## Perturbation theory:

In quantum mechanics, we often encounter problems that can be described by a Hamiltonian on the form

H= Ho+ AH,

where Ho describes at easy problem that we can solve, while Hy is a perturbation.

The perturbation parameter & must be small, 1461, for the perturbation theory to work.

Since we have 'solved' Ho (it could be, e.g., the harmonic oscillator), we know its eigenvalues E'n and leight states |4'n), where  $\hat{H}_0 | 4'_n > = E'_n | 4$ 

Below, we assume that there eigenenergies are not degenerate. Moreover, we assume that the eigenvalues and eigenstates can be expanded in the perturbation poraweter  $\lambda$  as

En = En+ XEn+ 12 En+ ... and 14h>= 14h>+ X14h1)+ 1214h(11)+... We now aim at calculating these corrections order by order in  $\lambda$ . To this end, we write the Schrödinger equation as

$$\rightarrow \left( \hat{H}_{0} + \lambda \hat{H}_{1} \right) \left( |4_{h}^{(0)}\rangle + \lambda |4_{h}^{(0)}\rangle + \lambda^{2} |4_{h}^{(0)}\rangle + \dots \right)^{2}$$

$$\left( E_{h}^{(0)} + \lambda E_{h}^{(0)} + \lambda^{2} E_{h}^{(0)} + \dots \right) \times$$

$$\left( |4_{h}^{(0)}\rangle + \lambda |4_{h}^{(0)}\rangle + \lambda^{2} |4_{h}^{(0)}\rangle + \dots \right)$$

and collect terms to same order in X:

We are free normalize Itn > so that (4") Itn >= 1

Or

$$\langle \Psi_{n}^{(\omega)} | \Psi_{n}^{(\omega)} \rangle + \lambda \langle \Psi_{n}^{(\omega)} | \Psi_{n}^{(\omega)} \rangle + \lambda^{2} \langle \Psi_{n}^{(\omega)} | \Psi_{n}^{(\omega)} \rangle + \dots = 1$$

for all  $\Lambda \ll L$ 

$$= \int \langle \Psi_{n}^{(\omega)} | \Psi_{n}^{(\omega)} \rangle = \langle \Psi_{n}^{(\omega)} | \Psi_{n}^{(\omega)} \rangle = \dots = 0$$

$$=) \left[ \frac{(1)}{(1)} = \left( \frac{4}{h}, \frac{(0)}{1}, \frac{1}{1}, \frac{4}{h}, \frac{(0)}{1} \right) \right]$$

We can also find the first-order correction to the eigenstate. To this eld, we rewrite it as

$$|4_{n}^{(4)}\rangle = \left(\frac{\sum_{m} |4_{m}^{(0)} \times 4_{m}^{(0)}|}{\sum_{m} |4_{m}^{(0)}|} |4_{m}^{(4)}\rangle |4_{m}^{$$

Since  $\langle 4_n^{(i)} | 4_n^{(i)} \rangle = 1$ . We now need to determine the coefficients  $\langle 4_m^{(i)} | 4_n^{(i)} \rangle$ .

For that, we use that

$$\langle 4_{m}^{(0)} | \hat{H}_{D} | 4_{n}^{(0)} \rangle + \langle 4_{m}^{(0)} | \hat{H}_{1} | 4_{n}^{(0)} \rangle =$$

$$= \frac{E_{n}^{(0)} \langle 4_{m}^{(0)} | 4_{n}^{(0)} \rangle + E_{n}^{(0)} \langle 4_{m}^{(0)} | 4_{n}^{(0)} \rangle =}{E_{n}^{(0)} \langle 4_{m}^{(0)} | 4_{n}^{(0)} \rangle + \langle 4_{m}^{(0)} | \hat{H}_{1}^{(1)} | 4_{n}^{(0)} \rangle =} E_{n}^{(0)} \langle 4_{m}^{(0)} | 4_{n}^{(0)} \rangle + \langle 4_{m}^{(0)} | \hat{H}_{1}^{(1)} | 4_{n}^{(0)} \rangle =} E_{n}^{(0)} \langle 4_{m}^{(0)} | 4_{n}^{(0)} \rangle + \langle 4_{m}^{(0)} | \hat{H}_{1}^{(1)} | 4_{n}^{(0)} \rangle =} E_{n}^{(0)} \langle 4_{m}^{(0)} | 4_{n}^{(0)} \rangle + \langle 4_{m}^{(0)} | \hat{H}_{1}^{(1)} | 4_{n}^{(0)} \rangle =} E_{n}^{(0)} \langle 4_{m}^{(0)} | 4_{n}^{(0)} \rangle + \langle 4_{m}^{(0)} | 4_{n}^{(0)} | 4_{n}^{(0)} \rangle + \langle 4_{m}^{(0)} | 4$$

$$= > \langle 4^{(\alpha)} | 4^{(\alpha)} \rangle = \frac{\langle 4^{(\alpha)} | f_{1} | 4^{(\alpha)} \rangle}{E_{n}^{(\alpha)} - E_{m}^{(\alpha)}}$$

so that

$$|Y_{h}^{(i)}\rangle = \frac{\sum_{m \neq h} \langle Y_{m}^{(i)} | \hat{H}_{n} | Y_{n}^{(i)} \rangle}{E_{n}^{(i)} - E_{m}^{(i)}} | Y_{m}^{(i)} \rangle$$

With the correction to the eigenstate, we can find the second-order correction to the eigeneuergy. To this end, we use that

$$E_{h}^{(0)} < \frac{4_{h}^{(0)} | 4_{h}^{(2)} > + E_{h}^{(1)} < \frac{4_{h}^{(0)} | 4_{h}^{(1)} > + E_{h}^{(2)} < \frac{4_{h}^{(1)} | 4_{h}^{(1)} > + E_{h}^{(2)} < \frac{4_{h}^{(2)} | 4_{h}^{(2)} > + E_{h}^{(2)} < \frac{4_{h$$

$$= \sum_{m \neq n} \frac{\langle \Psi_{n}^{(i)} | \Psi_{n} | \Psi_{n}^{(i)} \rangle \langle \Psi_{m}^{(i)} | \Psi_{n}^{(i)} \rangle}{\langle \Psi_{n}^{(i)} | \Psi_{n}^{(i)} | \Psi_{n}^{(i)} \rangle}$$

$$|E_{n}^{(2)}| = \sum_{m \neq n} \frac{|\langle 4_{m}^{(6)} | \hat{1}_{1} | 4_{n}^{(6)} \rangle|^{2}}{|E_{n}^{(6)} - E_{n}^{(6)}|}$$

Bue can in principle continue this perturbolism scheme to any order in  $\lambda$ . However, for most applications the first and second order eoverctions suffice. For that, the matrix elements  $\langle 4^{11}_{m}|4^{11}_{n}, 14^{11}_{n}\rangle$  should be small, i.e.

See text book for degenerate pertubolion theory!

C'onsider a quantum harmonic oscillator with a quartic perturbation, i.e.

H= H<sub>6</sub>+H<sub>1</sub>=  $\frac{\hat{p}^2}{2m}+\frac{1}{2}mw_s^2x^2+\lambda hw_s(\hat{x}_6)^4$ , where  $x_0=V_{t/mw_s}$  is the oscillator Dersth, and  $x\ll 1$  is a small perturbation parameter.

The unperturbed Hamiltonian can be written as

and corresponding eigenvectors h) =  $\frac{1}{\ln 1} (at)^h | 0 \rangle$ .

The perturbation can be written as

To first order in X, the corrections to the eigenenergies are

$$E_{n}^{(1)} = \langle n|\hat{H}_{n}|n \rangle = \lambda \frac{\hbar \omega_{0}}{4} \langle n| (\hat{a}^{+}+\hat{a})^{4} |n \rangle$$

$$= \lambda \frac{\hbar \omega_{0}}{4} \langle n| (\hat{a}^{+}+\hat{a})^{2} |n \rangle = \lambda \frac{\hbar \omega_{0}}{4} \langle n| (\hat{a}^{+}+\hat{a})^{2} |n \rangle$$

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$$|\tilde{h}\rangle = (\hat{q}^{\dagger} + \hat{q})^{2} |h\rangle$$

$$= [\hat{q}^{\dagger} + \hat{q}^{\dagger} + \hat{$$

Thus, we get

$$\langle \tilde{n} | \tilde{n} \rangle = (2n+1)^2 + (n+1)(n+2) + n(n-1)$$

=) 
$$E_n^{(1)} = \lambda \frac{3\hbar w}{9} (2n^2 + 2n + 1)$$

=) 
$$E_{h} = \frac{\hbar w_{o}(n+\frac{1}{2}) + \lambda \frac{3\hbar w_{o}(2n^{2}+24+1)}{4} + O(\lambda^{2})}{4}$$

We also find

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$$\Delta E_{h} = E_{h} - E_{h-1} = \hbar w_{o} \left(1 + \frac{34}{2}\right) + \hbar w_{o} \frac{34}{2} \left(h^{2} - (h-1)^{2}\right)$$

$$= \hbar w_{o} \left(1 + \frac{34}{2}\right) + \hbar w_{o} \frac{34}{2} \left(h^{2} - h^{2} + 2h^{-1}\right)$$

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2 hus (1561) Notice how the energy Splitting is Itwo Ithes (1+31) no longer constant! Perhaps this

can be used for ESR on the ground state?

## The Wentzel-Kramers-Brillonin method (WKB)

The WKB method provides a semi-classical Solution to the Schrödinger equation

To start with, we rewrite it as

Recalling the classical expressions  $\frac{1}{2}mv^2$  and pv for energy and momentum, we can identify  $E-V=\frac{1}{2}mv^2=P^2/am=$ 

P = + Vam(E-V) with the "classical" momentum if E)V

=) 
$$\nabla^2 4(\underline{r}) + \frac{1}{4^2} p^2(r) 4(\underline{r}) = 0$$

If the potential V(s) is constant, the solutions

to the Schrödinger equation would be

Now, if V(x) is slowly varying, the WKB method assumes that the solutions are of the form  $U(x) = A(x) e^{i \hat{S}(x)/\hbar}$ 

Inserting this ansatz into the equation

we find

$$0 = \nabla^2 (Ae^{iS/\hbar}) + \frac{1}{\hbar^2} p^2 A e^{iS/\hbar}$$

$$\times t^2 e^{iS/t}$$

$$A\left(\frac{h^2}{A}\nabla^2A - (\nabla S)^2 + \rho^2\right) + ih\left(2(\nabla A)\cdot(\nabla S) + A\nabla^2S\right) = 0$$

$$= ) \begin{cases} \frac{h^2}{A} \nabla^2 A - (\nabla S)^2 + \rho^2 = 0 \\ 2(\nabla A) - (\nabla S) + A \nabla^2 S = 0 \end{cases}$$

$$2(\nabla A) \cdot (\nabla S) + A \nabla^2 S = 0$$

where we have used too in the semi-classical limit. Here, it has been assumed that E)V such that the momentum p is ved.

We now ansider a one-dimensional problem, i.e.

$$(\nabla 5)^2 \rightarrow (\frac{dS}{dx})^2 = 2m(E-V) \Rightarrow \frac{dS}{dx} = \pm \rho = \pm \sqrt{2m(E-V)}$$

and

$$2\left(\frac{d}{dx}A\right)\frac{dS}{dx} + A\frac{d^2}{dx^2}S = 0$$

$$= 2\left(\frac{d}{dx}A\right)(\pm p) + A\frac{d}{dx}(\pm p)$$

$$= 2 \frac{1}{A} \frac{d}{dx} A + \frac{1}{P} \frac{d}{dx} P = 0$$

=) 
$$2 \frac{d}{dx} \ln A + \frac{d}{dx} \ln p - \frac{d}{dx} \ln \left( \frac{A^2 p}{a} \right) = 0$$

=) 
$$A^2 p = (oust. =) A(x) = \frac{C}{V[p[x]]}$$

Thus, we find solutions of the form  $4_{\pm}(x) = \frac{C^{\pm}}{|Ipu|} e^{\pm i \int dx} p(x)/t$ 

which holds for the classically allowed region, EXV(x).

For the classically forbidden region, E(V(x), a similar analysis is heeded, and one finds solutions of the form

Alternative derivation of the WKB approximation:

$$\frac{d^2}{dx^2} + (x) + \frac{1}{t^2} p^2 + (x) = 0, \quad p^2 = 2m (E-V)$$

We write the solution on the form

where flxt is a complex function and we think of these a small parameter (+10).

Indesting this expression above, we find

=> 
$$0 = -(f')^2 + i t_1 f'' + p^2 = i t_1 f'' - (f')^2 + p^2$$

Now, we expand flet in powers of to:

$$f(x) = f_0(x) + t_1f_1(x) + t_2f_2(x) + ...$$

Collecting terms to same order into, we find

Next, we solve these equations to first order in the theorem is the sequence of the sequence

We then have

$$4(x) = e^{i f(x)/h} = e^{\frac{1}{h} \left[ \frac{1}{h} \int_{A} dx \, p + h \left( i \ln h p - \frac{\alpha r_{3} p}{2} \right) \right]}$$

$$= \frac{C}{h p} e^{\frac{1}{h} i \int_{A} p \, dx / h}$$

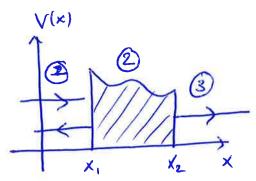
## Example of the WKB approximation: tunneling

Consider an incident

particle with momentum

Po = VIME hitting the

potential barrier shelched
in the figure, where E<Vmax



In region (1), the wave function reads  $4_1(x) = 4_{in}(x) + 4_{re}(x) = A e^{i p_i x/h} + B e^{-i p_i x/h}$ 

In region 3, we have

4311 = Meipsx/t

In region 2, we use the WKB approximation

and write

Yelx = = = + (x/dx/1plan) + D + (x/dx/1plan) + Vipan e + (x/dx/1plan)

-> blows up with barrier thickness, which is imphysical

We now want to evaluate the transmission co effe all

To this end, we use that the wave function and its first decirclive must be continuous at x, and x. At X=X1, we then have

and

where it has been assumed that  $\frac{d}{dx}|p(y)||_{X+x} \simeq 0$ 

At x=x2, we similarly find

From the case 
$$x=x_1$$
, we get

$$2Ae^{i} \frac{\rho_0 x_1/t_1}{r} = \frac{C}{|\nabla \rho_0 x_1|} - \frac{C}{|\partial \rho_0 x_1|} \frac{|\nabla \rho_0 x_1|}{|\partial \rho_0 x_1|}$$

$$= \frac{C}{|\nabla \rho_0 x_1|} \left(1 - \frac{|\rho_0 x_1|}{|\partial \rho_0 x_1|}\right)$$

$$= C = 2A |\nabla \rho_0 x_1| e^{i} \frac{\rho_0 x_1/t_1}{|\partial \rho_0 x_1|} \left(1 - \frac{|\rho_0 x_1|}{|\partial \rho_0 x_1|}\right)$$

Insecting this expression into the result for X=X2,

we obtain

$$L e^{i Po \times 2 t t} = \frac{C}{|\nabla P(x)|} e^{-\frac{1}{t} \int_{x_1}^{x_2} dx' |P(x')|}$$

$$= 2A \sqrt{\frac{|P(x_1)|}{|P(x_1)|}} e^{i Po \times 1/t} + \int_{x_1}^{x_2} dx' |P(x')| / (1-\frac{|P(x)|}{|P(x_1)|})$$

=) 
$$\frac{M}{A} = \frac{2}{1+i\frac{1p(x,1)}{p_0}} \sqrt{\frac{1p(x,1)}{1p(x,2)}} e^{i\frac{x}{p_0}(x-x_2)/4} e^{-\frac{1}{4\pi}\int_{x_1}^{x_2} dx' |p(x')|}$$

We then arrive of

We then arrive of

$$\frac{|V|^2}{|A|^2} = \frac{4}{1 + \frac{|P|x||^2}{|P|x||^2}} \frac{|P|x||^2}{|P|x||^2} e^{-\frac{2}{4\pi} \int_{X_1}^{X_2} dx' |P|x'||^2} e^{-\frac{2}{4\pi} \int_{X_2}^{X_2} c|x'| |P|x'||^2} e^{-\frac{2}{4\pi} \int_{X_1}^{X_2} c|x'| |P|x'||^2} e^{-\frac{2}{4\pi} \int_{X_2}^{X_2} c|x'| |P|x'||^2} e^{-\frac{2}{4\pi} \int_{X_1}^{X_2} c|x'| |P|x'||^2} e^{-\frac{2}{4\pi} \int_{X_1}^{X_2} c|x'| |P|x'||^2}$$

$$= \frac{4}{|P|x||^2} = \frac{4}{1 + \frac{|P|x||^2}{|P|x||^2}} \frac{|P|x'||^2}{|P|x||^2} e^{-\frac{2}{4\pi} \int_{X_1}^{X_2} c|x'| |P|x'||^2} e^{-\frac{2}{4\pi} \int_{X_1}^{X_2} c|x'| |P|x'||^2}$$

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$$= \frac{4}{1 + \frac{|P|x||^2}{|P|x||^2}} \frac{|P|x||^2}{|P|x||^2} e^{-\frac{2}{4\pi} \int_{X_1}^{X_2} c|x'|} \frac{|P|x'||^2}{|P|x'|^2}$$

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As an example, let us consider  $V(x) = \begin{cases} 0, & x < 0 \end{cases} = \begin{cases} 0, & x < 0 \end{cases}$   $V(x) = \begin{cases} 0, & x > 0 \end{cases}$   $V(x) = \begin{cases} 0, & x > 0 \end{cases}$ tunneling through a barner of the form

In a crude approximation, we colculate the termeling rote of as

$$\gamma = \frac{1}{4\pi} \int_{0}^{V_{o}-E} dx \sqrt{2m(V_{o}-\lambda x-E)}$$

$$= \frac{\sqrt{2m}}{4\pi} \left[ \frac{2}{-3\lambda} \left( V_{o}-\lambda x-E \right)^{3/2} \right]_{0}^{V_{o}-E}$$

$$= \frac{2\sqrt{2m}}{3\pi\lambda} \left( V_{o}-E \right)^{3/2}$$

$$= \frac{2\sqrt{2m}}{3\pi\lambda} \left( V_{o}-E \right)^{3/2}$$

$$= \frac{4\sqrt{2m}}{3\pi\lambda} \left( V_{o}-E \right)^{3/2}$$

$$\rightarrow + \infty e^{-\frac{4\sqrt{2m}}{3\pi\lambda}} \left( V_{o}-E \right)^{3/2}$$