,.$$

I'll perform the rest of this step in-place for now, since it's important to get it right, although perhaps eventually it belongs in an appendix or something.

$$\frac{1}{\sqrt{1+\delta_{\alpha\beta}}\sqrt{1+\delta_{\gamma\xi}}}\langle 0|\,\tilde{r}_\alpha\tilde{r}_\beta\left(\sum_{a\geq b,c\geq d}^{N_{cav}}U_{abcd}\tilde{r}_a^\dagger\tilde{r}_b^\dagger\tilde{r}_c\tilde{r}_d\right)\tilde{r}_\gamma^\dagger\tilde{r}_\xi^\dagger\,|0\rangle = \frac{1}{G_{\alpha\beta}G_{\gamma\xi}}\langle 0|\left(\sum_{j>k}^{N_{at}}\left(\frac{g_{k\alpha}g_{j\beta}+g_{j\alpha}g_{k\beta}}{2\delta_2+U(|x_j-x_k|)}\right)^*\sigma_j^{gr}\sigma_k^{gr}\right)\left(\sum_{p>q}^{N_{at}}\sigma_p^{rr}\sigma_q^{rr}U\right.$$

where I've defined

$$G_{\gamma\xi} \equiv \sqrt{\sum_{j>k}^{N_{at}}\left|\frac{g_{k\gamma}g_{j\xi}+g_{j\gamma}g_{k\xi}}{2\delta_2+U(|x_j-x_k|)}\right|^2}.$$

The LHS is relatively easy to handle. Note that $c>d$, so if it is possible for c to equal γ then it is NOT possible for c to equal ξ UNLESS $\gamma=\xi$ as well.

$$LHS = \frac{1}{\sqrt{1+\delta_{\alpha\beta}}\sqrt{1+\delta_{\gamma\xi}}}\sum_{a\geq b,c\geq d}^{N_{cav}}U_{abcd}\,\langle 0|\,\tilde{r}_\alpha\tilde{r}_\beta\tilde{r}_a^\dagger\tilde{r}_b^\dagger\tilde{r}_c\tilde{r}_d\tilde{r}_\gamma^\dagger\tilde{r}_\xi^\dagger\,|0\rangle$$

The cleanest way to handle it is to remember that $r_\alpha r_\beta^\dagger = r_\beta^\dagger r_\alpha + \delta_{\alpha\beta}$:

$$LHS = \frac{1}{\sqrt{1+\delta_{\alpha\beta}}\sqrt{1+\delta_{\gamma\xi}}}\sum_{a\geq b,c\geq d}^{N_{cav}}U_{abcd}\,\langle 0|\,\tilde{r}_\alpha\left(\tilde{r}_a^\dagger\tilde{r}_\beta+\delta_{a\beta}\right)\tilde{r}_b^\dagger\tilde{r}_c\left(\tilde{r}_\gamma^\dagger\tilde{r}_d+\delta_{\gamma d}\right)\tilde{r}_\xi^\dagger\,|0\rangle$$

$$LHS = \frac{1}{\sqrt{1+\delta_{\alpha\beta}}\sqrt{1+\delta_{\gamma\xi}}}\sum_{a\geq b,c\geq d}^{N_{cav}}U_{abcd}\,\langle 0|\left(\tilde{r}_\alpha\tilde{r}_a^\dagger\tilde{r}_\beta\tilde{r}_b^\dagger\tilde{r}_c\left(\tilde{r}_\gamma^\dagger\tilde{r}_d+\delta_{\gamma d}\right)\tilde{r}_\xi^\dagger + \delta_{a\beta}\tilde{r}_\alpha\tilde{r}_b^\dagger\tilde{r}_c\left(\tilde{r}_\gamma^\dagger\tilde{r}_d+\delta_{\gamma d}\right)\tilde{r}_\xi^\dagger\right)|0\rangle$$

$$LHS = \frac{1}{\sqrt{1+\delta_{\alpha\beta}}\sqrt{1+\delta_{\gamma\xi}}}\sum_{a\geq b,c\geq d}^{N_{cav}}U_{abcd}\,\langle 0|\left(\tilde{r}_\alpha\tilde{r}_a^\dagger\tilde{r}_\beta\tilde{r}_b^\dagger\tilde{r}_c\tilde{r}_\gamma^\dagger\tilde{r}_d\tilde{r}_\xi^\dagger + \delta_{\gamma d}\tilde{r}_\alpha\tilde{r}_a^\dagger\tilde{r}_\beta\tilde{r}_b^\dagger\tilde{r}_c\tilde{r}_\xi^\dagger + \delta_{a\beta}\tilde{r}_\alpha\tilde{r}_b^\dagger\tilde{r}_c\tilde{r}_\gamma^\dagger\tilde{r}_d\tilde{r}_\xi^\dagger + \delta_{\gamma d}\delta_{a\beta}\tilde{r}_\alpha\tilde{r}_b^\dagger\tilde{r}_c\tilde{r}_\xi^\dagger\right)|0\rangle$$

$$LHS = \frac{1}{\sqrt{1+\delta_{\alpha\beta}}\sqrt{1+\delta_{\gamma\xi}}} \sum_{a\geq b, c\geq d}^{N_{cav}} U_{abcd} \langle 0| \left(\delta_{a\alpha}\delta_{b\beta}\delta_{c\gamma}\delta_{d\xi} + \delta_{a\alpha}\delta_{b\beta}\delta_{c\xi}\delta_{d\gamma} + \delta_{a\beta}\delta_{b\alpha}\delta_{c\gamma}\delta_{d\xi} + \delta_{a\beta}\delta_{b\alpha}\delta_{c\xi}\delta_{d\gamma}\right) |0\rangle$$

$$LHS = \frac{1}{\sqrt{1+\delta_{\alpha\beta}}\sqrt{1+\delta_{\gamma\xi}}} \left(\sum_{a\geq \beta, c\geq d}^{N_{cav}} U_{a\beta cd} \langle 0| \left(\delta_{a\alpha}\delta_{c\gamma}\delta_{d\xi} + \delta_{a\alpha}\delta_{c\xi}\delta_{d\gamma}\right) + \sum_{a\geq \alpha, c\geq d}^{N_{cav}} U_{a\alpha cd} \langle 0| \left(\delta_{a\beta}\delta_{c\gamma}\delta_{d\xi} + \delta_{a\beta}\delta_{c\xi}\delta_{d\gamma}\right) \right) |0\rangle$$

$$LHS = \frac{1}{\sqrt{1+\delta_{\alpha\beta}}\sqrt{1+\delta_{\gamma\xi}}} \langle 0| \left(\sum_{a\geq \beta, c\geq \xi}^{N_{cav}} U_{a\beta c\xi} \left(\delta_{a\alpha}\delta_{c\gamma}\right) + \sum_{a\geq \beta, c\geq \gamma}^{N_{cav}} U_{a\beta c\gamma} \left(\delta_{a\alpha}\delta_{c\xi}\right) + \sum_{a\geq \alpha, c\geq \xi}^{N_{cav}} U_{a\alpha c\xi} \left(\delta_{a\beta}\delta_{c\gamma}\right) + \sum_{a\geq \alpha, c\geq \gamma}^{N_{cav}} U_{a\alpha c\gamma} \left(\delta_{a\beta}\delta_{c\xi}\right)$$

It is never possible for both $\xi > \gamma$ and $\gamma > \xi$ to be true. Therefore, either $\xi = \gamma$, in which case we get non-zero terms from all of the sums, or $\xi \neq \gamma$, in which case only half of the sums can yield a non-zero term. The same is true for α and β. Therefore (and requiring $U_{abcd} \equiv U_{abdc} \equiv U_{bacd}$):

$$LHS = \frac{1}{\sqrt{1+\delta_{\alpha\beta}}\sqrt{1+\delta_{\gamma\xi}}} \langle 0| \left((1+\delta_{\gamma\xi}) \sum_{a\geq \beta}^{N_{cav}} U_{a\beta\gamma\xi} \left(\delta_{a\alpha}\right) + (1+\delta_{\gamma\xi}) \sum_{a\geq \alpha}^{N_{cav}} U_{a\alpha\gamma\xi} \left(\delta_{a\beta}\right) \right) |0\rangle$$

$$LHS = \frac{1}{\sqrt{1+\delta_{\alpha\beta}}\sqrt{1+\delta_{\gamma\xi}}} \left(1+\delta_{\gamma\xi}\right)\left(1+\delta_{\alpha\beta}\right) U_{a\beta\gamma\xi}$$

$$LHS = \sqrt{\left(1+\delta_{\gamma\xi}\right)\left(1+\delta_{\alpha\beta}\right)} U_{a\beta\gamma\xi}$$

This was a very long derivation for something that we might have guessed, but I wanted to be absolutely certain that I had it right - those extra factors can be sneaky! Now let's move on to handle the RHS:

$$\frac{1}{G_{\alpha\beta}G_{\gamma\xi}} \langle 0| \left(\sum_{j>k}^{N_{at}} \left(\frac{g_{k\alpha}g_{j\beta} + g_{j\alpha}g_{k\beta}}{2\delta_2 + U(|x_j - x_k|)} \right)^* \sigma_j^{gr}\sigma_k^{gr} \right) \left(\sum_{p>q}^{N_{at}} \sigma_p^{rr}\sigma_q^{rr} U(|x_p - x_q|) \right) \left(\sum_{m>n}^{N_{at}} \left(\frac{g_{n\gamma}g_{m\xi} + g_{m\gamma}g_{n\xi}}{2\delta_2 + U(|x_m - x_n|)} \right) \sigma_m^{rg}\sigma_n^{rg} \right) |0\rangle$$

$$\frac{1}{G_{\alpha\beta}G_{\gamma\xi}} \langle 0| \left(\sum_{j>k}^{N_{at}} \left(\frac{g_{k\alpha}g_{j\beta} + g_{j\alpha}g_{k\beta}}{2\delta_2 + U(|x_j - x_k|)} \right)^* \sigma_j^{gr}\sigma_k^{gr} \right) \sum_{m>n}^{N_{at}} \sum_{p>q}^{N_{at}} \sigma_p^{rr}\sigma_q^{rr}\sigma_m^{rg}\sigma_n^{rg} U(|x_p - x_q|) \frac{g_{n\gamma}g_{m\xi} + g_{m\gamma}g_{n\xi}}{2\delta_2 + U(|x_m - x_n|)} |0\rangle$$

$$\frac{1}{G_{\alpha\beta}G_{\gamma\xi}} \langle 0| \left(\sum_{j>k}^{N_{at}} \left(\frac{g_{k\alpha}g_{j\beta} + g_{j\alpha}g_{k\beta}}{2\delta_2 + U(|x_j - x_k|)} \right)^* \sigma_j^{gr}\sigma_k^{gr} \right) \sum_{m>n}^{N_{at}} \sum_{p>q}^{N_{at}} \left(\delta_{pm}\delta_{qn} + \delta_{pn}\delta_{qm}\right) \sigma_m^{rg}\sigma_n^{rg} U(|x_p - x_q|) \frac{g_{n\gamma}g_{m\xi} + g_{m\gamma}g_{n\xi}}{2\delta_2 + U(|x_m - x_n|)} |0\rangle$$

Here, the inequalities in our summation indices are *exclusive*, so we never have $p = q$ or $m = n$. For given values of m and n, it is only possible to have $\delta_{pm}\delta_{qn}$ be satisfied; it is never possible the other way around. Therefore this resolves to:

$$\frac{1}{G_{\alpha\beta}G_{\gamma\xi}} \langle 0| \left(\sum_{j>k}^{N_{at}} \left(\frac{g_{k\alpha}g_{j\beta} + g_{j\alpha}g_{k\beta}}{2\delta_2 + U(|x_j - x_k|)} \right)^* \sigma_j^{gr}\sigma_k^{gr} \right) \sum_{m>n}^{N_{at}} \sum_{p>q}^{N_{at}} \left(\delta_{pm}\delta_{qn}\right) \sigma_m^{rg}\sigma_n^{rg} U(|x_p - x_q|) \frac{g_{n\gamma}g_{m\xi} + g_{m\gamma}g_{n\xi}}{2\delta_2 + U(|x_m - x_n|)} |0\rangle$$

$$\frac{1}{G_{\alpha\beta}G_{\gamma\xi}}\left\langle 0\right|\left(\sum_{j>k}^{N_{at}}\left(\frac{g_{k\alpha}g_{j\beta}+g_{j\alpha}g_{k\beta}}{2\delta_2+U(|x_j-x_k|)}\right)^*\sigma_j^{gr}\sigma_k^{gr}\right)\sum_{m>n}^{N_{at}}\sigma_m^{rg}\sigma_n^{rg}U(|x_m-x_n|)\frac{g_{n\gamma}g_{m\xi}+g_{m\gamma}g_{n\xi}}{2\delta_2+U(|x_m-x_n|)}\left|0\right\rangle$$

Essentially the same thing happens here, yielding:

$$RHS=\frac{1}{G_{\alpha\beta}G_{\gamma\xi}}\sum_{j>k}^{N_{at}}\left(\frac{g_{k\alpha}g_{j\beta}+g_{j\alpha}g_{k\beta}}{2\delta_2+U(|x_j-x_k|)}\right)^*\left(\frac{g_{j\gamma}g_{k\xi}+g_{k\gamma}g_{j\xi}}{2\delta_2+U(|x_j-x_k|)}\right)U(|x_j-x_k|)$$

Now, let's return to equating the LHS and RHS:

$$\sqrt{(1+\delta_{\gamma\xi})(1+\delta_{\alpha\beta})}U_{\alpha\beta\gamma\xi}=\frac{1}{G_{\alpha\beta}G_{\gamma\xi}}\sum_{j>k}^{N_{at}}\left(\frac{g_{k\alpha}g_{j\beta}+g_{j\alpha}g_{k\beta}}{2\delta_2+U(|x_j-x_k|)}\right)^*\left(\frac{g_{j\gamma}g_{k\xi}+g_{k\gamma}g_{j\xi}}{2\delta_2+U(|x_j-x_k|)}\right)U(|x_j-x_k|)$$

which finally yields the formula for the desired parameter:

$$\boxed{U_{\alpha\beta\gamma\xi}=\frac{1}{G_{\alpha\beta}G_{\gamma\xi}\sqrt{(1+\delta_{\gamma\xi})(1+\delta_{\alpha\beta})}}\sum_{j>k}^{N_{at}}\left(\frac{g_{k\alpha}g_{j\beta}+g_{j\alpha}g_{k\beta}}{2\delta_2+U(|x_j-x_k|)}\right)^*\left(\frac{g_{j\gamma}g_{k\xi}+g_{k\gamma}g_{j\xi}}{2\delta_2+U(|x_j-x_k|)}\right)U(|x_j-x_k|)}$$

B. Omega coefficient

Once again we want to satisfy

$$\left\langle\psi_y\right|H_E^{(1)}+H_E^{(2)}\left|\psi_x\right\rangle=\left\langle\psi_y\right|H_0\left|\psi_x\right\rangle$$

but now with $|\psi_x\rangle=|R_\gamma E_\xi\rangle$ and $\langle\psi_y|=\langle R_\alpha R_\beta|$. This one is a bit trickier, because the $H_E^{(1)}$ contribution is not negligible.

$$\left\langle R_\alpha R_\beta\right|\sum_a^{n_{cav}}\Omega\left(\tilde r_a^\dagger p_a+p_a^\dagger\tilde r_a\right)\left|R_\gamma E_\xi\right\rangle+\left\langle R_\alpha R_\beta\right|\sum_{a\geq b,c,d}^{N_{cav}}\left(\delta\Omega_{abcd}\tilde r_a^\dagger\tilde r_b^\dagger\tilde r_c p_d+\delta\Omega_{abcd}^*p_d^\dagger\tilde r_c^\dagger\tilde r_b\tilde r_a\right)\left|R_\gamma E_\xi\right\rangle=\left\langle R_\alpha R_\beta\right|\sum_j^{N_{at}}\left(\Omega\sigma_j^{re}+\Omega^*\sigma_j^{er}\right)\left|R_\gamma\right.$$

First the LHS:

$$LHS=\left\langle R_\alpha R_\beta\right|\sum_a^{n_{cav}}\Omega\left(\tilde r_a^\dagger p_a+p_a^\dagger\tilde r_a\right)\left|R_\gamma E_\xi\right\rangle+\left\langle R_\alpha R_\beta\right|\sum_{a\geq b,c,d}^{N_{cav}}\left(\delta\Omega_{abcd}\tilde r_a^\dagger\tilde r_b^\dagger\tilde r_c p_d+\delta\Omega_{abcd}^*p_d^\dagger\tilde r_c^\dagger\tilde r_b\tilde r_a\right)\left|R_\gamma E_\xi\right\rangle$$

$$\frac{1}{\sqrt{1+\delta_{\alpha\beta}}}\left\langle 0\right|\tilde r_\alpha\tilde r_\beta\sum_a^{n_{cav}}\Omega\left(\tilde r_a^\dagger p_a+p_a^\dagger\tilde r_a\right)\tilde r_\gamma^\dagger p_\xi^\dagger\left|0\right\rangle+\frac{1}{\sqrt{1+\delta_{\alpha\beta}}}\left\langle 0\right|\tilde r_\alpha\tilde r_\beta\sum_{a\geq b,c,d}^{N_{cav}}\left(\delta\Omega_{abcd}\tilde r_a^\dagger\tilde r_b^\dagger\tilde r_c p_d+\delta\Omega_{abcd}^*p_d^\dagger\tilde r_c^\dagger\tilde r_b\tilde r_a\right)\tilde r_\gamma^\dagger p_\xi^\dagger\left|0\right\rangle$$

$$\frac{1}{\sqrt{1+\delta_{\alpha\beta}}}\left\langle 0\right|\tilde r_\alpha\tilde r_\beta\sum_a^{n_{cav}}\Omega\left(\tilde r_a^\dagger\tilde r_\gamma^\dagger\delta_{a\xi}+p_a^\dagger\delta_{a\gamma}p_\xi^\dagger\right)\left|0\right\rangle+\frac{1}{\sqrt{1+\delta_{\alpha\beta}}}\left\langle 0\right|\tilde r_\alpha\tilde r_\beta\sum_{a\geq b,c,d}^{N_{cav}}\left(\delta\Omega_{abcd}\tilde r_a^\dagger\tilde r_b^\dagger\tilde r_c p_d+\delta\Omega_{abcd}^*p_d^\dagger\tilde r_c^\dagger\tilde r_b\tilde r_a\right)\tilde r_\gamma^\dagger p_\xi^\dagger\left|0\right\rangle$$

$$\frac{\Omega}{\sqrt{1+\delta_{\alpha\beta}}}\left(\delta_{\alpha\gamma}\delta_{\beta\xi}+\delta_{\alpha\xi}\delta_{\beta\gamma}\right)+\frac{1}{\sqrt{1+\delta_{\alpha\beta}}}\left\langle 0\right|\tilde r_\alpha\tilde r_\beta\sum_{a\geq b,c,d}^{N_{cav}}\left(\delta\Omega_{abcd}\tilde r_a^\dagger\tilde r_b^\dagger\tilde r_c p_d+\delta\Omega_{abcd}^*p_d^\dagger\tilde r_c^\dagger\tilde r_b\tilde r_a\right)\tilde r_\gamma^\dagger p_\xi^\dagger\left|0\right\rangle$$

$$\frac{\Omega}{\sqrt{1+\delta_{\alpha\beta}}}\left(\delta_{\alpha\gamma}\delta_{\beta\xi}+\delta_{\alpha\xi}\delta_{\beta\gamma}\right)+\frac{1}{\sqrt{1+\delta_{\alpha\beta}}}\left\langle 0\right|\tilde{r}_{\alpha}\tilde{r}_{\beta}\sum_{a\geq b,c,d}^{N_{cav}}\delta\Omega_{abcd}\tilde{r}_{a}^{\dagger}\tilde{r}_{b}^{\dagger}\tilde{r}_{c}p_{d}\tilde{r}_{\gamma}^{\dagger}p_{\xi}^{\dagger}\left|0\right\rangle$$

$$\frac{\Omega}{\sqrt{1+\delta_{\alpha\beta}}}\left(\delta_{\alpha\gamma}\delta_{\beta\xi}+\delta_{\alpha\xi}\delta_{\beta\gamma}\right)+\frac{1}{\sqrt{1+\delta_{\alpha\beta}}}\left\langle 0\right|\tilde{r}_{\alpha}\tilde{r}_{\beta}\sum_{a\geq b,c,d}^{N_{cav}}\delta\Omega_{abcd}\tilde{r}_{a}^{\dagger}\tilde{r}_{b}^{\dagger}\delta_{c\gamma}\delta_{d\xi}\left|0\right\rangle$$

$$\frac{\Omega}{\sqrt{1+\delta_{\alpha\beta}}}\left(\delta_{\alpha\gamma}\delta_{\beta\xi}+\delta_{\alpha\xi}\delta_{\beta\gamma}\right)+\frac{1}{\sqrt{1+\delta_{\alpha\beta}}}\left\langle 0\right|\sum_{a\geq b}^{N_{cav}}\delta\Omega_{ab\gamma\xi}\tilde{r}_{\alpha}\tilde{r}_{\beta}\tilde{r}_{a}^{\dagger}\tilde{r}_{b}^{\dagger}\left|0\right\rangle$$

$$\frac{\Omega}{\sqrt{1+\delta_{\alpha\beta}}}\left(\delta_{\alpha\gamma}\delta_{\beta\xi}+\delta_{\alpha\xi}\delta_{\beta\gamma}\right)+\frac{1}{\sqrt{1+\delta_{\alpha\beta}}}\left\langle 0\right|\sum_{a\geq\beta}^{N_{cav}}\delta\Omega_{a\beta\gamma\xi}\delta_{\alpha a}+\sum_{a\geq\alpha}^{N_{cav}}\delta\Omega_{a\alpha\gamma\xi}\delta_{\beta a}\left|0\right\rangle$$

$$\frac{\Omega}{\sqrt{1+\delta_{\alpha\beta}}}\left(\delta_{\alpha\gamma}\delta_{\beta\xi}+\delta_{\alpha\xi}\delta_{\beta\gamma}\right)+\frac{1}{\sqrt{1+\delta_{\alpha\beta}}}\left(1+\delta_{\alpha\beta}\right)\delta\Omega_{\alpha\beta\gamma\xi}$$

$$\delta\Omega_{\alpha\beta\gamma\xi}\equiv\delta\Omega_{\beta\alpha\gamma\xi}$$

$$LHS=\frac{\Omega}{\sqrt{1+\delta_{\alpha\beta}}}\left(\delta_{\alpha\gamma}\delta_{\beta\xi}+\delta_{\alpha\xi}\delta_{\beta\gamma}\right)+\sqrt{1+\delta_{\alpha\beta}}\delta\Omega_{\alpha\beta\gamma\xi}$$

Now for the RHS:

$$-i\frac{1}{G_{\alpha\beta}}\frac{1}{G_{\gamma}G_{\xi}}\left\langle 0\right|\left(\sum_{j>k}^{N_{at}}\left(\frac{g_{k\alpha}g_{j\beta}+g_{j\alpha}g_{k\beta}}{2\delta_{2}+U(|x_{j}-x_{k}|)}\right)^{*}\sigma_{j}^{gr}\sigma_{k}^{gr}\sum_{m}^{N_{at}}\left(\Omega\sigma_{m}^{re}+\Omega^{*}\sigma_{m}^{er}\right)\sum_{p}^{N_{at}}g_{p\gamma}\sigma_{p}^{eg}\sum_{q}^{N_{at}}g_{q\xi}\sigma_{q}^{rg}\right)\left|0\right\rangle$$

$$-i\frac{1}{G_{\alpha\beta}}\frac{1}{G_{\gamma}G_{\xi}}\left\langle 0\right|\left(\sum_{j>k}^{N_{at}}\left(\frac{g_{k\alpha}g_{j\beta}+g_{j\alpha}g_{k\beta}}{2\delta_{2}+U(|x_{j}-x_{k}|)}\right)^{*}\sigma_{j}^{gr}\sigma_{k}^{gr}\sum_{m}^{N_{at}}\sum_{p}^{N_{at}}\sum_{q}^{N_{at}}\left(\Omega\sigma_{m}^{re}+\Omega^{*}\sigma_{m}^{er}\right)\sigma_{p}^{eg}\sigma_{q}^{rg}g_{p\gamma}g_{q\xi}\right)\left|0\right\rangle$$

$$-i\frac{1}{G_{\alpha\beta}}\frac{1}{G_{\gamma}G_{\xi}}\left\langle 0\right|\left(\sum_{j>k}^{N_{at}}\left(\frac{g_{k\alpha}g_{j\beta}+g_{j\alpha}g_{k\beta}}{2\delta_{2}+U(|x_{j}-x_{k}|)}\right)^{*}\sigma_{j}^{gr}\sigma_{k}^{gr}\sum_{m}^{N_{at}}\sum_{p}^{N_{at}}\sum_{q}^{N_{at}}\left(\Omega\delta_{mp}\sigma_{m}^{rg}\sigma_{q}^{rg}g_{p\gamma}g_{q\xi}+\Omega^{*}\delta_{mq}\sigma_{m}^{eg}\sigma_{p}^{eg}g_{p\gamma}g_{q\xi}\right)\right)\left|0\right\rangle$$

$$-i\frac{1}{G_{\alpha\beta}}\frac{1}{G_{\gamma}G_{\xi}}\left\langle 0\right|\left(\sum_{j>k}^{N_{at}}\left(\frac{g_{k\alpha}g_{j\beta}+g_{j\alpha}g_{k\beta}}{2\delta_{2}+U(|x_{j}-x_{k}|)}\right)^{*}\sigma_{j}^{gr}\sigma_{k}^{gr}\sum_{p}^{N_{at}}\sum_{q}^{N_{at}}\left(\Omega\sigma_{p}^{rg}\sigma_{q}^{rg}g_{p\gamma}g_{q\xi}+\Omega^{*}\sigma_{q}^{eg}\sigma_{p}^{eg}g_{p\gamma}g_{q\xi}\right)\right)\left|0\right\rangle$$

$$-i\frac{1}{G_{\alpha\beta}}\frac{1}{G_{\gamma}G_{\xi}}\left\langle 0\right|\left(\sum_{j>k}^{N_{at}}\left(\frac{g_{k\alpha}g_{j\beta}+g_{j\alpha}g_{k\beta}}{2\delta_{2}+U(|x_{j}-x_{k}|)}\right)^{*}\sigma_{j}^{gr}\sigma_{k}^{gr}\sum_{p}^{N_{at}}\sum_{q}^{N_{at}}\left(\Omega\sigma_{p}^{rg}\sigma_{q}^{rg}g_{p\gamma}g_{q\xi}\right)\right)\left|0\right\rangle$$

$$-i\frac{1}{G_{\alpha\beta}}\frac{1}{G_{\gamma}G_{\xi}}\left\langle 0\right|\left(\sum_{j>k}^{N_{at}}\left(\frac{g_{k\alpha}g_{j\beta}+g_{j\alpha}g_{k\beta}}{2\delta_{2}+U(|x_{j}-x_{k}|)}\right)^{*}\sum_{p}^{N_{at}}\sum_{q}^{N_{at}}\left(\Omega\left(\delta_{jp}\delta_{kq}+\delta_{jq}\delta_{kp}\right)g_{p\gamma}g_{q\xi}\right)\right)\left|0\right\rangle$$

$$-i\frac{1}{G_{\alpha\beta}}\frac{1}{G_{\gamma}G_{\xi}}\left(\sum_{p}^{N_{at}}\sum_{q}^{N_{at}}\left(\Omega\left(\delta_{jp}\delta_{kq}+\delta_{jq}\delta_{kp}\right)g_{p\gamma}g_{q\xi}\right)\sum_{j>k}^{N_{at}}\left(\frac{g_{k\alpha}g_{j\beta}+g_{j\alpha}g_{k\beta}}{2\delta_{2}+U(|x_{j}-x_{k}|)}\right)^{*}\right)$$

$$-i\frac{\Omega}{G_{\alpha\beta}}\frac{1}{G_{\gamma}G_{\xi}}\left(\sum_{q}^{N_{at}}\sum_{p>q}^{N_{at}}\left(\frac{g_{q\alpha}g_{p\beta}+g_{p\alpha}g_{q\beta}}{2\delta_{2}+U(|x_{p}-x_{q}|)}\right)^{*}g_{p\gamma}g_{q\xi}+\sum_{p}^{N_{at}}\sum_{q>p}^{N_{at}}\left(\frac{g_{p\alpha}g_{q\beta}+g_{q\alpha}g_{p\beta}}{2\delta_{2}+U(|x_{q}-x_{p}|)}\right)^{*}g_{p\gamma}g_{q\xi}\right)$$

$$RHS=-i\frac{\Omega}{G_{\alpha\beta}}\frac{1}{G_{\gamma}G_{\xi}}\left(\sum_{q}^{N_{at}}\sum_{p\neq q}^{N_{at}}\left(\frac{g_{q\alpha}g_{p\beta}+g_{p\alpha}g_{q\beta}}{2\delta_{2}+U(|x_{p}-x_{q}|)}\right)^{*}g_{p\gamma}g_{q\xi}\right)$$

Now set LHS and RHS equal and solve for the desired parameter:

$$\frac{\Omega}{\sqrt{1+\delta_{\alpha\beta}}}\left(\delta_{\alpha\gamma}\delta_{\beta\xi}+\delta_{\alpha\xi}\delta_{\beta\gamma}\right)+\sqrt{1+\delta_{\alpha\beta}}\delta\Omega_{\alpha\beta\gamma\xi}=-i\frac{\Omega}{G_{\alpha\beta}}\frac{1}{G_{\gamma}G_{\xi}}\left(\sum_{q}^{N_{at}}\sum_{p\neq q}^{N_{at}}\left(\frac{g_{q\alpha}g_{p\beta}+g_{p\alpha}g_{q\beta}}{2\delta_{2}+U(|x_{p}-x_{q}|)}\right)^{*}g_{p\gamma}g_{q\xi}\right)$$

$$\sqrt{1+\delta_{\alpha\beta}}\delta\Omega_{\alpha\beta\gamma\xi}=\frac{-i\Omega}{G_{\alpha\beta}}\frac{1}{G_{\gamma}G_{\xi}}\left(\sum_{q}^{N_{at}}\sum_{p\neq q}^{N_{at}}\left(\frac{g_{q\alpha}g_{p\beta}+g_{p\alpha}g_{q\beta}}{2\delta_{2}+U(|x_{p}-x_{q}|)}\right)^{*}g_{p\gamma}g_{q\xi}\right)-\frac{\Omega}{\sqrt{1+\delta_{\alpha\beta}}}\left(\delta_{\alpha\gamma}\delta_{\beta\xi}+\delta_{\alpha\xi}\delta_{\beta\gamma}\right)$$

$$\boxed{\delta\Omega_{\alpha\beta\gamma\xi}=\frac{1}{\sqrt{1+\delta_{\alpha\beta}}}\left(\frac{-i\Omega}{G_{\alpha\beta}}\frac{1}{G_{\gamma}G_{\xi}}\left(\sum_{q}^{N_{at}}\sum_{p\neq q}^{N_{at}}\left(\frac{g_{q\alpha}g_{p\beta}+g_{p\alpha}g_{q\beta}}{2\delta_{2}+U(|x_{p}-x_{q}|)}\right)^{*}g_{p\gamma}g_{q\xi}\right)-\frac{\Omega}{\sqrt{1+\delta_{\alpha\beta}}}\left(\delta_{\alpha\gamma}\delta_{\beta\xi}+\delta_{\alpha\xi}\delta_{\beta\gamma}\right)\right)}$$

Again, it would've been possible to make a good guess based on physical intuitions, but this way I can have a lot more confidence that I'm not missing any δ's or other picky factors.

Let me summarize what we have so far. We have the form of an effective Hamiltonian, and we have a way to calculate parameters of that Hamiltonian from microscopic physical parameters for some arrangement of atoms. The effective Hamiltonian is exactly identical to the original Hamiltonian within this limited manifold of states; the manifold contains the ordinary collective states (one for each cavity mode) except in the RR manifold where the collective states are modified by the interactions using this hokey (but physically not absurd) NHPT-based approximation. However, the effective Hamiltonian does not capture any couplings to states outside of the chosen manifold, and such couplings not only exist but are quite likely relevant when interactions are strong, for instance providing extra loss channels via the eventual formation of P-state excitations that do not have any coupling to a cavity mode. I would like to treat these additional modes as a (Markovian) bath, to the degree that I can roughly justify it. I will attempt to do so in the next section.

C. Numerical integrals

Initial thoughts and calculations (quite good and useful) in lyx note; cleaner version below.

When you're done, don't forget to check simple things like the non-interacting case, known/intuitive cases, comparison to NHPT...

1. *Cleaning up the form of the integrals that need to be calculated; ignoring longitudinal d.o.f. (see LyX note above)*

$$\delta\Omega_{\alpha\beta\gamma\xi}=\frac{1}{\sqrt{1+\delta_{\alpha\beta}}}\left(\frac{-i\Omega}{G_{\alpha\beta}}\frac{1}{G_{\gamma}G_{\xi}}\left(\int d^3x_1\int d^3x_2\left(\frac{g_\alpha(x_1)g_\beta(x_2)+g_\alpha(x_2)g_\beta(x_1)}{2\delta_2+U(|x_1-x_2|)}\right)^* g_\gamma(x_1)g_\xi(x_2)\right)-\frac{\Omega}{\sqrt{1+\delta_{\alpha\beta}}}\left(\delta_{\alpha\gamma}\delta_{\beta\xi}+\delta_{\alpha\xi}\delta_{\beta\right.$$

$$\delta\Omega_{\alpha\beta\gamma\xi}\equiv\frac{\Omega}{\sqrt{1+\delta_{\alpha\beta}}}\left(-i\frac{B_{\alpha\beta\gamma\xi}}{G_{\alpha\beta}G_\gamma G_\xi}-\frac{1}{\sqrt{1+\delta_{\alpha\beta}}}\left(\delta_{\alpha\gamma}\delta_{\beta\xi}+\delta_{\alpha\xi}\delta_{\beta\gamma}\right)\right)$$

$$B_{\alpha\beta\gamma\xi}=\int d^3x_1\int d^3x_2\left(\frac{g_\alpha(x_1)g_\beta(x_2)+g_\alpha(x_2)g_\beta(x_1)}{2\delta_2+U(|x_1-x_2|)}\right)^* g_\gamma(x_1)g_\xi(x_2)$$

$$G_{\gamma\xi}\equiv\sqrt{\frac{1}{2}A_{\gamma\xi}}.$$

$$A_{\gamma\xi}=\int d^3x_1\int d^3x_2\left|\frac{g_\gamma(x_1)g_\xi(x_2)+g_\gamma(x_2)g_\xi(x_1)}{2\delta_2+U(|x_1-x_2|)}\right|^2$$

Note: when convering $\sum_{j>k}^{N_{at}}$ from a sum to a double integral, I'm taking advantage of the symmetry between the atoms and simply cutting in half and using the naive double integral with simple limits (rather than an integral actually using $j>k$). I suppose the numerical integral would be faster the other way... but if I need a factor of 2 then I can change that later.

$$U_{a\beta\gamma\xi}=\frac{1}{G_{\alpha\beta}G_{\gamma\xi}\sqrt{(1+\delta_{\gamma\xi})(1+\delta_{\alpha\beta})}}\sum_{j>k}^{N_{at}}\left(\frac{g_{k\alpha}g_{j\beta}+g_{j\alpha}g_{k\beta}}{2\delta_2+U(|x_j-x_k|)}\right)^*\left(\frac{g_{j\gamma}g_{k\xi}+g_{k\gamma}g_{j\xi}}{2\delta_2+U(|x_j-x_k|)}\right)U(|x_j-x_k|)$$

$$U_{a\beta\gamma\xi}\equiv\frac{C_{\alpha\beta\gamma\xi}}{2G_{\alpha\beta}G_{\gamma\xi}\sqrt{(1+\delta_{\gamma\xi})(1+\delta_{\alpha\beta})}}$$

$$C_{\alpha\beta\gamma\xi}=\int dr_1dr_2d\theta_1d\theta_2r_1r_2\left(\frac{g_\alpha(x_1)g_\beta(x_2)+g_\alpha(x_2)g_\beta(x_1)}{2\delta_2+U(|x_1-x_2|)}\right)^*\left(\frac{g_\gamma(x_1)g_\xi(x_2)+g_\gamma(x_2)g_\xi(x_1)}{2\delta_2+U(|x_1-x_2|)}\right)U(|x_j-x_k|)$$

Next steps:

- re-jigger into physically transparent units (and ideally dimensionless integrals)
- reduce to 3D integrals (again)

2. *Physically transparent units*

The properly normalized Lowest Landau Level wavefunction with angular momentum l is

$$\phi_l(z)\equiv\frac{1}{\sqrt{2\pi 2^l l!}}z^le^{-|z|^2/4},$$

satisfying

$$\int dr_1d\theta_1r_1|\phi_l(r_1e^{i\theta_1})|^2=1.$$

Define

$$g_l(z) \equiv G\phi_l(z)$$

which we want to satisfy (assuming a homogeneous atomic sample)

$$G_{phys}^2 = \int d^2z|g_l(z)|^2 = G^2 \int d^2z|\phi_l(r_1e^{i\theta_1})|^2 = G^2$$

where G_{phys} is the total atom-photon coupling for a single mode, which should be independent of the mode as long as the sample is homogeneous. Therefore, the introduced parameter G is indeed equivalent to the total atom-photon coupling per mode G_{phys}, as long as we properly convert from the physical coordinate x to the dimensionless coordinate z. The easiest way is to note $|\phi_0(z)|^2 \sim e^{-|z|^2/2}$, and that our physical intensity profile should be $e^{-2|x|^2/w^2}$ since the waist w is the radius at which the intensity drops to e^{-2}. Therefore, we should have (being liberal with my variables)

$$z \equiv \frac{x}{w/2}$$

$$g_l(x)d^2x = \left(\frac{w}{2}\right)^2 G\phi_l(z)d^2z$$

I will use capital R as the dimensionless radius ($z \equiv R \times e^{i\theta}$)

$$C_{\alpha\beta\gamma\xi} = \left(\frac{w}{2}\right)^4 G^4 \int dR_1dR_2d\theta_1d\theta_2R_1R_2 \left(\frac{\phi_\alpha(z_1)\phi_\beta(z_2)+\phi_\alpha(z_2)\phi_\beta(z_1)}{2\delta_2+C_6\left(\frac{w}{2}\right)^{-6}|z_1-z_2|^{-6}}\right)^* \left(\frac{\phi_\gamma(z_1)\phi_\xi(z_2)+\phi_\gamma(z_2)\phi_\xi(z_1)}{2\delta_2+C_6\left(\frac{w}{2}\right)^{-6}|z_1-z_2|^{-6}}\right) C_6\left(\frac{w}{2}\right)^{-6} |z_1-z_2|^{-}$$

$$C_{\alpha\beta\gamma\xi} = \frac{\left(\frac{w}{2}\right)^{10}G^4}{C_6}\int dR_1dR_2d\theta_1d\theta_2R_1R_2\frac{|z_1-z_2|^{-6}}{|H+|z_1-z_2|^{-6}|^2}\left(\phi_\alpha(z_1)\phi_\beta(z_2)+\phi_\alpha(z_2)\phi_\beta(z_1)\right)^*\left(\phi_\gamma(z_1)\phi_\xi(z_2)+\phi_\gamma(z_2)\phi_\xi(z_1)\right)$$

$$H \equiv \frac{2\delta_2}{C_6\left(\frac{w}{2}\right)^{-6}}$$

In this form it is clear that there is only a single dimensionless parameter H which has non-trivial effects. In fact, calculating C for any set of modes as a function of H would completely characterize the problem (limited by the assumptions made wayy above). Note that the strong interaction limit is $H \ll 1$. The weak interaction limit is not as simple to specify since there is always a distance small enough that H is less than $|z_1 - z_2|^{-6}$; but I suspect a useful expansion or something could still be done for that limit. Anyway, for the moment my focus is on elsewhere, but I should return to those limiting cases, especially as a function of mode choices.

$$B_{\alpha\beta\gamma\xi} = \left(\frac{w}{2}\right)^4 G^4 \int dR_1dR_2d\theta_1d\theta_2R_1R_2\left(\frac{\phi_\alpha(z_1)\phi_\beta(z_2)+\phi_\alpha(z_2)\phi_\beta(z_1)}{2\delta_2+C_6\left(\frac{w}{2}\right)^{-6}|z_1-z_2|^{-6}}\right)^*\phi_\gamma(z_1)\phi_\xi(z_2)$$

$$B_{\alpha\beta\gamma\xi} = \frac{\left(\frac{w}{2}\right)^{10}G^4}{C_6}\int dR_1dR_2d\theta_1d\theta_2R_1R_2\left(\frac{\phi_\alpha(z_1)\phi_\beta(z_2)+\phi_\alpha(z_2)\phi_\beta(z_1)}{H+|z_1-z_2|^{-6}}\right)^*\phi_\gamma(z_1)\phi_\xi(z_2)$$

..

$$G_{\gamma\xi} \equiv \sqrt{\frac{1}{2}A_{\gamma\xi}}.$$

$$A_{\gamma\xi} = \int d^3x_1 \int d^3x_2 \left|\frac{g_\gamma(x_1)g_\xi(x_2)+g_\gamma(x_2)g_\xi(x_1)}{2\delta_2+U(|x_1-x_2|)}\right|^2$$

$$A_{\gamma\xi} = \frac{\left(\frac{w}{2}\right)^{16} G^4}{C_6^2} \int dR_1 dR_2 d\theta_1 d\theta_2 R_1 R_2 \left| \frac{\phi_\gamma(z_1)\phi_\xi(z_2) + \phi_\gamma(z_2)\phi_\xi(z_1)}{H + |z_1 - z_2|^{-6}} \right|^2$$

Also the simple single mode integral:

$$G_m^2 \equiv \sum_k^{N_{at}} |g_{km}|^2$$

$$G_\alpha = \sqrt{\int d^2x \, |g_\alpha(x)|^2}$$

$$G_\alpha = \left(\frac{w}{2}\right) G \sqrt{\int d^2z \, |\phi_\alpha(z)|^2}$$

$$G_\alpha = \frac{w}{2} G$$

This form is correct for a **homogeneous atomic sample** in which every mode has total coupling G.

Now, of course, one thing this is revealing is that I forgot the spacing factor when converting my discrete sums to integrals, and so I ended up with a bunch of extra factors of $w/2$. Since I made the same mistake everywhere, they should all cancel out lol. But let's just redefine things:

Remember that the "physical" G, which you would want to actually use in the effective Hamiltonian, is simply G :) Here I will use the most convenient things to make the formulae transparent.

$$\tilde{G}_\alpha \equiv 1$$

$$\tilde{G}_{\gamma\xi} \equiv \sqrt{\frac{1}{2}\tilde{A}_{\gamma\xi}}.$$

$$\tilde{A}_{\gamma\xi} = \int dR_1 dR_2 d\theta_1 d\theta_2 R_1 R_2 \left| \frac{\phi_\gamma(z_1)\phi_\xi(z_2) + \phi_\gamma(z_2)\phi_\xi(z_1)}{H + |z_1 - z_2|^{-6}} \right|^2$$

$$\tilde{B}_{\alpha\beta\gamma\xi} = \int dR_1 dR_2 d\theta_1 d\theta_2 R_1 R_2 \left(\frac{\phi_\alpha(z_1)\phi_\beta(z_2) + \phi_\alpha(z_2)\phi_\beta(z_1)}{H + |z_1 - z_2|^{-6}} \right)^* \phi_\gamma(z_1)\phi_\xi(z_2)$$

$$\delta\Omega_{\alpha\beta\gamma\xi} = \Omega \left(-i \frac{\tilde{B}_{\alpha\beta\gamma\xi}}{\tilde{G}_{\alpha\beta}\tilde{G}_\gamma\tilde{G}_\xi\sqrt{1+\delta_{\alpha\beta}}} - \frac{1}{1+\delta_{\alpha\beta}} \left(\delta_{\alpha\gamma}\delta_{\beta\xi} + \delta_{\alpha\xi}\delta_{\beta\gamma}\right) \right)$$

$$\tilde{C}_{\alpha\beta\gamma\xi} = \int dR_1 dR_2 d\theta_1 d\theta_2 R_1 R_2 \frac{|z_1 - z_2|^{-6}}{|H + |z_1 - z_2|^{-6}|^2} \left(\phi_\alpha(z_1)\phi_\beta(z_2) + \phi_\alpha(z_2)\phi_\beta(z_1)\right)^* \left(\phi_\gamma(z_1)\phi_\xi(z_2) + \phi_\gamma(z_2)\phi_\xi(z_1)\right)$$

$$U_{a\beta\gamma\xi} = C_6 \left(\frac{w}{2}\right)^{-6} \left(\frac{\tilde{C}_{\alpha\beta\gamma\xi}}{2\tilde{G}_{\alpha\beta}\tilde{G}_{\gamma\xi}\sqrt{(1+\delta_{\gamma\xi})(1+\delta_{\alpha\beta})}} \right)$$

3. Reduction to 3D integrals

We've made great progress, simplifying the problem to three dimensionless integrals. Just one more step (as basically done in the lyx note above): using the rotation ~symmetry with LLL wavefunctions to reduce the 4D integrals to 3D integrals. In case we ever want to look at non-lowest LL, I'll use a generic form of the radial wavefunction here, but labeled with a single index for convenience.

$$\phi_\gamma(r,\theta) = \Phi_\gamma(r)e^{i\gamma\theta}$$

$$z \equiv re^{i\theta}$$

UPDATE: I'm adding factors of H in numerators so that the relevant physical parameters all come out the same but the integrals are always O(1) regardless of H

$$\tilde{A}_{\gamma\xi}(H) = \int dR_1 dR_2 d\Delta\theta \times H^2 2\pi R_1 R_2 \left| \frac{\Phi_\gamma(R_1)\Phi_\xi(R_2)e^{i(\gamma-\xi)\Delta\theta} + \Phi_\gamma(R_2)\Phi_\xi(R_1)}{H + |(R_1^2 \sin^2\Delta\theta) + (R_1\cos(\Delta\theta) - R_2)^2|^{-3}} \right|^2$$

$$\tilde{B}_{\alpha\beta\gamma\xi}(H) = \delta_{\alpha+\beta,\gamma+\xi} \int dR_1 dR_2 d\Delta\theta \times H 2\pi R_1 R_2 \left(\frac{\Phi_\alpha(r_1)\Phi_\beta(r_2)e^{i\alpha\Delta\theta} + \Phi_\alpha(r_2)\Phi_\beta(r_1)e^{i\beta\Delta\theta}}{H + \left|(R_1^2 \sin^2\Delta\theta) + (R_1\cos(\Delta\theta) - R_2)^2\right|^{-3}} \right)^* e^{i\gamma\Delta\theta}\Phi_\gamma(r_1)\Phi_\xi(r_2)$$

$$\tilde{C}_{\alpha\beta\gamma\xi}(H) = \delta_{\alpha+\beta,\gamma+\xi} \int dR_1 dR_2 d\theta_1 \times H^2 2\pi R_1 R_2 \frac{\left((R_1^2 \sin^2\Delta\theta) + (R_1\cos(\Delta\theta) - R_2)^2\right)^{-3}}{\left|H + \left((R_1^2 \sin^2\Delta\theta) + (R_1\cos(\Delta\theta) - R_2)^2\right)^{-3}\right|^2} \left(\Phi_\alpha(r_1)\Phi_\beta(r_2)e^{i\alpha\Delta\theta} + \Phi_\alpha(r_2)\Phi_\beta\right.$$

Note that the "integrand" functions in python will include everything after the cross. Don't forget the 2π when calculating the complete value!

D. Numerical integration using scipy; testing code

https://docs.scipy.org/doc/scipy/reference/tutorial/integrate.html
Looks like a fantastic package! Can see how long it takes to do the 3D integrals, and if it's fast you can go ahead with the full 5D version including longitudinal instead.
Seriously, looks so convenient to use. You just define the limits of inner integrals as functions of the values of the outer variables (each step further into the integral chain means your limits should be a function of an additional variable). Copious use of lambda functions is convenient. But seriously, this is such an intuitively convenient approach to numerical integration. **And it returns an error bound!** Love it!
(as it turns out, matlab actually has an equivalent integrate3 which works the same way)
Also, an intriguing package option for handling units: https://pint.readthedocs.io/en/0.11/
Want to try that sometime :)

- initial tests worked well; everything is basically in order
- but once I implemented some of the real integrands (ex. the integrand of C) the scipy integrate function seemed to run interminably
  - not sure if the default tolerances are unreasonable or if there is some bug in my code
  - confirmed that the integrand shrinks sufficiently quickly that the integral should converge
  - confirmed that with sufficiently generous tolerance the integral converges quickly
  - found a tolerance at which the integral only takes about 20 seconds
    - tightening tolerance by another factor of 10 caused runtime to balloon to 90 seconds (next was 170 seconds, so the scaling is actually favorable)

- **and increasing tolerance does seem to produce compatible results**
- pasted1.png

- **SO, besides wanting it to run faster (good thing I reduced to 3D at least!), I'll need better tests to decide whether or not it's really working**

- I need some better tests! Do I have any preconceived expectations?
  - Here's a good place to start

$$\delta\Omega_{\alpha\beta\gamma\xi} = \Omega\left(-i\frac{\tilde{B}_{\alpha\beta\gamma\xi}}{\tilde{G}_{\alpha\beta}\sqrt{1+\delta_{\alpha\beta}}} - \frac{1}{1+\delta_{\alpha\beta}}\left(\delta_{\alpha\gamma}\delta_{\beta\xi} + \delta_{\alpha\xi}\delta_{\beta\gamma}\right)\right)$$

* when the interactions are negligible ($H \gg 1$) then $\delta\Omega_{\alpha\beta\gamma\xi}$ should go to zero. So: **[UPDATE: PASSES]**
  - if $\alpha = \gamma$ and $\beta = \xi$ (or vice versa), but $\alpha \neq \beta$, we should have $\tilde{B}_{\alpha\beta\gamma\xi} == \tilde{G}_{\alpha\beta}$
  - yup it works!
  - if we also have $\alpha = \beta$ (which thne implies ALL indices are equal), then we expect $\tilde{B}_{\alpha\beta\gamma\xi} == \sqrt{2}\tilde{G}_{\alpha\beta}$
  - first attempts failed, and I found a bug: was conjugating twice in B lol
  - ended up being pretty damn obvious because B was coming out negative
  - **after fixing that bug, with H=1000,** $B \approx\approx \sqrt{2}G$ **!! Yay** (with all in mode 6)
  - if angular momentum conserved but modes don't match, expect B/G to approach 0
  - that is indeed what I found as well!
* when the interactions are huge ($H \ll 1$), I expect $B/G \to 0$; so it's not super specific, but it's certainly a thing to check
  - takes much longer for integral to converge when interactions are strong!
  - may just be a result of my tolerance settings, not really sure
  - well, with $H = 0.1$, still get $B/G = 0.96$, when using an L=6 and an L=2
  - how about for two excitations in the same mode? interactions probably more relevant:
  - nope, still didn't see much suppression
  - switching to imaginary H because that's what we have when we're mostly considering Rydberg decay (not energy shift)
  - maybe $H = 0.1$ just isn't small enough?
  - Yeah, this limit behaves as expected, it just gets there more slowly than I expected
  - even with all in L=0 and $H = 10^{-6}i$, B/G=0.31; it's shrinking, but quite slowly
  - when $H = 10^{-12}i$, B/G=0.32 still... **that's fishy, maybe an issue of the integration tolerance**
  - **Nope I made the tolerance a lot tighter and got no change... it seems like over a WIDE range of H I get the same result, B/G~=0.316**
  - Is this real?! or do I have some issues?
  - Okay, I think it's real, which is hilarious:
    Lolz let's see if this limit of ~0.32 is actually real (it's probably mode dependent, but anyway):

$$\tilde{G}_{\gamma\xi} \equiv \sqrt{\frac{1}{2}\tilde{A}_{\gamma\xi}}$$

$$\tilde{A}_{\gamma\xi}(H) = \int dR_1 dR_2 d\Delta\theta \times H^2 2\pi R_1 R_2 \left| \frac{\Phi_\gamma(R_1)\Phi_\xi(R_2)e^{i(\gamma-\xi)\Delta\theta} + \Phi_\gamma(R_2)\Phi_\xi(R_1)}{H + |(R_1^2 \sin^2\Delta\theta) + (R_1\cos(\Delta\theta) - R_2)^2|^{-3}} \right|^2$$

$$\tilde{B}_{\alpha\beta\gamma\xi}(H) = \delta_{\alpha+\beta,\gamma+\xi} \int dR_1 dR_2 d\Delta\theta \times H 2\pi R_1 R_2 \left(\frac{\Phi_\alpha(r_1)\Phi_\beta(r_2)e^{i\alpha\Delta\theta} + \Phi_\alpha(r_2)\Phi_\beta(r_1)e^{i\beta\Delta\theta}}{H + \left|(R_1^2 \sin^2\Delta\theta) + (R_1\cos(\Delta\theta) - R_2)^2\right|^{-3}} \right)^* e^{i\gamma\Delta\theta}\Phi_\gamma(r_1$$

$$\frac{B_{\alpha\beta\gamma\xi}}{G_{\alpha\beta}} = \delta_{\alpha+\beta,\gamma+\xi}\sqrt{4\pi}\frac{\int dR_1 dR_2 d\Delta\theta \times R_1 R_2 \left(\frac{\Phi_\alpha(r_1)\Phi_\beta(r_2)e^{i\alpha\Delta\theta} + \Phi_\alpha(r_2)\Phi_\beta(r_1)e^{i\beta\Delta\theta}}{H + \left|(R_1^2 \sin^2\Delta\theta) + (R_1\cos(\Delta\theta) - R_2)^2\right|^{-3}} \right)^* e^{i\gamma\Delta\theta}\Phi_\gamma(r_1)\Phi_\xi(r_2)}{\sqrt{\int dR_1 dR_2 d\Delta\theta \times R_1 R_2 \left| \frac{\Phi_\alpha(r_1)\Phi_\beta(r_2)e^{i(\gamma-\xi)\Delta\theta} + \Phi_\alpha(r_2)\Phi_\beta(r_1)(R_1)}{H + |(R_1^2 \sin^2\Delta\theta) + (R_1\cos(\Delta\theta) - R_2)^2|^{-3}} \right|^2}}$$

$$\frac{B_{\alpha\beta\gamma\xi}}{G_{\alpha\beta}} = \delta_{\alpha+\beta,\gamma+\xi}\sqrt{4\pi}\frac{\int dR_1 dR_2 d\Delta\theta \times R_1 R_2 \left|(R_1^2 \sin^2\Delta\theta) + (R_1\cos(\Delta\theta) - R_2)^2\right|^3 \left(\frac{\Phi_\alpha(r_1)\Phi_\beta(r_2)e^{i\alpha\Delta\theta} + \Phi_\alpha(r_2)\Phi}{H\left|(R_1^2 \sin^2\Delta\theta) + (R_1\cos(\Delta\theta)\right.} \right.}{\sqrt{\int dR_1 dR_2 d\Delta\theta \times R_1 R_2 \left|(R_1^2 \sin^2\Delta\theta) + (R_1\cos(\Delta\theta) - R_2)^2\right|^6 \left| \frac{\Phi_\alpha(r_1)\Phi_\beta(r_2)e^{i(\gamma}}{H\left|(R_1^2 \sin^2\Delta\theta)\right.} \right.}}$$

The case that I used in the numerics was $\alpha = \beta = \gamma = \xi = 0$, so let's just start there for convenience, because it will definitely make it easy to focus on certain areas:

$$\frac{B_{0000}}{G_{00}} = \sqrt{4\pi}\frac{\int dR_1 dR_2 d\Delta\theta \times R_1 R_2 \left|(R_1^2 \sin^2\Delta\theta) + (R_1\cos(\Delta\theta) - R_2)^2\right|^3 \left(\frac{\Phi_\alpha(r_1)\Phi_\beta(r_2) + \Phi_\alpha(r_2)\Phi_\beta(r_1)}{H\left|(R_1^2 \sin^2\Delta\theta) + (R_1\cos(\Delta\theta) - R_2)^2\right|^3 + 1} \right.}{\sqrt{\int dR_1 dR_2 d\Delta\theta \times R_1 R_2 \left|(R_1^2 \sin^2\Delta\theta) + (R_1\cos(\Delta\theta) - R_2)^2\right|^6 \left| \frac{\Phi_\alpha(r_1)\Phi_\beta(r_2) + \Phi_\alpha(r_2)\Phi_\beta}{H\left|(R_1^2 \sin^2\Delta\theta) + (R_1\cos(\Delta\theta) -\right.} \right.}}$$

- We have (apologies, but capital R and lowercase r indicate the same variable here... lazy to fix)
-

$$\Phi_0(r) = \frac{1}{\sqrt{2\pi}} e^{-|z|^2/4}$$

$$\frac{B_{0000}}{G_{00}} = \sqrt{4\pi}\frac{\int dR_1 dR_2 d\Delta\theta \times R_1 R_2 \left|(R_1^2 \sin^2\Delta\theta) + (R_1\cos(\Delta\theta) - R_2)^2\right|^3 \frac{1}{4\pi^2} \left(\frac{2e^{-(r_1^2+r_2^2)/4}}{H\left|(R_1^2 \sin^2\Delta\theta) + (R_1\cos(\Delta\theta) - R_2)^2\right|} \right.}{\sqrt{\int dR_1 dR_2 d\Delta\theta \times R_1 R_2 \left|(R_1^2 \sin^2\Delta\theta) + (R_1\cos(\Delta\theta) - R_2)^2\right|^6 \frac{1}{4\pi^2} \left| \frac{2e^{-(r_1^2+r_2^2)/4}}{H\left|(R_1^2 \sin^2\Delta\theta) + (R_1\cos(\Delta\theta)\right.} \right.}}$$

- Easiest version would be if you can drop H because it's small... I'm a smidge worried about that, since there should be some R where that term is not small, but perhaps the gaussian has already killed it at that point. Let's proceed and we can always try again if the result is not self-consistent:

$$\frac{B_{0000}}{G_{00}} = \frac{\sqrt{4\pi}}{2\pi}\frac{\int dR_1 dR_2 d\Delta\theta \times R_1 R_2 \left|(R_1^2 \sin^2\Delta\theta) + (R_1\cos(\Delta\theta) - R_2)^2\right|^3 e^{-(r_1^2+r_2^2)/2}}{\sqrt{\int dR_1 dR_2 d\Delta\theta \times R_1 R_2 \left|(R_1^2 \sin^2\Delta\theta) + (R_1\cos(\Delta\theta) - R_2)^2\right|^6 e^{-(r_1^2+r_2^2)/2}}}$$

$$\frac{B_{0000}}{G_{00}} = \frac{\sqrt{\pi}}{\pi}\frac{\int dR_1 dR_2 d\Delta\theta \times R_1 R_2 \left|(R_1^2 \sin^2\Delta\theta) + (R_1\cos(\Delta\theta) - R_2)^2\right|^3 e^{-(r_1^2+r_2^2)/2}}{\sqrt{\int dR_1 dR_2 d\Delta\theta \times R_1 R_2 \left|(R_1^2 \sin^2\Delta\theta) + (R_1\cos(\Delta\theta) - R_2)^2\right|^6 e^{-(r_1^2+r_2^2)/2}}}$$

$$\frac{B_{0000}}{G_{00}} = \frac{1}{\sqrt{\pi}}\frac{\int dR_1 dR_2 d\Delta\theta \times R_1 R_2 \left|\left(R_1^2 + R_2^2 - 2R_1R_2\cos\theta\right)\right|^3 e^{-(r_1^2+r_2^2)/2}}{\sqrt{\int dR_1 dR_2 d\Delta\theta \times R_1 R_2 \left|(R_1^2 + R_2^2 - 2R_1R_2\cos\theta)\right|^6 e^{-(r_1^2+r_2^2)/2}}}$$

·

$$\sqrt{\int dR_1 dR_2 d\Delta\theta \times R_1 R_2 \left|(R_1^2+R_2^2-2R_1R_2\cos\theta)\right|^6 e^{-(r_1^2+r_2^2)/2}} ==== \sqrt{\frac{1}{2}\int dR_1 dR_2 d\Delta\theta \times H^2 2\pi R_1 R_2 \left|\frac{\Phi}{H}\right.}$$

·

$$\sqrt{\int dR_1 dR_2 d\Delta\theta \times R_1 R_2 \left|(R_1^2+R_2^2-2R_1R_2\cos\theta)\right|^6 e^{-(r_1^2+r_2^2)/2}} ==== \sqrt{\frac{1}{2}H^2 2\pi \left(2\frac{1}{\sqrt{2\pi}}\frac{1}{\sqrt{2\pi}}\right)^2 \int dR_1 dR_2}$$

·

$$\sqrt{\int dR_1 dR_2 d\Delta\theta \times R_1 R_2 \left|(R_1^2+R_2^2-2R_1R_2\cos\theta)\right|^6 e^{-(r_1^2+r_2^2)/2}} ==== \pi^{-1/2}\sqrt{H^2 \int dR_1 dR_2 d\Delta\theta \times R_1 R_2 |(}$$

- **So the result I'm getting is a constant B/G=0.14; That's not the same as my other integrals, BUT I have numerically confirmed that the difference from a small but finite H is indeed negligible. So whatever's wrong is something else =P Could be in my functions for A and B, or it could be here, perhaps in some power or simply some constant factor... which is close to 9/4, fwiw.**
- - found 1st error, was taking sqrt inside the integrand... oy vey that was rough
- - now overall result is off by a factor of pi... so let's hunt some more! But we should be close:
- .ROFL I found two more problems with my test integral. That's what I get for being lazy! And not properly handling taking things in and out of my sqrt =P Anyway, the original numerical code seems good, and now the test agrees with it!
- **.turns out the correct OVERALL answer is $B_{0000}/G_{00} = 1/\pi$. The result is mode dependent, but it's always some non-zero constant**
- .
- Anyway, this was all very helpful. It's a nice verification of the original code, and it also gave me a chance to go through and check all that code thoroughly by hand after a night's sleep. Everything looks correct to me.
- For context, what is H typically in our real experiments? For Laughlin we typically had $\delta_2 \approx I\frac{\gamma_R}{2} \approx I * 0.05$ MHz; C6 =1.5×10^8MHz*microns^6. $w = 20$microns.

$$H \equiv \frac{2\delta_2}{C_6\left(\frac{w}{2}\right)^{-6}} \approx 0.0007i$$

Let me now check on the limit of contact interactions and look at the interaction strengths U as a function of the chosen modes

First, some results from a super old matlab code for the contact interaction limit (I consider this a nice "independent" check... though it'll be a pain if they turn out not to agree):

- old matlab integrals:
  - U_{3333}/U_{6666} =1.385
  - U_{3333}/U_{3636}=0.952
  - U_{3333}/U_{9999}=1.685
- new python code with $H = 100$ limit (updated 04/23/20 at 11:32 am):
  - pasted4.png

– **the only disagreement is a factor of 2 on U3333/U3636, but that's just a difference of definitions between here and MATLAB (MATLAB effective model had terms like$|33\rangle U_{3333} \langle 33|$; here it's $U_{3333}a_3^\dagger a_3^\dagger a_3 a_3$; so overall this result constitutes AGREEMENT on the actual Hamiltonian terms =D)**

So, let's take a closer look at the C integral in the limit of huge H:

$$\tilde{C}_{\alpha\beta\gamma\xi}(H) = \delta_{\alpha+\beta,\gamma+\xi} \int dR_1 dR_2 d\theta_1 \times H^2 2\pi R_1 R_2 \frac{\left((R_1^2 \sin^2 \Delta\theta) + (R_1 \cos(\Delta\theta) - R_2)^2\right)^{-3}}{\left|H + \left((R_1^2 \sin^2 \Delta\theta) + (R_1 \cos(\Delta\theta) - R_2)^2\right)^{-3}\right|^2} \left(\Phi_\alpha(r_1)\Phi_\beta(r_2)e^{i\alpha\Delta\theta} + \Phi_\alpha(r_2)\Phi_\beta\right.$$

We certainly do NOT just want to drop the other term in the denominator, because for small enough separation it diverges, so it's not negligible no matter how huge H becomes. BUT we can note that our integral will be dominated by tiny separations between the atoms, meaning small $|R_1 - R_2|$ and small $\Delta\theta$.

$$\tilde{C}_{\alpha\beta\gamma\xi}(H) = \delta_{\alpha+\beta,\gamma+\xi} \int dR_1 dR_2 d\theta_1 \times H^2 2\pi R_1 R_2 \frac{\left(R_1^2 \Delta\theta^2 + (R_1 - R_2)^2\right)^{-3}}{\left|H + \left(R_1^2 \Delta\theta^2 + (R_1 - R_2)^2\right)^{-3}\right|^2} \left(\Phi_\alpha(r_1)\Phi_\beta(r_2) + \Phi_\alpha(r_2)\Phi_\beta(r_1)\right)^* \left(\Phi_\gamma(r_1)\Phi_\xi(r_2\right.$$

$$\tilde{C}_{\alpha\beta\gamma\xi}(H) = \delta_{\alpha+\beta,\gamma+\xi} \int dR_1 dR_2 d\theta_1 \times H^2 2\pi R_1 R_2 \frac{\left(R^2 \Delta\theta^2 + \Delta R^2\right)^{-3}}{\left|H + \left(R^2 \Delta\theta^2 + \Delta R^2\right)^{-3}\right|^2} \left(\Phi_\alpha(r_1)\Phi_\beta(r_2) + \Phi_\alpha(r_2)\Phi_\beta(r_1)\right)^* \left(\Phi_\gamma(r_1)\Phi_\xi(r_2) + \Phi_\gamma\right.$$

$$\tilde{C}_{\alpha\beta\gamma\xi}(H) = \delta_{\alpha+\beta,\gamma+\xi} \int dR d\Delta R d\Delta\theta \times H^2 2\pi R^2 \frac{\left(R^2 \Delta\theta^2 + \Delta R^2\right)^3}{\left|H \left(R^2 \Delta\theta^2 + \Delta R^2\right)^3 + 1\right|^2} 4 \left(\Phi_\alpha(R)\Phi_\beta(R)\right)^* \left(\Phi_\gamma(R)\Phi_\xi(R)\right)$$

$$\tilde{C}_{\alpha\beta\gamma\xi}(H) = \delta_{\alpha+\beta,\gamma+\xi} \int dR d\Delta R d\Delta\theta \times H^2 8\pi R^2 \frac{\left(R^2 \Delta\theta^2 + \Delta R^2\right)^3}{\left|H \left(R^2 \Delta\theta^2 + \Delta R^2\right)^3 + 1\right|^2} \left(\Phi_\alpha(R)\Phi_\beta(R)\right)^* \left(\Phi_\gamma(R)\Phi_\xi(R)\right)$$

I'm going to press forward with this because it's interesting, BUT keep in mind that in reality short range potential becomes $C_3 R^{-3}$ and then eventually breaks down even further... so it's not clear that this limit is realistic or relevant. BUT at the moment I'm more interested in just checking my calculation. And I am curious about whether an R^{-6} potential becomes contact-like when it is sufficiently weak. My intuition is that it should... "long range" doesn't start until R^{-3} in 3 dimensions. Anyway, let's use LLL wavefunctions because it should allow further simplification:

$$\tilde{C}_{\alpha\beta\gamma\xi}(H) = \delta_{\alpha+\beta,\gamma+\xi} \int dR d\Delta R d\Delta\theta \times H^2 8\pi R^2 \frac{\left(R^2 \Delta\theta^2 + \Delta R^2\right)^3}{\left|H \left(R^2 \Delta\theta^2 + \Delta R^2\right)^3 + 1\right|^2} R^{2(\alpha+\beta)} e^{-R^2} \frac{(2\pi)^{-2}}{\sqrt{2^\alpha \alpha! 2^\beta \beta! 2^\gamma \gamma! 2^\xi \xi!}}$$

$$\tilde{C}_{\alpha\beta\gamma\xi}(H) = \delta_{\alpha+\beta,\gamma+\xi} \int dR d\Delta R d\Delta\theta \times H^2 \frac{8\pi (2\pi)^{-2}}{\sqrt{2^\alpha \alpha! 2^\beta \beta! 2^\gamma \gamma! 2^\xi \xi!}} \frac{\left(R^2 \Delta\theta^2 + \Delta R^2\right)^3}{\left|H \left(R^2 \Delta\theta^2 + \Delta R^2\right)^3 + 1\right|^2} R^{2(\alpha+\beta+1)} e^{-R^2}$$

The integral should be dominated by the value near the peak (hokey explanation: integral is 3D and the ratio has Δ^6 in the numerator and Δ^{12} in the denominator which are steep power laws). What is that value?

My original attempt (in LyX note) was fine, but it then became clear that I should have gone to a new ~polar coordinate system. (I'm going to ignore the θ integration limits; since the integrand near its peak will dominate the entire integral, they can be expanded to $\pm\infty$ or whatever makes you happy). And ΔR can also be integrated between $\pm\infty$, so our new angle Θ goes over a full 2π.

$$\tilde{C}_{\alpha\beta\gamma\xi}(H) = \delta_{\alpha+\beta,\gamma+\xi} \int dR d\Delta R d(R\Delta\theta) \times H^2 \frac{8\pi(2\pi)^{-2}}{\sqrt{2^\alpha \alpha! 2^\beta \beta! 2^\gamma \gamma! 2^\xi \xi!}} \frac{\left(R^2\Delta\theta^2 + \Delta R^2\right)^3}{\left|H\left(R^2\Delta\theta^2 + \Delta R^2\right)^3 + 1\right|^2} R^{2(\alpha+\beta)+1} e^{-R^2}$$

$$\rho^2 \equiv R^2\Delta\theta^2 + \Delta R^2$$

$$\tilde{C}_{\alpha\beta\gamma\xi}(H) = \delta_{\alpha+\beta,\gamma+\xi} \int dR d\rho d\Theta \times H^2 \frac{8\pi(2\pi)^{-2}}{\sqrt{2^\alpha \alpha! 2^\beta \beta! 2^\gamma \gamma! 2^\xi \xi!}} \frac{\rho\left(\rho\right)^6}{\left|H\left(\rho\right)^6 + 1\right|^2} R^{2(\alpha+\beta)+1} e^{-R^2}$$

$$\tilde{C}_{\alpha\beta\gamma\xi}(H) = \delta_{\alpha+\beta,\gamma+\xi} \int dR d\rho d\Theta \times H^2 \frac{2}{\pi\sqrt{2^\alpha \alpha! 2^\beta \beta! 2^\gamma \gamma! 2^\xi \xi!}} \frac{\rho^7}{\left|H\rho^6 + 1\right|^2} R^{2(\alpha+\beta)+1} e^{-R^2}$$

Notice that the integral over the new angle is trivial

$$\tilde{C}_{\alpha\beta\gamma\xi}(H) = \delta_{\alpha+\beta,\gamma+\xi} \int dR d\rho \times H^2 \frac{4\pi}{\pi\sqrt{2^\alpha \alpha! 2^\beta \beta! 2^\gamma \gamma! 2^\xi \xi!}} \frac{\rho^7}{\left|H\rho^6 + 1\right|^2} R^{2(\alpha+\beta)+1} e^{-R^2}$$

$$H \equiv i|H|$$

$$\tilde{C}_{\alpha\beta\gamma\xi}(H) = \delta_{\alpha+\beta,\gamma+\xi} \int dR d\rho \times H^2 \frac{4\pi}{\pi\sqrt{2^\alpha \alpha! 2^\beta \beta! 2^\gamma \gamma! 2^\xi \xi!}} \frac{\rho^7}{\left|H\right|^2 \rho^{12} + 1} R^{2(\alpha+\beta)+1} e^{-R^2}$$

And now also notice that the whole thing factorizes

$$\tilde{C}_{\alpha\beta\gamma\xi}(H) = \delta_{\alpha+\beta,\gamma+\xi} H^2 \frac{4\pi}{\pi\sqrt{2^\alpha \alpha! 2^\beta \beta! 2^\gamma \gamma! 2^\xi \xi!}} \int_0^\infty dR R^{2(\alpha+\beta)+1} e^{-R^2} \int_0^\infty d\rho \frac{\rho^7}{\left|H\right|^2 \rho^{12} + 1}$$

This is looking a LOT like the contact interaction limit, where there is some geometric factor from the ρ integral and the R integral captures the single particle wavefunction shapes. **In other words, I think we have indeed recovered the contact interaction limit.** There was probably a nicer way to do this, and maybe we could define a scattering length or something... but whatever I'm pretty happy with this. We should get some H dependence from that last integral, so let's check it out:

$$\int_0^\infty d\rho \frac{\rho^7}{\left|H\right|^2 \rho^{12} + 1}$$

Should be dominated by the peak of the integrand; find the peak:

$$F(\rho) = \rho^7 \left(|H|^2\rho^{12} + 1\right)^{-1}$$

$$F'(\rho) = 7\rho^6 \left(|H|^2\rho^{12} + 1\right)^{-1} - 12\rho^7|H|^{-2}\rho^{11} \left(|H|^2\rho^{12} + 1\right)^{-2}$$

$$0 = 7\left(|H|^2\rho^{12} + 1\right) - 12|H|^2\rho^{12}$$

$$0 = 7 - 5|H|^2\rho^{12}$$

$$\rho_0 = \left(\frac{7}{5}\right)^{1/12} |H|^{-1/6}$$

$$F(\rho_0) = \frac{(7/5)^{7/12} H^{-7/6}}{(7/5)+1}$$

$$F(\rho_0) = \frac{5^{5/12} 7^{7/12}}{12 H^{7/6}}$$

$$\rho \approx \rho_0 + \delta$$

$$\int_{-\infty}^{\infty} d\delta \frac{(\rho_0+\delta)^7}{|H|^2 (\rho_0+\delta)^{12} + 1}$$

$$\int_{-\infty}^{\infty} d\rho \frac{\rho_0^7 \left(1 + 7\rho_0^{-1}\delta\right)}{\left(|H|^2 \rho_0^{12} + 1\right)\left(1 + \frac{12H^2\rho_0^{11}\delta}{|H|^2\rho_0^{12}+1}\right)}$$

$$F(\rho_0) \int_{-\infty}^{\infty} d\rho \frac{\left(1 + 7\rho_0^{-1}\delta\right)}{\left(1 + \frac{12H^2\rho_0^{11}\delta}{|H|^2\rho_0^{12}+1}\right)}$$

$$F(\rho_0) \left(|H|^2 \rho_0^{12} + 1\right) \int_{-\infty}^{\infty} d\rho \frac{\left(1 + 7\rho_0^{-1}\delta\right)}{(12/5 + 12H^2\rho_0^{11}\delta)}$$

This integral should be tractable. But I'm a smidge worried that I made the wrong move, because this integrand does not decay sufficiently with δ. And yet I think it SHOULD be okay to assume $\delta \ll 1$. Maybe the large H saves me? As long as I don't integrate to infinity?

Okay that whole thing was fun, but maybe I [Mathematica] can just integrate the original expression...

$$\int_{0}^{\infty} d\rho \frac{\rho^7}{|H|^2 \rho^{12} + 1}$$

Lolz mathematica is struggling. Maybe I can make it easier

$$|H|^{-2} \int_{0}^{\infty} d\rho \frac{\rho^7}{\rho^{12} + \epsilon}$$

$$\epsilon \equiv |H|^{-2} \ll 1$$

$$\rho \approx \rho_0 + \delta$$

$$\rho_0 = \left(\frac{7}{5}\right)^{1/12} |H|^{-1/6}$$

sooo ρ_0 is also small-ish.

$$|H|^{-2} \int_0^\infty d\rho \frac{\rho^7}{\rho^{12} + \epsilon} \approx$$

Okay I don't like that either. How about this:

$$\int_{-\infty}^{\infty} d\delta \frac{\rho_0^7 \left(1 + \delta/\rho_0\right)^7}{|H|^2 \rho_0^{12} \left(1 + \delta/\rho_0\right)^{12} + 1}$$

$$\int_{-\infty}^{\infty} d\delta \frac{\rho_0^7 \left(1 + \delta/\rho_0\right)^7}{\left(|H|^2 \rho_0^{12} + 1\right) \left(1 + \delta/\rho_0\right)^{12} - \left(1 + \delta/\rho_0\right)^{12} + 1}$$

$$\int_{-\infty}^{\infty} d\delta \frac{\rho_0^7 \left(1 + \delta/\rho_0\right)^7}{\left(|H|^2 \rho_0^{12} + 1\right) \left(1 + \delta/\rho_0\right)^{12} - \left(1 + \delta/\rho_0\right)^{12} + 1}$$

THIS IS AN APPROX THAT I REALLY HAVE TO CHECK AFTERWARD:

$$\int_{-\infty}^{\infty} d\delta \frac{\rho_0^7 \left(1 + \delta/\rho_0\right)^7}{\left(|H|^2 \rho_0^{12} + 1\right) \left(1 + \delta/\rho_0\right)^{12}}$$

$$F(\rho_0)\rho_0^5 \int_{-\infty}^{\infty} d\delta \left(\rho_0 + \delta\right)^{-5}$$

$$F(\rho_0)\rho_0^5(-1/6) \int_{-\infty}^{\infty} d\delta \left(\rho_0 + \delta\right)^{-6}$$

LOL ANOTHER TRY: **[function is scale invariant: if you scale the x coordinate by rho_0 then the plot is independent of H] THIS ONE IS THE WINNER!!**

$$\int_0^\infty d\rho \frac{\rho^7}{|H|^2 \rho^{12} + 1}$$

$$\rho = \rho_0(\delta)$$

$$\int_0^\infty d\rho \frac{\rho^7}{|H|^2 \rho^{12} + 1} = \rho_0^8 \int_0^\infty d\delta \frac{(\delta)^7}{(7/5)(\delta)^{12} + 1}$$

OKAY THIS WAS THE RIGHT APPROACH. We have one "hard" integral that we can solve numerically, but it is totally independent of problem parameters (all captured in the coefficient out front) so we just need to calculate that integral once.

FWIW, Mathematica says:

$$\int_0^\infty d\delta \frac{(\delta)^7}{(7/5)(\delta)^{12}+1} = \frac{\left(\frac{5}{7}\right)^{2/3}\pi}{6\sqrt{3}}$$

$$\int_0^\infty d\rho \frac{\rho^7}{|H|^2\rho^{12}+1} = \rho_0^8 \frac{\left(\frac{5}{7}\right)^{2/3}\pi}{6\sqrt{3}}$$

$$\int_0^\infty d\rho \frac{\rho^7}{|H|^2\rho^{12}+1} = |H|^{-4/3}\left(\frac{7}{5}\right)^{2/3} \frac{\left(\frac{5}{7}\right)^{2/3}\pi}{6\sqrt{3}}$$

$$\int_0^\infty d\rho \frac{\rho^7}{|H|^2\rho^{12}+1} = \rho_0^8 \int_0^\infty d\delta \frac{(\delta)^7}{(7/5)(\delta)^{12}+1} = \frac{\pi}{6\sqrt{3}}|H|^{-4/3}$$

You might think that 5/7 can just be replaced based on that factor multiplying δ^{12}, but it's not that simple (Mathematica struggles with the integral when 5/7 is left as a free variable).

I verified this final result using Mathematica.

$$\boxed{\int_0^\infty d\rho \frac{\rho^7}{|H|^2\rho^{12}+1} = \frac{\pi}{6\sqrt{3}}|H|^{-4/3}}$$

Which brings us back to the original problem; the large H limit and the degree to which it looks like contact interactions:

$$\tilde{C}_{\alpha\beta\gamma\xi}(H) = \delta_{\alpha+\beta,\gamma+\xi} H^2 |H|^{-4/3} \frac{4\pi}{6\sqrt{3}} \frac{1}{\sqrt{2^\alpha \alpha! 2^\beta \beta! 2^\gamma \gamma! 2^\xi \xi!}} \int_0^\infty dR R^{2(\alpha+\beta)+1} e^{-R^2}$$

Actually, for that matter, I'm sure Mathematica (or even ME BY HAND lolz) can handle that Gaussian integral. I'll let Mathematica take the general case

$$\boxed{\tilde{C}_{\alpha\beta\gamma\xi}(H) = -\delta_{\alpha+\beta,\gamma+\xi} |H|^{2/3} \frac{\pi}{3\sqrt{3}} \frac{1}{\sqrt{2^\alpha \alpha! 2^\beta \beta! 2^\gamma \gamma! 2^\xi \xi!}} (\alpha+\beta)!}$$

This absolutely looks like contact interactions. Look at the entire derivation: we treated ΔR and $\Delta\theta$ as small, and got a simple numerical coefficient from their finite spread. Other than that coefficient, this is precisely the integral we would perform in the limit of contact interactions. Neat!!

Naturally this does NOT agree with my full result for C. Taking it one step at a time:

- UPDATE: I think it was just an issue with error tolerance. I'm now getting results that agree across the board, in the H=10^4-10^6 range; don't go crazy with 10^12, it's possible but makes error tricky
- **What is the proper pre-factor to make the integrals H-independent?**
  - .

$$\tilde{C}_{\alpha\beta\gamma\xi}(H) = \delta_{\alpha+\beta,\gamma+\xi} \int dR_1 dR_2 d\theta_1 \times H^2 2\pi R_1 R_2 \frac{\left((R_1^2 \sin^2\Delta\theta) + (R_1\cos(\Delta\theta) - R_2)^2\right)^{-3}}{\left|H + \left((R_1^2 \sin^2\Delta\theta) + (R_1\cos(\Delta\theta) - R_2)^2\right)^{-3}\right|^2} \left(\Phi_\alpha(r_1)\Phi_\beta(r_2)e^{i\alpha\Delta\theta}\right.$$

    * In the large H limit we need $|H|^{(4/3)}$ out front, which cancels the $|H|^{-4/3}$ from the integral itself.
    * In the small H limit we drop H (as was done for A and B above) and end up with a constant asymptote. So in the small H limit we want the prefactor to become 1

*

$$(1+|H|^{4/3})$$

* **SO HERE'S A BETTER DEFINITION FOR $\tilde{C}$; should update the code to reflect this one**

–

$$\tilde{C}_{\alpha\beta\gamma\xi}(H) = \delta_{\alpha+\beta,\gamma+\xi}\int dR_1 dR_2 d\theta_1 \times (1+|H|^{4/3}) 2\pi R_1 R_2 \frac{\left((R_1^2\sin^2\Delta\theta) + (R_1\cos(\Delta\theta) - R_2)^2\right)^{-3}}{\left|H + \left((R_1^2\sin^2\Delta\theta) + (R_1\cos(\Delta\theta) - R_2)^2\right)^{-3}\right|^2} \left(\Phi_\alpha(r_1)\Phi_\beta(r\right.$$

– NOW let's check the same limit for the others; each will have different ρ dependence so it seems safest to just take the limit directly

$$\tilde{G}_{\gamma\xi} \equiv \sqrt{\frac{1}{2}\tilde{A}_{\gamma\xi}}$$

$$\tilde{A}_{\gamma\xi}(H) = \int dR_1 dR_2 d\Delta\theta \times H_A 2\pi R_1 R_2 \left|\frac{\Phi_\gamma(R_1)\Phi_\xi(R_2)e^{i(\gamma-\xi)\Delta\theta} + \Phi_\gamma(R_2)\Phi_\xi(R_1)}{H + |(R_1^2\sin^2\Delta\theta) + (R_1\cos(\Delta\theta) - R_2)^2|^{-3}}\right|^2$$

lol turns out the approach above is not suitable here. On reflection it is physically obvious why: in the limit of contact interactions the interaction strength was dominated by nearby atoms, but in the same limit these normalization constants (and Omega) will be *unaffected* by interactions, certainly not dominated by nearby atoms. The thing to do then is drop the interaction potential range term entirely

$$\tilde{A}_{\gamma\xi}(H) = \int dR_1 dR_2 d\Delta\theta \times H_A 2\pi R_1 R_2 \left|\frac{\Phi_\gamma(R_1)\Phi_\xi(R_2)e^{i(\gamma-\xi)\Delta\theta} + \Phi_\gamma(R_2)\Phi_\xi(R_1)}{H}\right|^2$$

$$\tilde{A}_{\gamma\xi}(H) = \int dR_1 dR_2 d\Delta\theta \times \frac{H_A}{|H|^2} 2\pi R_1 R_2 \left|\Phi_\gamma(R_1)\Phi_\xi(R_2)e^{i(\gamma-\xi)\Delta\theta} + \Phi_\gamma(R_2)\Phi_\xi(R_1)\right|^2$$

$$\Phi_l(r) \equiv \frac{1}{\sqrt{2\pi 2^l l!}} r^l e^{-|r|^2/4},$$

$$\tilde{A}_{\gamma\xi}(H) = \int dR_1 dR_2 d\Delta\theta \times \frac{H_A}{|H|^2} 2\pi R_1 R_2 \left|\Phi_\gamma(R_1)\Phi_\xi(R_2)e^{i(\gamma-\xi)\Delta\theta} + \Phi_\gamma(R_2)\Phi_\xi(R_1)\right|^2$$

Honestly, I don't see how to simplify this that much more. Could plug it into mathematica, but whatever.

$$\tilde{B}_{\alpha\beta\gamma\xi}(H) = \delta_{\alpha+\beta,\gamma+\xi}\int dR_1 dR_2 d\Delta\theta \times H_B 2\pi R_1 R_2 \left(\frac{\Phi_\alpha(r_1)\Phi_\beta(r_2)e^{i\alpha\Delta\theta} + \Phi_\alpha(r_2)\Phi_\beta(r_1)e^{i\beta\Delta\theta}}{H + \left|(R_1^2\sin^2\Delta\theta) + (R_1\cos(\Delta\theta) - R_2)^2\right|^{-3}}\right)^* e^{i\gamma\Delta\theta}\Phi_\gamma(r_1)\Phi_\xi(r_2)$$

$$\tilde{B}_{\alpha\beta\gamma\xi}(H) = \delta_{\alpha+\beta,\gamma+\xi}\int dR_1 dR_2 d\Delta\theta \times \frac{H_B}{H} 2\pi R_1 R_2 \left(\Phi_\alpha(R_1)\Phi_\beta(R_2)e^{i\alpha\Delta\theta} + \Phi_\alpha(R_2)\Phi_\beta(R_1)e^{i\beta\Delta\theta}\right)^* e^{i\gamma\Delta\theta}\Phi_\gamma(R_1)\Phi_\xi(R_2)$$

BUT I'm still going to change them so that in the SMALL H limit they are O(1). Here are my latest set of definitions/summary of results:

UPDATE: Actually I think it's a great idea to plug in the LLL wavefunctions and stick them in mathematica =P

$$B_{\alpha\beta\gamma\xi} = \delta_{\alpha+\beta,\gamma+\xi} \int dR_1 dR_2 d\Delta\theta \times (1+|H|) 2\pi R_1 R_2 \left|(R_1^2 \sin^2 \Delta\theta) + (R_1 \cos(\Delta\theta) - R_2)^2\right|^3 \left(\Phi_\alpha(r_1)\Phi_\beta(r_2)e^{i\alpha\Delta\theta} + \Phi_\alpha(r_2)\Phi_\beta(r_1)e^{i\beta\Delta}\right.$$

$$G_{\alpha\beta} = \sqrt{\frac{1}{2}\int dR_1 dR_2 d\Delta\theta \times (1+|H|)^2 2\pi R_1 R_2 \left|(R_1^2 \sin^2 \Delta\theta) + (R_1 \cos(\Delta\theta) - R_2)^2\right|^6 \left|\Phi_\alpha(r_1)\Phi_\beta(r_2)e^{i(\gamma-\xi)\Delta\theta} + \Phi_\alpha(r_2)\Phi_\beta(r_1)(R_1\right.}$$

- trying C
  - Mathematica clearly CAN handle these ANALYTICALLY, at least when given specific integers. Now the trick is getting it to handle arbitrary integers...
  - tried to poke at the form of the integrand a little bit and give mathematica lots of assumptions to help it find a sufficiently simple form
    - $$\tilde{C}_{\alpha\beta\gamma\xi}(H) = \delta_{\alpha+\beta,\gamma+\xi} \int dR_1 dR_2 d\Delta\theta \times 2\pi R_1 R_2 \left(R_1^2 + R_2^2 - 2R_1 R_2 \cos\Delta\theta\right)^3 \left(\Phi_\alpha(r_1)\Phi_\beta(r_2)e^{i\alpha\Delta\theta} + \Phi_\alpha(r_2)\Phi_\beta(r_1\right.$$
    - and still couldn't get it to evaluate :(
  - but it gives such nice simple forms for specific integers! Maybe I can figure out the proper form from that...
    - AT LEAST WHEN ALL INTEGERS ARE EQUAL, SEEMS LIKE I MAY WANT AN EVEN AND AN ODD VERSION :D
    - a=b=c=d=0 $\rightarrow$ 1536
      - remove the 2^-(a+b+c+d)/2 and Sqrt[a!b!c!d!]:
      - 1536
      - 1x
    - a=b=c=d=1 $\rightarrow$ 8448 [11/2x]
      - remove the 2^-(a+b+c+d)/2 and Sqrt[a!b!c!d!]:
      - 33792
      - 22x
      - has an 11 and a 2^2
    - a=b=c=d=2 $\rightarrow$ 6144 [4x]
      - remove the 2^-(a+b+c+d)/2=1/16 and Sqrt[a!b!c!d!]=(2!)^2=4:
      - 393216
      - 256x
      - has a 2^8 OR view as a 16 and a 2^4
    - a=b=c=d=3 $\rightarrow$ 4480/3 [35/36 x]

      - remove the 2^-(a+b+c+d)/2=1/64 and Sqrt[a!b!c!d!]=(3!)^2=36:
      - 3440640
      - 2240x
      - has a 2^6 and 35=5*7
    - a=b=c=d=4 → 520/3 [65/576 x]
      - remove the Sqrt[a!b!c!d!]=(4!)^2=576:
      - 65x
      - remove the 2^-(a+b+c+d)/2=1/256:
      - 16640x
      - has a 13, a 5, and 2^8
    - a=b=c=d=5 → 868/75
      - remove factorial part
      - 217/2x
      - remove exponential part
      - 56 885 248 x
      - has a 55552 and a 2^{10}
    - I didn't find it, and it's very strange. But this is the solution when a=b=c=d from a veeery slow mathematica calculation:
      - pasted6.png

- **Okay Mathematica has helped me see the light. Look again - when you expand, you just get back a bunch of separable integrals. That's why it takes that form, i.e. the sum of lots of different random-looking things.:**
  -
$$\tilde{C}_{\alpha\beta\gamma\xi}(H) = \delta_{\alpha+\beta,\gamma+\xi} \int dR_1 dR_2 d\Delta\theta \times 2\pi R_1 R_2 \left(R_1^2 + R_2^2 - 2R_1 R_2 \cos\Delta\theta\right)^3 \left(\Phi_\alpha(r_1)\Phi_\beta(r_2)e^{i\alpha\Delta\theta} + \Phi_\alpha(r_2)\Phi_\beta(r_1)e^{i\beta\Delta\theta}\right.$$
  - pasted7.png

- **Seems like Mathematica actually kinda struggles with these θ integrals, but I can help! Because they're actually pretty easy.** There are four types, for arbitrary integer n:

$$\int_{-\pi}^{\pi} d\theta e^{in\theta} = 2\pi\delta_{n,0}$$

$$\int_{-\pi}^{\pi} d\theta e^{in\theta} \cos\theta$$

$$\int_{-\pi}^{\pi} d\theta e^{in\theta} \cos^2\theta$$

$$\int_{-\pi}^{\pi} d\theta e^{in\theta} \cos^3\theta$$

Frankly, all of these are pretty easy to handle by hand... and maybe Mathematica would handle them right if I gave it the right assumptions, but I tried and failed lolz:

$$\int_{-\pi}^{\pi} d\theta e^{in\theta} \cos\theta$$

$$\int_{-\pi}^{\pi} d\theta e^{in\theta} \frac{e^{i\theta} + e^{-i\theta}}{2} = 2\pi \frac{\delta_{n,1} + \delta_{n,-1}}{2}$$

Next:

$$\int_{-\pi}^{\pi} d\theta e^{in\theta} \cos^2\theta$$

$$\int_{-\pi}^{\pi} d\theta e^{in\theta} \frac{e^{2i\theta} + 2 + e^{-2i\theta}}{4} = 2\pi \frac{\delta_{n,2} + 2\delta_{n,0} + \delta_{n,-2}}{4}$$

Fun with binomial coefficients! If you wanted a general form you could use that.

$$\int_{-\pi}^{\pi} d\theta e^{in\theta} \cos^3\theta$$

$$\int_{-\pi}^{\pi} d\theta e^{in\theta} \frac{e^{3i\theta} + 3e^{i\theta} + 3e^{-i\theta} + e^{-3i\theta}}{8} = 2\pi \frac{\delta_{n,3} + 3\delta_{n,1} + 3\delta_{n,-1} + \delta_{n,-3}}{8}$$

And all of the radial parts are handled by (I suspect all of the n's that we care about are integer multiples of 2, and so this will just be a factorial, but we'll see, no big deal either way):

pasted8.png

$$\tilde{G}_\alpha \equiv 1$$

$$\tilde{G}_{\gamma\xi} \equiv \sqrt{\frac{1}{2}\tilde{A}_{\gamma\xi}}$$

$$\tilde{A}_{\gamma\xi}(H) = \int dR_1 dR_2 d\Delta\theta \times (1+|H|)^2 2\pi R_1 R_2 \left| \frac{\Phi_\gamma(R_1)\Phi_\xi(R_2)e^{i(\gamma-\xi)\Delta\theta} + \Phi_\gamma(R_2)\Phi_\xi(R_1)}{H + |(R_1^2 \sin^2\Delta\theta) + (R_1\cos(\Delta\theta) - R_2)^2|^{-3}} \right|^2$$

$$\tilde{B}_{\alpha\beta\gamma\xi}(H) = \delta_{\alpha+\beta,\gamma+\xi} \int dR_1 dR_2 d\Delta\theta \times (1+|H|) 2\pi R_1 R_2 \left(\frac{\Phi_\alpha(r_1)\Phi_\beta(r_2)e^{i\alpha\Delta\theta} + \Phi_\alpha(r_2)\Phi_\beta(r_1)e^{i\beta\Delta\theta}}{H + \left|(R_1^2\sin^2\Delta\theta) + (R_1\cos(\Delta\theta) - R_2)^2\right|^{-3}} \right)^* e^{i\gamma\Delta\theta}\Phi_\gamma(r_1)\Phi_\xi(r_2)$$

- $$\tilde{C}_{\alpha\beta\gamma\xi}(H) = \delta_{\alpha+\beta,\gamma+\xi} \int_0^\infty dR_1 \int_{-R_1}^\infty d\Delta_R \int_0^{2\pi} d\Delta\theta \times (1+|H|)^{4/3} 2\pi R_1(R_1+\Delta R) \frac{\left(2R_1(R_1+\Delta R)(1-\cos\Delta\theta) + (\Delta R)^2\right)^{-}}{\left|H + (2R_1(R_1+\Delta R)(1-\cos\Delta\theta) + (\Delta R)^2\right.}$$

$$\delta\Omega_{\alpha\beta\gamma\xi} = \Omega\left(-i\frac{\tilde{B}_{\alpha\beta\gamma\xi}}{\tilde{G}_{\alpha\beta}\tilde{G}_\gamma\tilde{G}_\xi\sqrt{1+\delta_{\alpha\beta}}} - \frac{1}{1+\delta_{\alpha\beta}}\left(\delta_{\alpha\gamma}\delta_{\beta\xi} + \delta_{\alpha\xi}\delta_{\beta\gamma}\right)\right)$$

$$U_{\alpha\beta\gamma\xi} = C_6\left(\frac{w}{2}\right)^{-6}(1+|H|)^{2/3}\left(\frac{\tilde{C}_{\alpha\beta\gamma\xi}}{2\tilde{G}_{\alpha\beta}\tilde{G}_{\gamma\xi}\sqrt{(1+\delta_{\gamma\xi})(1+\delta_{\alpha\beta})}}\right)$$

$$H \equiv \frac{2\delta_2}{C_6\left(\frac{w}{2}\right)^{-6}}$$

In the small H limit all integrals should become constant (but require not-obviously-trivial integration):

$$B_{\alpha\beta\gamma\xi} = \delta_{\alpha+\beta,\gamma+\xi}\int dR_1 dR_2 d\Delta\theta \times 2\pi R_1 R_2 \left|(R_1^2\sin^2\Delta\theta) + (R_1\cos(\Delta\theta) - R_2)^2\right|^3 \left(\Phi_\alpha(r_1)\Phi_\beta(r_2)e^{i\alpha\Delta\theta} + \Phi_\alpha(r_2)\Phi_\beta(r_1)e^{i\beta\Delta\theta}\right)^* e^{i\gamma}$$

$$G_{\gamma\xi} = \sqrt{\frac{1}{2}\int dR_1 dR_2 d\Delta\theta \times 2\pi R_1 R_2 \left|(R_1^2\sin^2\Delta\theta) + (R_1\cos(\Delta\theta) - R_2)^2\right|^6 \left|\Phi_\alpha(r_1)\Phi_\beta(r_2)e^{i(\gamma-\xi)\Delta\theta} + \Phi_\alpha(r_2)\Phi_\beta(r_1)(R_1)\right|^2}$$

- $$B_{0000}/G_{00} = 1/\pi$$

- $$\tilde{C}_{\alpha\beta\gamma\xi}(H) = \delta_{\alpha+\beta,\gamma+\xi}\int dR_1 dR_2 d\Delta\theta \times 2\pi R_1 R_2 \left(R_1^2 + R_2^2 - 2R_1R_2\cos\Delta\theta\right)^3 \left(\Phi_\alpha(r_1)\Phi_\beta(r_2)e^{i\alpha\Delta\theta} + \Phi_\alpha(r_2)\Phi_\beta(r_1)e^{i\beta\Delta\theta}\right)^* (\Phi$$

- **The small H limit requires veeeery small H (< 10^-6) before it starts to become decently valid**
  - so apparently "H=1" isn't really the "center"; good to know...
  - and therefore the values of A, B, and C in the small H limit ARE CONSTANT but aren't that close to 1 (they are large =P) but they do become independent of H, so this is all plausibly consistent
    - I suppose instead of (1+H) I could use something else... and then they would be O(1)

Large H limit should be constant:

Okay I think this still isn't QUITE the proper way to make the numerical integrals "easy". For that I might need to change coordinates to a center of mass and a distance, or something... Otherwise the C integrals with large H will always be hard, I think, because it has to find the places where the R are veeery similar and the θ is small. Well so let's try it, use R_1 and $R_2 - R_1$; the trick being that you need to SHIFT THE LIMITS OF R_2 by R_1!!!!. Now updated above..

***ALSO, DON'T FORGET TO UPDATE THE LIMITING CASES GIVEN YOUR NEW DEFINITIONS!!! ***

HERE'S THE TRICK I DIDNT UNDERSTAND ABOUT SCIPY QUAD ERROR TOLERANCES: IT'S AN ***OR*, not and**. so set the absolute tolerance to something really small like 1e-8, and then the relative tolerance is the only bound that matters

..

LIMITATIONS AT THE MOMENT:

- I assume that H is pure imaginary
- **NEXT STEPS:**
  - once you're satisfied, try implementing unittest so that you have your tests ready for later modifications
  - **PRE-COMPUTE A, B, and C over a sufficiently dense set of H values and for a useful set of modes** (like 0, 1, 2, 3, 4, 5, 6, 9, 12, 15)
    - use H from ~10^{-7} to 10^3
      - extrapolating from there is quite safe using the limiting formulae
      - otherwise you can interpolate the pre-computed results and whenever someone needs a value they get it quickly
    - finish the U and Ω parts and see what things look like for our real physical parameters... do they make sense?
  - **Once precomputed, make nice plots so you can see cool physical things!**
    - show the two limits for all integrals
    - try all of the "different kinds" of sets of modes to show the different kinds of behaviors :)
    - plot everything vs. H! =D
  - **if you get tired of the numerics, the question about Lindblad terms below remains very interesting and potentially important :)**
    - more generally, it would be helpful to be able to convert the imaginary parts of any effective model terms directly into jump operators for lindblad terms
  - **Because our approximation is hokey, I think the choice of basis matters a lot**
    - try investigating this and see what you find...
    - in particular, try simulating the same strongly-interacting system in two different bases; how much difference does it make?

III. HANDLING LOSS VIA "OTHER" ATOMIC STATES

i.e. not the primary collective modes

Thoughts:

- ideally, you should end up with Lindblad terms that capture the couplings to all of the out-of-manifold R-R, R-E, and E-E states (and R and E alone, for that matter, since that's what RR RE and EE decay toward)

  - but it's subtle because the out-of-manifold RR are not in 1:1 correspondence with the out-of-manifold EE; and in principle some of the out-of-manifold RR could have non-negligible coupling to in-manifold RE

- does model ever capture something like a "shelved Rydberg"?
  - it would be hard - a Rydberg should only be shelved if it is in an internal state that does not couple to a short-lived internal intermediate state...and our model only includes a single "relevant" Rydberg spin state at the moment
  - so I probably won't try to include these effects

A. First attempt at Lindblad terms

Define the collective states treated above as the "primary" atomic states; extra loss channels will therefore go through "secondary" atomic states; there may be (likely will be) additional states which are entirely irrelevant, so non-primary is not necessarily equal to secondary.

My first attempt will go as follows:

- define a projector onto non-primary atomic states
- calculate the RR, RE, EE, R, and E secondary states to which the primary states are coupled
  - it might be convenient to assume that the secondary states corresponding to each primary state are nearly orthogonal; so I may indeed try proceeding with that assumption (which is easy to check later, once I have the form of the secondary states)
- ... figure out how to capture those with additional Lindblad terms
  - I'll be using https://ocw.mit.edu/courses/nuclear-engineering/22-51-quantum-theory-of-radiation-interactions-fall-2012/lecture-notes/MIT22_51F12_Ch8.pdf to guide me on this step

The projector onto non-primary states is:

$$P_{np} = I - |0\rangle\langle 0| - \sum_{\alpha} \left(|E_\alpha\rangle\langle E_\alpha| + |R_\alpha\rangle\langle R_\alpha|\right) - \sum_{\alpha\beta}\left(|E_\alpha E_\beta\rangle\langle E_\alpha E_\beta| + |R_\alpha E_\beta\rangle\langle R_\alpha E_\beta| + |R_\alpha R_\beta\rangle\langle R_\alpha R_\beta|\right).$$

For each primary state $|\psi_1\rangle$ there is a secondary state $|\psi_2\rangle$ such that:

$$|\psi_2\rangle = N P_{np} H_0 |\psi_1\rangle$$

where N is a normalization factor.

...

Where are we going with this? Ideally we want to define a system (the primary states) and a bath (the secondary states) governed by a Hamiltonian

$$H_{SB} = H_S + H_B + C$$

where C is the coupling between the system and the bath. I'm going to assume that excitations in the bath decay fairly rapidly, and that relevant couplings induced by C are relatively small compared to the decays encoded in H_B. I'm going to start without thinking too hard, and then come back and think harder later as needed. I'm going to try to diagonalize within H_B first, for convenience, and then account for the couplings between primary states and the bath via C. Assume the bath starts in its empty state, and never goes above one excitation. **One tricky point is that my bath is already governed by a non-Hermitian Hamiltonian, or else I need to include the environment EM modes directly, which sounds yucky. But maybe it will actually be obvious how to handle this as I go along... In fact, under Markov approximation, it may not even matter what's in the bath...**

I'm pretty sure I can do this, but I'll return to it later; for one thing, it may be that the modified Ω captures the most important physics anyway. For another thing, I just feel more interested in working on the numerical integral right now.

IV. RESTORING BASIS INDEPENDENCE

just a note here - we need a better approximation which is at least basis independent, because that is way more likely to capture physical reality