kpm expansion of second order perturbation matrix elements

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$\mathbf{H^0}$ initial Hamiltonian

We start with an initial system H^0, and solve the initial eigenvalues problem

$$H^0|\psi_n\rangle = \epsilon_n|\psi_n\rangle.$$

We express the initial Hamiltonian in it's diagonal basis

$$\tilde{H^0}_{i,j} = \delta_{i,j}\epsilon_i.$$

Perturbation

We add a perturbation λH^1, where λ is a real parameter in $[0,1]$.

and we want to know what is the effect of this perturbation on the spectrum of $H = H^0 + \lambda H^1$.

From non-degenerate perturbation theory, we can get the correction to the eigenstates and eigenvalues of H^0 by expanding in a series of powers in λ. Since degeneracies can occur, we must find an effective Hamiltonian that couples the degenerate states.

First order

The first thing we can do is to express H^1 in the basis diagonalises H^0,

$$\tilde{H^1}_{i,j} = \langle\psi_i|H^1|\psi_j\rangle.$$

The diagonal elements $\tilde{H^1}_{i,i}$ are the first order corrections to the energy of the perturbed system, and the effective Hamiltonian up to first order is

$$H^1_{eff} = \tilde{H^0} + \lambda\tilde{H^1},$$

(Actually, diagonalising the effective Hamiltonian up to first order will include some corrections of second order, since the perturbation is mixing the initial states, and giving non-diagonal elements in H^1_{eff}. The energy correction will depend on λ^2 if $V = \lambda H^1$.)

Second order

After expanding the perturbation up to second order for the eigenstates of the system we can arrive at the second order term of the effective Hamiltonian, where we have separated the system into two substates A and B expanded by $\{|\psi_i\rangle\}_i$ and $\{|\psi_\mu\rangle\}_\mu$, respectively.

$$\tilde{H^2}_{i,j} = \sum_\mu \frac{\langle\psi_i|H^1|\psi_\mu\rangle\langle\psi_\mu|H^1|\psi_j\rangle}{\epsilon_j - \epsilon_\mu}$$

This correction is derived for the degenerate case of the initial states in the small system expanded by the states $|i\rangle$. Then, it must be symmetrized for the general "not-only" degenerate case, when $\epsilon_i \neq \epsilon_j$.

$$\tilde{H^2}_{i,j} = \sum_\mu \frac{1}{2}\left(\frac{\langle\psi_i|H^1|\psi_\mu\rangle\langle\psi_\mu|H^1|\psi_j\rangle}{\epsilon_j - \epsilon_\mu} + \frac{\langle\psi_i|H^1|\psi_\mu\rangle\langle\psi_\mu|H^1|\psi_j\rangle}{\epsilon_i - \epsilon_\mu}\right) \tag{1}$$

$$\tilde{H^2}_{i,j} = \sum_\mu \frac{1}{2}\langle\psi_i|H^1|\psi_\mu\rangle\langle\psi_\mu|H^1|\psi_j\rangle\left(\frac{1}{\epsilon_j - \epsilon_\mu} + \frac{1}{\epsilon_i - \epsilon_\mu}\right) \tag{2}$$

Effective Hamiltonian

The effective Hamiltonian up to second order is

$$H^2_{eff} = \tilde{H}^0 + \lambda\tilde{H}^1 + \lambda^2\tilde{H}^2 \tag{3}$$

$$(H^2_{eff})_{i,j} = \delta_{i,j}\epsilon_i + \lambda\langle\psi_i|H^1|\psi_j\rangle \tag{4}$$

$$+\sum_\mu \frac{1}{2}\langle\psi_i|H^1|\psi_\mu\rangle\langle\psi_\mu|H^1|\psi_j\rangle\left(\frac{1}{\epsilon_j-\epsilon_\mu}+\frac{1}{\epsilon_i-\epsilon_\mu}\right) \tag{5}$$

kpm expansion
The second order contribution to the effective Hamiltonian can be expressed as

$$\tilde{H^2}_{i,j} = \frac{1}{2}\langle\psi_i|H^1\left[\sum_\mu\frac{|\psi_\mu\rangle\langle\psi_\mu|}{\epsilon_j-\epsilon_\mu}\right]H^1|\psi_j\rangle + \frac{1}{2}\langle\psi_i|H^1\left[\sum_\mu\frac{|\psi_\mu\rangle\langle\psi_\mu|}{\epsilon_i-\epsilon_\mu}\right]H^1|\psi_j\rangle \tag{6}$$

$$= \frac{1}{2}\langle\psi_i|H^1\left[P_B\frac{1}{\epsilon_j-H^0}P_B\right]H^1|\psi_j\rangle + \frac{1}{2}\langle\psi_i|H^1\left[P_B\frac{1}{\epsilon_i-H^0}P_B\right]H^1|\psi_j\rangle, \tag{7}$$

where P_B is a projector over the space B defined by $\{\psi_\mu\}_\mu$, and we see the action of a Green's function defined as

$$G(\epsilon, H^0) = \frac{1}{\epsilon - H^0}.$$

This function can be expanded with the KPM, with the vectors of the expansion being

$$|\phi_i\rangle = P_B H^1|\psi_i\rangle,$$

such that

$$\tilde{H^2}_{i,j} = \frac{1}{2}\langle\phi_i|G(\epsilon_j, H^0)|\phi_j\rangle + \frac{1}{2}\langle\phi_i|G(\epsilon_i, H^0)|\phi_j\rangle \tag{8}$$

Green's function expansion with KPM
A function of a parameter and a Hamiltonian is expressed as

$$f(\epsilon, H) = \sum_k f(\epsilon, E_k)|\psi_k\rangle\langle\psi_k|,$$

where the funcion f is expanded in KPM as

$$f(\epsilon, E_k) = \frac{2}{\pi}\sum_m c_m(\epsilon)T_m(E_k) \tag{9}$$

$$c_m(\epsilon) = \frac{1}{1+\delta_{m,0}}\int_{-1}^{1}\frac{f(\epsilon,E_k)T_m(E_k)}{\sqrt{1-E_k^2}}\mathrm{d}E_k. \tag{10}$$

To simplify the calculations we can instead expand

$$\sqrt{1-E_k^2}f(\epsilon, E_k) = \frac{2}{\pi}\sum_m c_m(\epsilon)T_m(E_k) \tag{11}$$

$$c_m(\epsilon) = \frac{1}{1+\delta_{m,0}}\int_{-1}^{1}f(\epsilon,E_k)T_m(E_k)\mathrm{d}E_k. \tag{12}$$

The solution is expanded elsewhere[1] for the rescaled Hamiltonian $\tilde{H} = (H - bI)/a$, and rescaled energies $\tilde{\epsilon} = (\epsilon - b)/a$.

$$f(\epsilon,H)^{\pm}=\frac{1}{\epsilon-H\pm i0} \tag{13}$$

$$f(\epsilon,H)^{\pm}=\frac{1}{\tilde{\epsilon}a+b-\tilde{H}a-b\pm i0} \tag{14}$$

$$f(\epsilon,H)^{\pm}=a^{-1}\frac{1}{\tilde{\epsilon}-\tilde{H}\pm i0} \tag{15}$$

$$f(\epsilon,H)^{\pm}_{M}=\mp\frac{2i}{a\sqrt{1-\epsilon^2}}\sum_{m=0}^{M}\frac{g_m}{1+\delta_{m,0}}\exp(\pm i\,m\arccos(\epsilon))T_m(H) \tag{16}$$

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[1] Real-space calculation of the conductivity tensor for disordered topological matter Jose H. Garcia, Lucian Covaci, Tatiana G. Rappoport. Phys. Rev. Lett. 114, 116602 (2015)