Title: PSI 2016/2017 Quantum Theory - Lecture 12

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Abstract:

Quantum Mechanics

Perturbation Theory – Schrieffer-Wolff

Lecture 11

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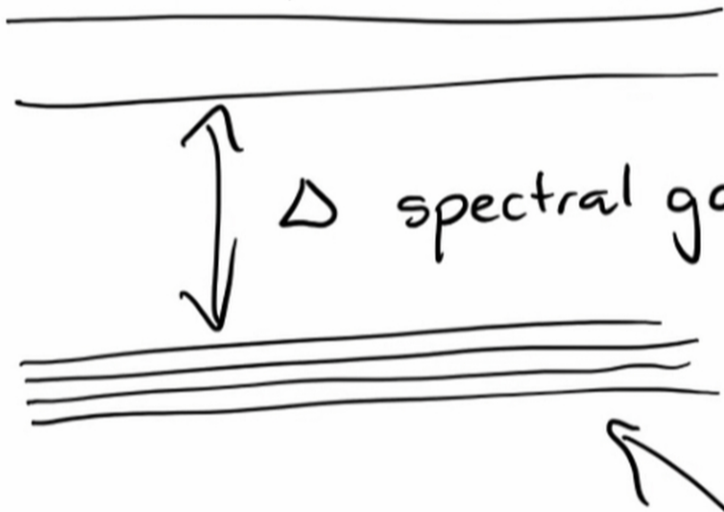
Low-energy effective theories

Q. many body system



high energy states } not (very?) relevant

Δ spectral gap

low energy states
ground state } relevant to low-energy physics

g.s. could be degenerate (topological)
or low energy space all very close in energy wrt Δ
"Degenerate"

‘Degenerate’ Perturbation Theory

Simple   Complex model

H_0 easy to solve

$\underbrace{H = H_0 + \epsilon V}_{\text{hard to solve}} \Leftarrow$ bound on $\epsilon\|V\|$

Construct H_{eff} on P_0

$$H_{eff} = U(H_0 + \epsilon V)U^{-1}\big|_{P_0}$$

as Taylor series in ϵ

Direct rotation between a pair of subspaces – one-dimensional

Finite dimensional Hilbert space $\mathcal{H}$

For any $|\psi\rangle \in \mathcal{H}$

$$R_\psi = I - 2|\psi\rangle\langle\psi|$$ flips sign of $|\psi\rangle$, acts trivially on complement

Given a pair $|\psi\rangle, |\phi\rangle$ we want $U_{\psi\to\phi}$ mapping $|\psi\rangle \to |\phi\rangle$ (up to an overall phase)

Double reflection $R_\phi R_\psi$ – rotates span$\{|\psi\rangle, |\phi\rangle\}$ by 2θ where $|\langle\psi|\phi\rangle| = \cos\theta$
– identity elsewhere

$$U_{\psi\to\phi} = \sqrt{R_\phi R_\psi}$$

Lemma: $|\phi\rangle, |\psi\rangle$ nonorthogonal $\Rightarrow$ $R_\phi R_\psi$ has no eigenvalues on real neg axis

Fix $\langle\phi|\psi\rangle$ real, positive $\Rightarrow$ $U_{\psi\to\phi}|\psi\rangle = |\phi\rangle$

Corollary: Let $P = |\psi\rangle\langle\psi|$ $P_0 = |\phi\rangle\langle\phi|$

Write $U_{\psi\to\phi} = \exp(S)$ S anti-Hermitian

- $PSP = P_0 S P_0 = (1-P)S(1-P) = (1-P_0)S(1-P_0) = 0$
- $\|S\| < \pi/2$

Generator of the direction rotation

How do we find S?

What are some "nice" conditions defining S?

Lemma: Suppose $\|P - P_0\| < 1$.

Then $\exists$ unique anti-hermitian S s.t.

1) $e^{S} P e^{-S} = P_0$

2) S is block-offdiagonal wrt P_0 $\quad P_0 S P_0 = 0$, $(I-P_0)S(I-P_0) = 0$

3) $\|S\| < \pi/2$

Then $U = \exp(S)$ is the direct rotation from P to P_0

Proof sketch: We know S exists, just need to prove uniqueness.

Spectral gap

unperturbed Hamiltonian

Finite dim $\mathcal{H}$, H_0 Hermitian operator

$P_0 \subseteq \mathcal{H}$ subspace spanned by eigenvectors corresponding to all eigenvalues in some interval $\mathcal{I}_0$

H_0 has a spectral gap Δ iff for any pair of eigenvalues $\lambda \in \mathcal{I}_0$, $\eta \notin \mathcal{I}_0$ we have $|\lambda - \eta| \geq \Delta$

Consider $H = H_0 + \epsilon V$ $\quad V$ arb. Hermitian op. on $\mathcal{H}$

Restrict ϵ s.t. $|\epsilon| \leq \epsilon_c = \frac{\Delta}{2\|V\|}$

$\mathcal{I} = \mathcal{I}_{0-\Delta/2}^{+\Delta/2}$ $\quad P \subseteq \mathcal{H}$ eigenvectors of H with eigenvalue in $\mathcal{I}$

Then for $|\epsilon| < \epsilon_c$, $\mathcal{I}$ has positive gap with rest of the spectrum

P and P_0 have same dimension

Define P, P_0 projectors on $\mathcal{P}, \mathcal{P}_0$

$Q = I - P \quad Q_0 = I - P_0$

The Schrieffer-Wolff transformation

Lemma: Suppose ϵ real, $|\epsilon| < \epsilon_c$. Then $\|P_0 - P\| \lesssim \frac{2\|\epsilon V\|}{\Delta} < 1$.

A direct rotation from P to P_0 is well-defined $|\epsilon| < \epsilon_c$

$$\mathcal{U} P \mathcal{U}^{-1} = P_0 \qquad \mathcal{U} Q \mathcal{U}^{-1} = Q_0$$

Also, $H = H_0 + \epsilon V$ is block-diagonal wrt P and Q

then $\mathcal{U} H \mathcal{U}^{-1}$ " " " P_0 and Q_0

Def. The direct rotation $\mathcal{U}$ from P to P_0 is the <u>SW transformation</u> for the unperturbed Ham H_0, perturbation ϵV, low-energy subspace P_0

Def. $H_{eff} = P_0 \mathcal{U} (H_0 + \epsilon V) \mathcal{U}^{-1} P_0$ effective low-energy Ham

Derivation of the perturbative series

Some notation

Superoperators that pick out block off-diag/diag.

$$\mathcal{O}(X) = P_0 X Q_0 + Q_0 X P_0 \qquad \mathcal{D}(X) = P_0 X P_0 + Q_0 X Q_0$$

$$V_d = \mathcal{D}(V) \qquad V_{od} = \mathcal{O}(V)$$

$$\hat{Y}[X] = [Y, X]$$

Main idea: For $|\epsilon| < \epsilon_c$, $\mathcal{U}$ is well defined

Write $\mathcal{U} = \exp(S)$ $\quad S$ - antihermitian
- block-off-diag
- $\|S\| < \pi/2$

$$e^{S}(H_0 + \epsilon V)e^{-S} = \exp(\hat{S})(H_0 + \epsilon V) \text{ is block diagonal}$$

This condition gives S. $\Rightarrow$ Taylor series for S and so calculate H_{eff} as Taylor series.

$V = V_d + V_{od}$

Derivation of the perturbative series

$$\exp(\hat{S})(H_0 + \epsilon V) = \underbrace{\cosh \hat{S}(H_0 + \epsilon V_d) + \sinh \hat{S}(\epsilon V_{od})}_{\text{block diagonal } \checkmark} + \underbrace{\sinh \hat{S}(H_0 + \epsilon V_d) + \cosh \hat{S}(\epsilon V_{od})}_{\text{block-off-diag } = 0}$$

Block diag.

$$\exp(\hat{S})(H_0 + \epsilon V) = H_0 + \epsilon V_d + (\cosh \hat{S} - 1)(H_0 + \epsilon V_d) + \sinh \hat{S}(\epsilon V_d)$$

$$= H_0 + \epsilon V_d + \frac{(\cosh \hat{S} - 1)}{\tanh \hat{S}} \tanh \hat{S}(H_0 + \epsilon V_d) + \sinh \hat{S}(\epsilon V_{od})$$

$$= H_0 + \epsilon V_d + F(\hat{S})(\epsilon V_{od})$$

$$= H_0 + \epsilon V_d + \tanh(\hat{S}/2)(\epsilon V_{od})$$

Block-off-diag

$$\tanh \hat{S}(H_0 + \epsilon V_d) + \epsilon V_{od} = 0$$

This determines S

with $F(x) = \sinh x - \frac{\cosh x - 1}{\tanh x} = \tanh(x/2)$

Derivation of the perturbative series

Let $\{|i\rangle\}$ orthonormal eigenbasis for H_0

Define $\mathcal{L}(X) = \sum_{i,j} \frac{\langle i|\mathcal{O}(X)|j\rangle}{E_i - E_j} |i\rangle\langle j|$

Because $\mathcal{O}(X)$ is block-off-diag, we can choose sum s.t. $i \in \mathcal{I}_0, j \notin \mathcal{I}_0$ and vice versa

$|E_i - E_j| \geq \Delta$

Check: $\mathcal{L}([H_0, X]) = [H_0, \mathcal{L}(X)] = \mathcal{O}(X)$

Solve for S: $\hat{S}(H_0 + \epsilon V_d) + \hat{S}\coth\hat{S}(\epsilon V_{od}) = 0$

Using S block-od: $S = \mathcal{L}\hat{S}(\epsilon V_d) + \mathcal{L}\hat{S}\coth\hat{S}(\epsilon V_{od})$

Solve as $S = \sum_{n=1}^{\infty} S_n \epsilon^n$ $\quad S_n^+ = -S_n$

$S_0 = 0$

Derivation of the perturbative series

$$x\coth(x) = \sum_{n=0}^{\infty} a_{2n} x^{2n}, \quad a_m = \frac{2^m B_m}{m!},$$

$$\begin{aligned} S_1 &= \mathcal{L}(V_{\text{od}}), \\ S_2 &= -\mathcal{L}\hat{V}_{\text{d}}(S_1), \\ S_n &= -\mathcal{L}\hat{V}_{\text{d}}(S_{n-1}) + \sum_{j\geq 1} a_{2j}\mathcal{L}\,\hat{S}^{2j}(V_{\text{od}})_{n-1} \qquad \text{for } n \geq 3. \end{aligned}$$

$$\hat{S}^k(V_{\text{od}})_m = \sum_{\substack{n_1,\ldots,n_k\geq 1 \\ n_1+\ldots+n_k=m}} \hat{S}_{n_1}\cdots\hat{S}_{n_k}(V_{\text{od}}).$$

$$H_{\text{eff}} = H_0P_0 + \epsilon P_0 V P_0 + \sum_{n=2}^{\infty} \epsilon^n H_{\text{eff},n}, \quad H_{\text{eff},n} = \sum_{j\geq 1} b_{2j-1} P_0\,\hat{S}^{2j-1}(V_{\text{od}})_{n-1}P_0.$$

$$\tanh(x/2) = \sum_{n=1}^{\infty} b_{2n-1} x^{2n-1}, \quad b_{2n-1} = \frac{2(2^{2n}-1)B_{2n}}{(2n)!}.$$

$$\begin{aligned} H_{\text{eff},2} &= b_1 P_0 \hat{S}_1(V_{\text{od}})P_0, \\ H_{\text{eff},3} &= b_1 P_0 \hat{S}_2(V_{\text{od}})P_0, \\ H_{\text{eff},4} &= b_1 P_0 \hat{S}_3(V_{\text{od}})P_0 + b_3 P_0 \hat{S}_1^3(V_{\text{od}})P_0, \\ H_{\text{eff},5} &= b_1 P_0 \hat{S}_4(V_{\text{od}})P_0 + b_3 P_0(\hat{S}_2\hat{S}_1^2 + \hat{S}_1\hat{S}_2\hat{S}_1 + \hat{S}_1^2\hat{S}_2)(V_{\text{od}})P_0. \end{aligned}$$

Convergence radius

$$S = \sum_{j=1}^{\infty} S_j \epsilon^j \qquad H_{eff} = \sum_{j=1}^{\infty} H_{eff,j} \epsilon^j$$

Lemma: The series for S and H_{eff} converge absolutely in the disk $|\epsilon| < \rho_c$ where

$$\rho_c = \frac{\epsilon_c}{8\left(1 + \frac{2|\mathcal{I}_0|}{\pi \Delta}\right)}$$

where $\epsilon_c = \frac{\Delta}{2\|V\|}$ and $|\mathcal{I}_0|$ width of $\mathcal{I}_0$

Additivity of the effective Hamiltonian

$\mathcal{H} = \mathcal{H}^A \otimes \mathcal{H}^B \qquad H_0 = H_0^A \otimes I^B + I^A \otimes H_0^B \qquad V = V^A \otimes I^B + I^A \otimes V^B$

Option ①

Define $U^A P^A (U^A)^\dagger = P_0^A \qquad U^B P^B (U^B)^\dagger = P_0^B$

$H_{eff}^A = P_0^A U^A (H_0^A + \epsilon V^A)(U^A)^\dagger P_0^A$

" for B

Option ②

$U^{AB}(P^A \otimes P^B)(U^{AB})^{-1} = P_0^A \otimes P_0^B$

$$H_{eff}^A \otimes I^B + I^A \otimes H_{eff}^B \overset{?}{\Longleftrightarrow} H_{eff}^{AB} = (P_0^A \otimes P_0^B) U^{AB} (H_0 + \epsilon V)(U^{AB})^\dagger (P_0^A \otimes P_0^B)$$

Lemma (Additivity) $H_{eff}^{AB} = H_{eff}^A \otimes I^B + I^A \otimes H_{eff}^B$

Proof sketch: Follows from weak multiplicativity of direct rotation

$$U^{AB}(P_0^A \otimes P_0^B) = (U^A \otimes U^B)(P_0^A \otimes P_0^B)$$

S-W for quantum many-body systems

$\mathcal{H} = \bigotimes_{a=1}^{N} \mathcal{H}_a$ $\mathcal{H}_a$ a-th "spin"   N spins

Usual: H_0 sum of local terms (acting nontrivially on only one $\mathcal{H}_a$)

$\Rightarrow P_0 = \bigotimes_{i=1}^{N} P_{0,a}$ $P_{0,a} \subseteq \mathcal{H}_a$ low energy subspace of a-th spin

V sum of two-spin (or many) interactions

Two concerns:

① $\|eV\|$ is extensive $\|eV\| \sim N \Rightarrow D \Rightarrow$ divergent series

Solution: truncate series at fixed order n

② Is $H_{eff}^{(n)}$ ~~is~~ a sum of local interactions on P_0?

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Two concerns:

(1) $\|eV\|$ is extensive $\|eV\| \sim N \Rightarrow D$ $\Rightarrow$ divergent series

Solution: truncate series at fixed order n

(2) Is $H_{eff}^{(n)}$ a sum of local interactions on P_0?

$\Rightarrow$ Modify S

local SW perturbation theory