4/5/2015

7. PORUCHOVÁ TEORIE

7. PERTURBATION THEORY

= Systém matematických metod pro nalezení přibližného řešení složitého problému, známe-li přesné řešení souvisejícího jednoduššího problému.

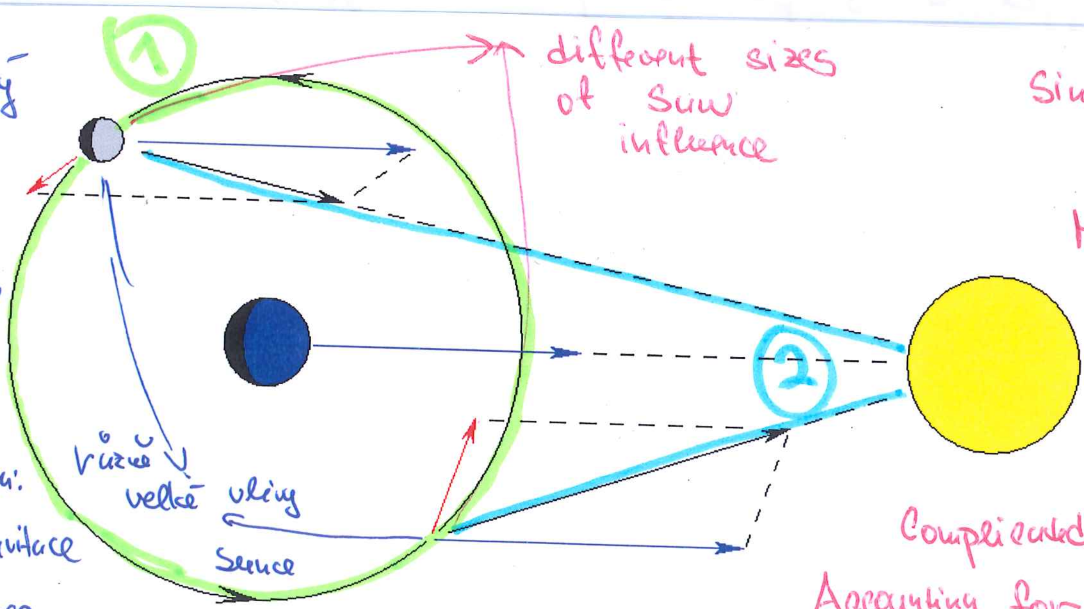
= System of mathematical methods for finding an approximate solution of a complicated problem on the basis of ~~the~~ an exact solution of an related, more simple problem

- Historicky poprvé použita v astronomii

- Historically used for the 1st time in astronomy

Jednoduchý problém: Měsíc v gravitačním poli Země.

Složitý problém: Započtení gravitace od Slunce



Simple problem: Moon in a gravitational field of Earth.

Complicated problem: Accounting for additional gravitation from the Sun.

7.1. ZÁKLADNÍ POPIS PROBLÉMU

7.1. BASIC PROBLEM DESCRIPTION

porušený / PERTURBED problem B $\longrightarrow$ problem A neporušený / UNPERTURBED

Hamiltonian $\hat{H} = \hat{H}_0 + \lambda \hat{H}'$ Hamiltonian $\hat{H}_0$

W_4, Φ_4 E_4, Ψ_4

W_{3-5}, Φ_{3-5} E_{3-5}, Ψ_{3-5}

W_2, Φ_2 E_2, Ψ_2

W_1, Φ_1 E_1, Ψ_1

Porušené řešení jako lineární kombinace neporušených řešení

Perturbed solution of as a linear combination unpert.

Příklad: Atom He bez repulze elektronů
↓ PORUCHA
Atom He s repulzí elektronů

Example: He atom without e-e repulsion
↓ PERTURBATION
He atom WITH e-e repulsion

$$0 \leq \lambda \leq 1$$

SKALÁRNÍ VELIČINA CHARAKTERIZUJE POSTUPNÉ (SPOJITÉ) ZAPÍNÁNÍ PORUCHY

SCALAR PROPERTY CHARACTERIZES CONTINUOUS SWITCHING-ON OF THE PERTURBATION

7.2. VYUŽITÍ TAYLOROVA ROZVOJE

7.2. APPLICATION OF TAYLOR EXPANSION

$$\hat{H}_0 \psi_i = E_i \psi_i$$

known
známe

$$\int \psi_i^* \psi_j \, d\tau = \delta_{ij}$$

Suppose ψ_i form an ORTHONORMAL SET

Předpoklad: ψ_i tvoří ORTHONORMÁLNÍ SYSTÉM

$$\hat{H} \phi_i = (\hat{H}_0 + \lambda \hat{H}') \phi_i = W \phi_i$$

unknown
neznáme

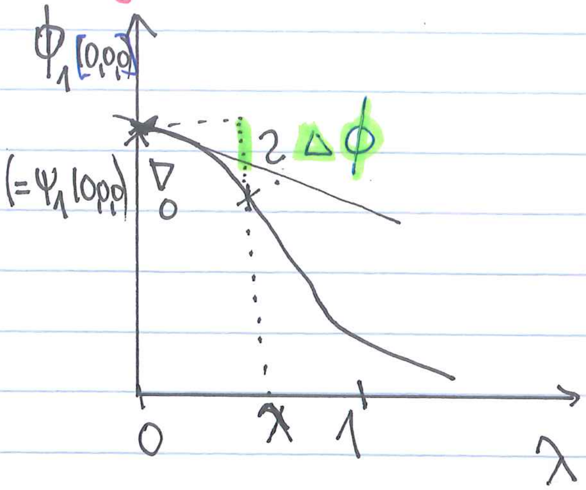
$\lambda = 0 \qquad \hat{H} = \hat{H}_0 \qquad \phi_i = \psi_i \qquad W_i = E_i$

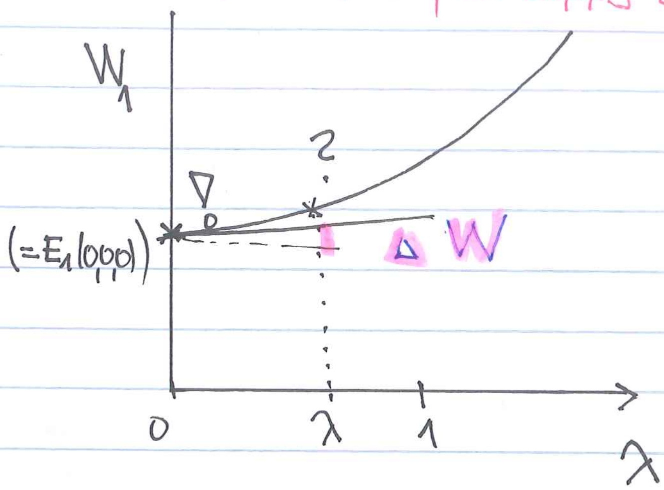
↓ spojitá změna ↓ continuous change ↓ ↓

$\lambda = 1 \qquad \hat{H} = \hat{H}_0 + \hat{H}' \qquad \phi_i \neq \psi_i \qquad W_i \neq E_i$

Např. chceme znát hodnotu vln. fce ϕ_1 v bodě [0,0,0] a energii W_1

E.g. We want to know the value of WF ϕ_1 in point [0,0,0] and energy W_1





1. aproximace:

Položím $\phi_1(\lambda)$ rovno $\phi_1(\lambda=0)$

$$\phi_1[0,0,0,\lambda] = \Psi_1[0,0,0,\lambda]$$

$W_1(\lambda)=W_1(\lambda=0)$

$$W_1[\lambda] = E_1(\lambda) \equiv W_1\big|_{\lambda=0}$$

1st approximation | set $\phi_1(\lambda)=\phi_1(0)$

i.e. $\phi_1(\lambda) = \phi_1(0) = \Psi_1 \equiv \phi_1\big|_{\lambda=0}$

$W_1(\lambda)=W_1(\lambda=0)$

2. aproximace:

změnu funkce $\Delta\phi$, ΔW mezi 0 a λ vyjádřím pomocí 1. derivace v $\lambda=0$

2nd approximation:

change in function $\Delta\phi_1$, ΔW between 0 and λ | express as the 1st derivative in $\lambda=0$

$$\phi_1(\lambda) = \phi_1\big|_{\lambda=0} + \frac{\partial\phi_1}{\partial\lambda}\bigg|_{\lambda=0}\cdot\frac{\lambda}{1!}$$

$$W_1(\lambda) = W_1\big|_{\lambda=0} + \frac{\partial W_1}{\partial\lambda}\bigg|_{\lambda=0}\cdot\frac{\lambda}{1!}$$

3. aproximace

změnu funkce mezi 0 a λ vyjádřím pomocí 1. a 2. derivace v $\lambda=0$

3rd approximation:

change in function between 0 and λ | express as the 1st and 2nd derivative in $\lambda=0$

$$\phi_1(\lambda) = \phi_1\big|_{\lambda=0} + \frac{\partial\phi_1}{\partial\lambda}\bigg|_{\lambda=0}\cdot\frac{\lambda}{1!} + \frac{\partial^2\phi_1}{\partial\lambda^2}\bigg|_{\lambda=0}\cdot\frac{\lambda^2}{2!}$$

$$W_1(\lambda) = W_1\big|_{\lambda=0} + \frac{\partial W_1}{\partial\lambda}\bigg|_{\lambda=0}\cdot\frac{\lambda}{1!} + \frac{\partial^2 W_1}{\partial\lambda^2}\bigg|_{\lambda=0}\cdot\frac{\lambda^2}{2!}$$

atd.

etc...

Obecně

In general

$$* \quad \phi_i(\lambda) = \underbrace{\overbrace{\phi_i\Big|_{\lambda=0}}^{\text{označíme } \phi_i(0)}}_{\text{we label } \phi_i(0)} + \underbrace{\overbrace{\frac{\partial\phi_i}{\partial\lambda}\Big|_{\lambda=0}}^{\text{označíme } \phi_i(1)}}_{\text{we label } \phi_i(1)}\cdot\frac{\lambda}{1!} + \underbrace{\overbrace{\frac{\partial^2\phi_i}{\partial\lambda^2}\Big|_{\lambda=0}}^{\text{označíme } \phi_i(2)}}_{\text{we label } \phi_i(2)}\cdot\frac{\lambda^2}{2!} + \underbrace{\overbrace{\frac{\partial^3\phi_i}{\partial\lambda^3}\Big|_{\lambda=0}}^{\text{označíme } \phi_i(3)}}_{\text{we label } \phi_i(3)}\cdot\frac{\lambda^3}{3!} + \dots$$

exponent

$$** \quad W_i(\lambda) = \underbrace{\overbrace{W_i\Big|_{\lambda=0}}^{\text{označíme } W_i(0)}}_{\text{we label } W_i(0)} + \underbrace{\overbrace{\frac{\partial W_i}{\partial\lambda}\Big|_{\lambda=0}}^{\text{označíme } W_i(1)}}_{\text{we label } W_i(1)}\cdot\frac{\lambda}{1!} + \underbrace{\overbrace{\frac{\partial^2 W_i}{\partial\lambda^2}\Big|_{\lambda=0}}^{\text{označíme } W_i(2)}}_{\text{we label } W_i(2)}\cdot\frac{\lambda^2}{2!} + \underbrace{\overbrace{\frac{\partial^3 W_i}{\partial\lambda^3}\Big|_{\lambda=0}}^{\text{označíme } W_i(3)}}_{\text{we label } W_i(3)}\cdot\frac{\lambda^3}{3!} + \dots$$

Můžeme pak psát: Then we can write:

$$\phi_i(\lambda) = \underbrace{\overbrace{\phi_i(0)}^{\text{VF v nultém řádu}}}_{\text{WF in 0th order}} + \underbrace{\overbrace{\phi_i(1)\cdot\lambda^1}^{\text{Oprava 1. řádu k VF}}}_{\text{1st order correction}} + \phi_i(2)\cdot\lambda^2 + \phi_i(3)\cdot\lambda^3 + \dots$$

$$W_i(\lambda) = \underbrace{\overbrace{W_i(0)}^{\text{energie v nultém řádu}}}_{\text{WF in 0th order}} + \underbrace{\overbrace{W_i(1)\cdot\lambda^1}^{\text{Oprava 1. řádu k energii}}}_{\text{1st order correction to energy}} + \underbrace{\overbrace{W_i(2)\cdot\lambda^2}^{\text{Oprava 2. řádu k energii}}}_{\text{2nd order correction to energy}} + W_i(3)\cdot\lambda^3 + \dots$$

Taylorova věta říká, že výrazy (*) a (**) mohou aproximovat funkci s libovolnou přesností.

Taylor theorem says that expressions (*) and (**) can provide ϕ_i and W_i with any desirable accuracy.

SCHRÖDINGEROVA ROVNICE PRO PORUŠENÝ PROBLÉM:

SCHRÖDINGER EQUATION FOR THE PERTURBED PROBLEM:

$$(H_0 + \lambda H')\,\phi_i = W_i\,\phi_i$$

dosadím rozvoj * — I insert expansion *

dosadím rozvoj ** — I insert expansion **

Tato rovnice může pro všechna λ platit jen tehdy, rovnají-li se koeficienty u každé mocniny λ zvlášť

$$\left(H_0 + \lambda H'\right)\left(\phi_i^{(0)} + \lambda\phi_i^{(1)} + \lambda^2\phi_i^{(2)} + \cdots\right)$$
$$= \left(W_i^{(0)} + \lambda W_i^{(1)} + \lambda^2 W_i^{(2)} + \cdots\right)\left(\phi_i^{(0)} + \lambda\phi_i^{(1)} + \lambda^2\phi_i^{(2)} + \cdots\right) \quad (12\text{-}7)$$

The variable in Eq. (12-7) is λ, and each power of λ is linearly independent of all other powers of λ. As indicated in Section 3-4D, this means that Eq. (12-7) can be satisfied for all values of λ only if it is satisfied for *each power* of λ separately. Collecting terms having the zeroth power of λ gives

λ^0:

$$H_0\phi_i^{(0)} = W_i^{(0)}\phi_i^{(0)} \quad (12\text{-}8)$$

However, we have already recognized that

$$\phi_i^{(0)} = \psi_i, \quad W_i^{(0)} = E_i \quad (12\text{-}9)$$

neříká nic nového.

and Eq. (12-8) is simply a restatement of Eq. (12-1). Collecting terms from Eq. (12-7) containing λ to the first power we obtain

$$\lambda H'\phi_i^{(0)} + \lambda H_0\phi_i^{(1)} = \lambda W_i^{(1)}\phi_i^{(0)} + \lambda\phi_i^{(1)} W_i^{(0)}$$

λ^1:

$$\lambda\left(H'\underbrace{\phi_i^{(0)}}_{=\psi_i} + H_0\phi_i^{(1)} - W_i^{(0)}\phi_i^{(1)} - W_i^{(1)}\underbrace{\phi_i^{(0)}}_{=\psi_i}\right) = 0 \quad (12\text{-}10)$$

This equality must hold for any value of λ, so the term in parentheses is zero. Hence, rearranging and making use of Eqs. (12-9), we have the first-order equation

$$\left(H' - W_i^{(1)}\right)\psi_i + \left(H_0 - E_i\right)\phi_i^{(1)} = 0 \quad (12\text{-}11)$$

$$\int \psi_i^* \left(H' - W_i^{(1)}\right)\psi_i\, d\tau + \int \psi_i^* \left(H_0 - E_i\right)\phi_i^{(1)}\, d\tau = 0$$

Let us multiply this from the left by ψ_i^* and integrate:

$$\int \psi_i^* H'\psi_i\, d\tau - W_i^{(1)}\underbrace{\int \psi_i^*\psi_i\, d\tau}_{1} + \int \psi_i^* H_0\phi_i^{(1)}\, d\tau - E_i\int \psi_i^*\phi_i^{(1)}\, d\tau = 0 \quad (12\text{-}12)$$

$$\int \psi_i^* H_0 \phi_i^{(1)}\, d\tau = \int \phi_i^{(1)} \left(H_0\psi_i^{(1)}\right)^* d\tau = \int \phi_i^{(1)} \left(E_i\psi_i\right)^* d\tau = E_i\int \phi_i^{(1)}\psi_i\, d\tau$$

Using the hermitian property of H_0, it is easy to show that the third and fourth terms cancel, leaving

$$\boxed{W_i^{(1)} = \int \psi_i^* H'\psi_i\, d\tau} \quad (12\text{-}13\text{a})$$

zelený člen se odečte s modrým