Perturbation theory

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1 Notes on Perturbation Theory for a Two-Ensemble Dicke Model

(Donors + Acceptors coupled to a single quantised mode)

These notes build up the machinery we need to do **effective-Hamiltonian perturbation theory** properly, including the appearance of **folded-diagram (derivative) terms at 4th order**. We keep the discussion general first, then later we will plug in our specific Dicke Hamiltonian and basis.

1.1 1) The model

We consider a Hamiltonian split into "bare" and "interaction" parts:

$H = H_0 + V$.

A convenient Dicke-like choice is:

- Single bosonic mode: $a, a^\dagger$ with frequency ω_c.
- Two ensembles of two-level systems (TLS): donors D and acceptors A.
- Collective spin operators (Dicke operators) for each ensemble:
  - $S_D^\pm, S_D^z$ for donors, size N_D.
  - $S_A^\pm, S_A^z$ for acceptors, size N_A.

A standard "Rabi/Dicke" style Hamiltonian is:

$$H_0 = \omega_c a^\dagger a + \omega_0 \big(S_D^z + S_A^z\big) \tag{1}$$

$$V = (a + a^\dagger)\Big[v_D(S_D^+ + S_D^-) + v_A(S_A^+ + S_A^-)\Big]. \tag{2}$$

Here v_D and v_A are the single-particle couplings for donors and acceptors (not assumed equal).

1.2 2) Choice of basis and the P/Q split

1.2.1 Dicke basis (conceptual)

A convenient label for basis states is:

$|N_D^*, N_A^*, n\rangle$,

where: - N_D^* is the number of donor excitations in the symmetric Dicke ladder $(0, 1, \ldots, N_D)$, - N_A^* is the number of acceptor excitations $(0, 1, \ldots, N_A)$, - n is the photon number.

The bare energies take the schematic form:

$$E^{(0)}(N_D^*, N_A^*, n) = \omega_0(N_D^* + N_A^*) + \omega_c n \quad \text{(up to constant offsets).} \tag{3}$$

1.2.2 The two-dimensional P space

We choose a "model space" P consisting of the two single-excitation states at a chosen photon sector (often $k = 0$, i.e. photon number fixed to some reference n):

- Donor-like state:

$|D\rangle \equiv |1, 0, n\rangle$

- Acceptor-like state:

$|A\rangle \equiv |0, 1, n\rangle$

So P is 2D and is spanned by $\{|D\rangle, |A\rangle\}$. Let Q be the complement:

$Q = 1 - P$.

We will write operator blocks like: - $H_{PP} \equiv PHP$ - $H_{PQ} \equiv PHQ$ - $H_{QP} \equiv QHP$ - $H_{QQ} \equiv QHQ$

and similarly for H_0 and V.

1.3 3) Exact elimination of Q space: Bloch–Horowitz effective Hamiltonian

Start from the Schrödinger equation:

$H|\Psi\rangle = E|\Psi\rangle$.

Decompose the state:

$|\Psi\rangle = |\psi_P\rangle + |\psi_Q\rangle$,

where $|\psi_P\rangle = P|\Psi\rangle$ and $|\psi_Q\rangle = Q|\Psi\rangle$.

Projecting onto P and Q gives the coupled block equations:

$$(H_{PP} - E)\,|\psi_P\rangle + H_{PQ}\,|\psi_Q\rangle = 0 \tag{4}$$

$$H_{QP}\,|\psi_P\rangle + (H_{QQ} - E)\,|\psi_Q\rangle = 0. \tag{5}$$

Assuming $(E - H_{QQ})$ is invertible on Q, solve the second equation:

$$|\psi_Q\rangle = (E - H_{QQ})^{-1} H_{QP}\,|\psi_P\rangle. \tag{6}$$

Insert into the P equation to obtain the **exact energy-dependent effective Hamiltonian**:

$$H_{\text{eff}}(E) = H_{PP} + H_{PQ}\,(E - H_{QQ})^{-1}\,H_{QP}. \tag{7}$$

This is often called the **Bloch–Horowitz (BH)** or **Feshbach** effective Hamiltonian.

Key point: $H_{\text{eff}}(E)$ depends on E, so the eigenvalue problem is nonlinear:

$$H_{\text{eff}}(E)\,|\psi_P\rangle = E\,|\psi_P\rangle. \tag{8}$$

Solving this self-consistently reproduces the exact full-space eigenvalues associated with the chosen P sector.

1.4 4) Perturbative expansion: resolvent and "unfolded" series

We now expand in powers of V.

Write:

$H = H_0 + V$,

and correspondingly:

$H_{QQ} = (H_0)_{QQ} + V_{QQ}$, etc.

Define an "unperturbed" Q-space resolvent:

$$G_0(E) \equiv (E - (H_0)_{QQ})^{-1}. \tag{9}$$

Then we expand the full resolvent:

$$(E-H_{QQ})^{-1} = \big(E-(H_0)_{QQ}-V_{QQ}\big)^{-1} = G_0(E)+G_0(E)V_{QQ}G_0(E)+G_0(E)V_{QQ}G_0(E)V_{QQ}G_0(E)+\cdots \tag{10}$$

Insert into BH:

$$H_{\text{eff}}(E) = H_{PP}+V_{PQ}G_0(E)V_{QP}+V_{PQ}G_0(E)V_{QQ}G_0(E)V_{QP}+V_{PQ}G_0(E)V_{QQ}G_0(E)V_{QQ}G_0(E)V_{QP}+\cdots \tag{11}$$

This produces an expansion in powers of V:

- 2nd order: $V_{PQ}G_0(E)V_{QP}$
- 3rd order: $V_{PQ}G_0(E)V_{QQ}G_0(E)V_{QP}$
- 4th order: $V_{PQ}G_0(E)V_{QQ}G_0(E)V_{QQ}G_0(E)V_{QP}$
- etc.

If we evaluate these terms at a fixed reference energy $E = E_0$ (typically the degenerate bare energy of the P states), we get what we will call the **unfolded** contributions (no intermediate return to P inside the resolvent expansion).

1.5 5) Why energy dependence matters: self-consistency vs energy-independent expansions

1.5.1 Self-consistent (BH) viewpoint

In BH, you compute $H_{\text{eff}}(E)$ and solve the nonlinear problem

$H_{\text{eff}}(E)\psi_P = E\psi_P$.

This automatically includes "folding" effects because you never expand away the E dependence: it is treated exactly (within the chosen truncation of Q).

1.5.2 Energy-independent perturbation theory viewpoint

Often we want an **energy-independent** effective Hamiltonian expanded order-by-order (Rayleigh–Schrödinger style). Then we must handle the fact that H_{eff} depends on E.

This is where **folded-diagram (derivative) terms** appear.

1.6 6) The origin of folded terms: Taylor expanding the self-energy

Define the BH self-energy operator:

$\Sigma(E) \equiv H_{PQ}(E - H_{QQ})^{-1} H_{QP}$.

Then:

$H_{\text{eff}}(E) = H_{PP} + \Sigma(E)$.

Choose a reference energy E_0 (for our degenerate P space this is the common bare energy of $|D\rangle$ and $|A\rangle$), and write:

$E = E_0 + \delta E$.

Now Taylor expand:

$$\Sigma(E) = \Sigma(E_0) + \delta E\, \Sigma'(E_0) + \frac{(\delta E)^2}{2} \Sigma''(E_0) + \cdots \tag{12}$$

Crucial power counting: - $\Sigma(E_0)$ starts at order V^2. - Typically δE is also order V^2 (it is an energy shift generated by the interaction).

Therefore the term

$\delta E\, \Sigma'(E_0)$

is of order V^4.

That is exactly the **leading folded contribution at 4th order**.

1.6.1 Why derivatives appear

The derivative comes from differentiating the resolvent:

$$\frac{d}{dE}(E - H_{QQ})^{-1} = (E - H_{QQ})^{-2}. \tag{13}$$

So folded terms correspond to squared denominators in the intermediate-state sums. Diagrammatically, they are associated with intermediate returns to the model space P that would otherwise produce zero denominators in naive time-ordered perturbation theory.

1.7 7) What "folded" means when P is two-dimensional

Here P contains two states, $|D\rangle$ and $|A\rangle$.

A process can "return to P" in the middle by landing on **either** state (with the correct photon sector).

- Returning early to $|D\rangle$ corresponds to "dressing the donor leg".
- Returning early to $|A\rangle$ corresponds to "dressing the acceptor leg".

This is why, in a 2D P space, the folded correction is naturally a **matrix product** structure (schematically):

$$H_{\text{eff}}^{(\leq 4)} \approx H_{PP} + \Sigma^{(2)}(E_0) + \Sigma^{(4)}_{\text{unfolded}}(E_0) + \Sigma^{(2)\prime}(E_0)\,\Sigma^{(2)}(E_0) \quad \text{(up to convention-dependent symmetrisation).} \tag{14}$$

When we look specifically at the **off-diagonal element** AD, the folded term contains contributions corresponding to "hit D early" and "hit A early":

- "hit D early" dressing contributes via the P-index $p = D$
- "hit A early" dressing contributes via the P-index $p = A$

This is exactly how "getting to the end point early" enters analytically: it is one of the allowed intermediate P states in the folded correction.

1.8 8) Stop point for the general formalism

At this stage we have:

1. A clear P/Q reduction to an exact $H_{\text{eff}}(E)$ (BH/Feshbach).
2. A perturbative expansion of $H_{\text{eff}}(E)$ in powers of V that yields "unfolded" contributions at fixed E_0.
3. A Taylor expansion in E showing that, at 4th order, we must include derivative terms (folded diagrams) because δE is itself order V^2.

Next step (in our Dicke model): - Choose the explicit Dicke basis states and compute $\Sigma^{(2)}_{DD}(E_0)$, $\Sigma^{(2)}_{AA}(E_0)$, $\Sigma^{(2)}_{AD}(E_0)$ keeping full $(n, n+1)$ dependence. - Then compute $\Sigma^{(2)\prime}(E_0)$ and assemble the 4th-order folded correction. - Compare "static at E_0" vs "self-consistent BH" and show the cancellations we observed numerically.
