PHOT 301: Quantum Photonics

LECTURE 17

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APPROXIMATIONS

	Method	Approximates?
1	Transfer matrix method	piece-wise constant $V(x)$
2	Finite basis method	limited ψ_n, E_n: Matrix-formalism
3	Finite difference method	discretizes wave function
4	Perturbation theory (stat.)	small perturbation known solutions
5	Time-dependent perturbation	small perturbation known solutions
6	Tight-binding approx.	electrons strongly bound (covalent)
7	Variational method	finding energy minima

David Miller's book Chapters 6 and 7

TIME-DEPENDENT PERTURBATION THEORY (DAVID MILLER’S BOOK, CHAPTER 7)

TIME-DEPENDENT PERTURBATION THEORY

- Method very similar to time-independent pertubation theory

Steps to reach to the solutions:

1. $\hat{H} = \hat{H}_0 + \gamma \hat{H}_p$ with the perturbation in time small
2. Expand wave function $\Psi(x,t) = \sum_n a_n(t) e^{-i\omega_n t} \psi_n(x)$
3. Then expand coefficients $a_n(t)$ into power series in γ
4. Calculate $a_n(t)$ up to some order to find Ψ

PERTURBING HAMILTONIAN

- Solve the time-dependent Schrodinger equation
- The time-dependent part is a (small) perturbation

$$\hat{H} = \hat{H}_0 + \gamma \hat{H}_p(t), \qquad i\hbar \frac{\partial}{\partial t}|\Psi\rangle = \hat{H}|\Psi\rangle$$

- Unperturbed $\hat{H}_0$ does **not depend on time**
- $\hat{H}_0$ has **known eigenvalues and eigenstates**

$$\hat{H}_0|\psi_n\rangle = E_n|\psi_n\rangle$$

The time-dependent wave function can be expanded in $|\psi_n\rangle$ with *extra* time factors

$$|\Psi\rangle = \sum_n a_n(t) e^{-iE_n t/\hbar} |\psi_n\rangle$$

SOME NOTATIONS

Notation: We will most of the time stop writing the time argument to simplify:

$$a_n(t) = a_n^{(0)} + \gamma\, a_n^{(1)} + \gamma^2\, a_n^{(2)} + \gamma^3\, a_n^{(3)} + \dots$$

Notation: We write a little dot on top of a function to indicate a derivative to time:

$$\frac{\partial a_q^{(j)}(t)}{\partial t} \equiv \dot{a}_q^{(j)}(t) \equiv \dot{a}_q^{(j)}$$

Notation: prime derivative notation for spacial derivatives (to x):

$$f'(x) \equiv \frac{\partial f(x)}{\partial x} \qquad f''(x) \equiv \frac{\partial^2 f(x)}{\partial x^2}$$

Notation: shorter partial derivative notation (I will try to avoid to use it):

$$\partial_x f(x) \equiv \frac{\partial f(x)}{\partial x} \qquad \partial_x^2 f(x) = \partial_{xx} f(x) \equiv \frac{\partial^2 f(x)}{\partial x \partial y} \qquad \partial_{xy} f(x) \equiv \frac{\partial^2 f(x)}{\partial x \partial y}$$

EQUATION IN THE COEFFICIENTS

We know everything except of $a_n(t)$, how to find them?

$$\hat{H} = \hat{H}_0 + \gamma \hat{H}_p(t), \qquad i\hbar \frac{\partial}{\partial t} |\Psi\rangle = \hat{H} |\Psi\rangle$$

- Fill in the wave function and our *approximate* Hamiltonian

$$i\hbar \frac{\partial}{\partial t} \sum_n a_n(t) e^{-iE_n t/\hbar} |\psi_n\rangle = \left(\hat{H}_0 + \gamma \hat{H}_p(t)\right) \sum_n a_n(t) e^{-iE_n t/\hbar} |\psi_n\rangle$$

$$\Rightarrow \quad \sum_n \left(i\hbar\, \dot{a}_n(t) e^{-iE_n t/\hbar} + a_n(t) E_n e^{-iE_n t/\hbar}\right) |\psi_n\rangle = \left(\hat{H}_0 + \gamma \hat{H}_p(t)\right) \sum_n a_n(t) e^{-iE_n t/\hbar} |\psi_n\rangle$$

EQUATION IN THE COEFFICIENTS CTU'D

$$\sum_n \left(i\hbar\, \dot{a}_n(t) e^{-iE_n t/\hbar} + a_n(t) E_n e^{-iE_n t/\hbar} \right) |\psi_n\rangle = \left(\hat{H}_0 + \gamma \hat{H}_p(t) \right) \sum_n a_n(t) e^{-iE_n t/\hbar} |\psi_n\rangle$$

$$\implies \sum_n \left(i\hbar \dot{a}_n + a_n E_n \right) e^{-iE_n t/\hbar} |\psi_n\rangle = \sum_n a_n \left(E_n + \gamma \hat{H}_p(t) \right) e^{-iE_n t/\hbar} |\psi_n\rangle$$

- Time-independent terms in energy E_n: **they cancel out**

$$\implies \sum_n i\hbar \dot{a}_n e^{-iE_n t/\hbar} |\psi_n\rangle = \sum_n a_n \gamma \hat{H}_p(t) e^{-iE_n t/\hbar} |\psi_n\rangle$$

EQUATION IN THE COEFFICIENTS CTU'D

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- Then left-multiply with $\langle \psi_q |$

$$\implies \quad \sum_n i\hbar \dot{a}_n e^{-iE_n t/\hbar} \langle \psi_q | \psi_n \rangle = \sum_n a_n \gamma e^{-iE_n t/\hbar} \langle \psi_q | \hat{H}_p(t) |\psi_n\rangle$$

$$\implies \quad i\hbar \dot{a}_q e^{-iE_q t/\hbar} = \sum_n a_n \gamma e^{-iE_n t/\hbar} \langle \psi_q | \hat{H}_p(t) |\psi_n\rangle$$

$$\implies \quad \dot{a}_q = \frac{1}{i\hbar} \sum_n a_n \gamma e^{-i(E_n - E_q)t/\hbar} \langle \psi_q | \hat{H}_p(t) |\psi_n\rangle$$

Now we will make the actual approximation using γ (perturbation)

PERTURBATION EXPANSION COEFFICIENTS

Power series of the expansion coefficients $a_n(t)$ in γ

$$a_n(t) = a_n^{(0)}(t) + \gamma\, a_n^{(1)}(t) + \gamma^2\, a_n^{(2)}(t) + \gamma^3\, a_n^{(3)}(t) + \ldots$$

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Power series of the expansion coefficients $a_n(t)$ in γ

$$a_n(t) = a_n^{(0)} + \gamma\, a_n^{(1)} + \gamma^2\, a_n^{(2)} + \gamma^3\, a_n^{(3)} + \dots$$

Derivative to time $\longrightarrow$ time-derivatives of the power series coefficients

$$\dot{a}_n(t) = \dot{a}_n^{(0)} + \gamma\, \dot{a}_n^{(1)} + \gamma^2\, \dot{a}_n^{(2)} + \gamma^3\, \dot{a}_n^{(3)} + \dots$$

$$\dot{a}_q^{(0)} + \gamma\, \dot{a}_q^{(1)} + \gamma^2\, \dot{a}_q^{(2)} + \dots = \\ \frac{1}{i\hbar} \sum_n \left(a_n^{(0)} + \gamma\, a_n^{(1)} + \gamma^2\, a_n^{(2)} + \dots \right) \gamma e^{-i(E_n - E_q)t/\hbar} \langle \psi_q | \hat{H}_p(t) | \psi_n \rangle$$

PERTURBATION EXPANSION COEFFS CTU'D

$$\dot{a}_q^{(0)} + \gamma\,\dot{a}_q^{(1)} + \gamma^2\,\dot{a}_q^{(2)} + \cdots =$$
$$\frac{1}{i\hbar}\sum_n \left(a_n^{(0)} + \gamma\,a_n^{(1)} + \gamma^2\,a_n^{(2)} + \ldots\right)\gamma e^{-i(E_n - E_q)t/\hbar}\langle\psi_q|\hat{H}_p(t)\,|\psi_n\rangle$$

Equate order 0 in γ lead to zero right hand side.

$$\frac{a_q^{(0)}(t)}{\partial t} \equiv \dot{a}_q^{(0)}(t) \equiv \dot{a}_q^{(0)} = 0$$

- If $\gamma = 0$ the coefficients $a_q^{(0)}(t)$ are constants.
- There is no perturbation in time

FIRST ORDER PERTURBATION

$$\dot{a}_q^{(0)} + \gamma\,\dot{a}_q^{(1)} + \gamma^2\,\dot{a}_q^{(2)} + \cdots = \frac{1}{i\hbar}\sum_n \left(a_n^{(0)} + \gamma\,a_n^{(1)} + \gamma^2\,a_n^{(2)} + \ldots\right)\gamma e^{-i(E_n - E_q)t/\hbar}\langle\psi_q|\hat{H}_p(t)\,|\psi_n\rangle$$

- First order perturbed coefficients

$$\dot{a}_q^{(1)} = \frac{1}{i\hbar}\sum_n a_n^{(0)}\gamma e^{i\omega_{qn}t}\langle\psi_q|\hat{H}_p(t)\,|\psi_n\rangle$$

- with $\omega_{qn} = (E_q - E_n)/\hbar$
- $a_n^{(0)}$ all constant in time

HIGHER ORDERS

- Higher order perturbed coefficients
- Suppose you calculated up to order p
- Next order $a_n^{(p+1)}$ computed from previous orders

$$\dot{a}_q^{(p+1)} = \frac{1}{i\hbar} \sum_n a_n^{(p)} \gamma e^{i\omega_{qn} t} \langle \psi_q | \hat{H}_p(t) | \psi_n \rangle$$

- with $\omega_{qn} = (E_q - E_n)/\hbar$

For examples: Chapter 7 of David Miller's book.