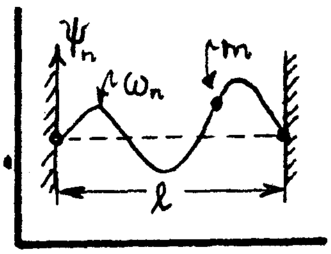
General idea of a perturbation theory

Stationary State Perturbation Theory ∫ ref. Davydov: ¶ 47-50, Sakurai: Secs. 5.1-5.2.

The key idea of a perturbation theory is to start with a well-defined and well-known system, add a small change (i.e perturbation), and then develop a method for specifying the presumably small excursions in system parameters.

In this general sense, the WKB approximation is a perturbation theory -- we start from free particle eigenfcns & eigenvalues (or from ψ's & E's in a cnst external potential), and document how things change when we add "small" (remember $|k'/k^2| \ll 1$) departures from a cnst potential.

A classical example ¶ of a perturbation is a string of length l & uniform mass density, pegged at both ends and set into vibration. The wave amplitudes ψ_n and eigenfrequencies ω_n are easy to get. Now a small point mass m (small means $m \ll$ string mass) is attached to the string -- this changes $\psi_n \to \psi_n'$ and $\omega_n \to \omega_n'$ by small amounts. The problem is to calculate the new ψ_n' & ω_n' from the old (unperturbed) ψ_n & ω_n.



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1) We shall now do the QM version of the above string problem, viz.

> Suppose a stationary (i.e. time-independent), bound-state (i.e. discrete energies) QM system with known eigenfcns $\psi_n^{(0)}$ & eigenenergies $E_n^{(0)}$ is described by: $\mathcal{H}_0(p,x)\,\psi_n^{(0)}(x) = E_n^{(0)}\,\psi_n^{(0)}(x)$. A "small" time-independent potential $V(x)$ is added to $\mathcal{H}_0$, i.e. $\mathcal{H}_0 \to \mathcal{H} = \mathcal{H}_0 + V$. The new QM problem is: $\mathcal{H}\psi_n = E_n\psi_n$. How are the perturbed (ψ_n, E_n) related to the known $(\psi_n^{(0)}, E_n^{(0)})$? (1)

¶ See Sec. 44 of A. Fetter & J. Walecka "Theoretical Mechanics..." (McGraw-Hill, 1980)

Basic perturbation equation.

REMARKS

1. For the unperturbed system, the $\{\psi_n^{(0)}\}$ are a complete orthonormal set. The energies $E_n^{(0)}$ are assumed non-degenerate (we'll treat degeneracy later).
2. $V(x)$ "small" means $|\langle\psi_n^{(0)}|V|\psi_n^{(0)}\rangle| << |E_n^{(0)}|$ within n^{th} state, or when $m \neq n$: $|\langle\psi_m^{(0)}|V|\psi_n^{(0)}\rangle| << |E_m^{(0)} - E_n^{(0)}|$. So V cannot change the spectrum much.

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2) With V added in, our perturbed problem is:

$$\mathcal{H}(p,x)\,\psi_k(x) = E_k\,\psi_k(x), \quad \text{w/ } \mathcal{H}(p,x) = \mathcal{H}_0(p,x) + V(x).$$

PROBLEM: Find ψ_k and E_k in terms of $\psi_n^{(0)}$, $E_n^{(0)}$ & V. (2)

Since $\{\psi_n^{(0)}\}$ are a complete set, we can expand the unknown ψ_k as...

$$\rightarrow \psi_k(x) = \sum_n a_{nk}\,\psi_n^{(0)}(x), \quad \text{w/ } a_{nk} = \langle\psi_n^{(0)}|\psi_k\rangle \tag{3}$$

at this point, the a_{nk} are unknown.

Plug this version of ψ_k into $\mathcal{H}\psi_k = E_k\psi_k$...

$$\sum_n a_{nk}\,(\mathcal{H}_0 + V)\,\psi_n^{(0)} = \sum_n a_{nk}\,E_k\,\psi_n^{(0)} \leftarrow \text{use } \mathcal{H}_0\psi_n^{(0)} = E_n^{(0)}\psi_n^{(0)},$$

and rearrange terms...

or/

$$\sum_n a_{nk}\,(E_k - E_n^{(0)})\,\psi_n^{(0)} = \sum_n a_{nk}\,V\,\psi_n^{(0)}. \tag{4}$$

Operate thru Eq. (4) by $\langle\psi_m^{(0)}|\ \ \rangle$, and use $\langle\psi_m^{(0)}|\psi_n^{(0)}\rangle = \delta_{mn}$. Then...

$$\boxed{(E_k - E_m^{(0)})\,a_{mk} = \sum_n V_{mn}\,a_{nk}}, \quad \text{w/ } V_{mn} = \langle\psi_m^{(0)}|V|\psi_n^{(0)}\rangle. \tag{5}$$

This is the <u>Fundamental Equation</u> of QM SS perturbation theory. It allows us -- at least in principle -- to solve for the set of coefficients $\{a_{nk}\}$ (which specify $\psi_k = \sum_n a_{nk}\psi_n^{(0)}$) from an ∞ set of linear coupled equations. The energies E_k are gotten from a secular eqtn, as follows...

Existence of solns $\{\psi_k, E_k\}$ from $\{\psi_n^{(0)}, E_n^{(0)}, V_{mn}\}$.

let/ $\rightarrow$ $$\mathbb{a}_k = \begin{pmatrix} \vdots \\ a_{nk} \\ \vdots \end{pmatrix}, \quad \underline{a_{nk} = \langle \psi_n^{(0)} | \psi_k \rangle} \ \left[\text{a rep}^{\text{n}} \text{ of } \psi_k \text{ on basis } \{\psi_n^{(0)}\}\right]; \tag{6a}$$

$\rightarrow$ $$\underset{\sim}{V} = \begin{pmatrix} & \vdots & \\ \cdots & V_{mn} & \cdots \\ & \vdots & \end{pmatrix}, \quad \underline{V_{mn} = \langle \psi_m^{(0)} | V | \psi_n^{(0)} \rangle} \ \left[\text{rep}^{\text{n}} \text{ of } V \text{ on } \{\psi_n^{(0)}\}\right]; \tag{6b}$$

$\rightarrow$ $$\underset{\sim}{\Delta}_k = \begin{pmatrix} \cdots (E_k - E_m^{(0)})\delta_{mn} \cdots \end{pmatrix}, \text{ a \underline{diagonal} energy matrix.} \tag{6c}$$

Then Eq. (5) reads, in these terms...

$$\underline{\underline{\underset{\sim}{\Delta}_k \mathbb{a}_k = \underset{\sim}{V} \mathbb{a}_k}}, \quad \text{or/} \ (\underset{\sim}{\Delta}_k - \underset{\sim}{V}) \mathbb{a}_k = 0;$$

and/ $$\det(\underset{\sim}{\Delta}_k - \underset{\sim}{V}) = \det\left[(E_k - E_m^{(0)})\delta_{mn} - V_{mn}\right] = 0. \quad \text{secular equation.} \tag{7}$$

The <u>secular eqtn</u> is imposed to avoid the trivial solution $\mathbb{a}_k \equiv 0$. It will evidently give a specific E_k in terms of all the $E_m^{(0)}$ & V_{mn}. Then, with the $\{E_k\}$, we can find the (normalized) eigenvectors $\{\mathbb{a}_k\}$ as usual.

This statement of the perturbation problem in Eq. (5) shows that solutions $\{\psi_k, E_k\}$ <u>exist</u>, and they can be gotten from the $\{\psi_n^{(0)}, E_n^{(0)}\}$ and V alone. But Eq. (7) is not a practical solution, since it involves $\infty \times \infty$ matrices like $\{V_{mn}\}$ and ∞-component eigenvectors $\mathbb{a}_k$.

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3) A practical method of dealing with Eq. (5) capitalizes on the "smallness" of V and the notion we can correct for it by a series of ever smaller terms. Let:

$$\underline{V \rightarrow \lambda V} \begin{cases} \text{parameter } \lambda = 0 \Rightarrow \text{no perturbation; solns are } \psi_n^{(0)} \text{ \& } E_n^{(0)}; \\ \quad " \quad \lambda = 1 \Rightarrow \text{full perturbation; solns are } \psi_k \text{ \& } E_k. \end{cases} \tag{8}$$

Expansion of Fund$^{\underline{l}}$ Eq. (5) in terms of order parameter λ

In what follows, we will always take $\lim_{\lambda\to 1}$ in the final result, to get the full solution of the $(\mathcal{H}_0+V)$ problem. λ is just a convenient parameter to keep track of what "order-of-approximation" we are doing; this will soon become clear.

If V is "small", E_k must be close to $E_k^{(0)}$, so we write...

$$\rightarrow E_k = E_k^{(0)} + \lambda E_k^{(1)} + \lambda^2 E_k^{(2)} + \cdots = \sum_{\mu=0}^{\infty} \lambda^\mu E_k^{(\mu)} \quad \Big/ \lim_{\lambda\to 1} \text{ is understood.} \tag{9}$$

$E_k^{(\mu)}$ is called the $\mu^{\underline{th}}$ order correction to $E_k^{(0)}$ [for $\mu \geq 1$].

Hope is: if V is "small", then $\underline{|E_k^{(\mu+1)}| \ll |E_k^{(\mu)}|}$, so series converges.

In the same spirit, we expand the unknown a_{nk}'s in Eq. (5), viz...

$$\rightarrow a_{nk} = a_{nk}^{(0)} + \lambda a_{nk}^{(1)} + \lambda^2 a_{nk}^{(2)} + \cdots = \sum_{\nu=0}^{\infty} \lambda^\nu a_{nk}^{(\nu)} \quad \Big/ \lim_{\lambda\to 1} \text{ is understood.} \tag{10}$$

Put the λ-expansions of Eqs. (9) & (10) into the Fundamental Equation (5);

$$\rightarrow (E_k - E_m^{(0)})\, a_{mk} = \sum_n \lambda V_{mn} a_{nk}, \text{ becomes:}$$

$$\underbrace{\Big(\sum_{\mu=0}^{\infty} E_k^{(\mu)} \lambda^\mu\Big)\Big(\sum_{\nu=0}^{\infty} a_{mk}^{(\nu)} \lambda^\nu\Big)} - \sum_{\nu=0}^{\infty} E_m^{(0)} a_{mk}^{(\nu)} \lambda^\nu = \sum_n \lambda V_{mn} \Big(\sum_{\nu=0}^{\infty} a_{nk}^{(\nu)} \lambda^\nu\Big). \tag{11}$$

[use general formula for product of power series] $\Big(\sum_{\mu=0}^{\infty} A_\mu \lambda^\mu\Big)\Big(\sum_{\nu=0}^{\infty} B_\nu \lambda^\nu\Big) = \sum_{\mu=0}^{\infty} C_\mu \lambda^\mu, \quad C_\mu = \sum_{\sigma=0}^{\mu} A_{\mu-\sigma} B_\sigma$

so// $1^{\underline{st}}$ term LHS in Eq. (11) $= \displaystyle\sum_{\mu=0}^{\infty} \Big(\sum_{\sigma=0}^{\mu} E_k^{(\mu-\sigma)} a_{mk}^{(\sigma)}\Big) \lambda^\mu$,

and Eq. (11) can be written...

$$\left[\!\left[\sum_{\mu=0}^{\infty} \Big[\sum_{\sigma=0}^{\mu} E_k^{(\mu-\sigma)} a_{mk}^{(\sigma)} - E_m^{(0)} a_{mk}^{(\mu)} \Big] \lambda^\mu = \sum_{\nu=0}^{\infty} \Big[\sum_n V_{mn} a_{nk}^{(\nu)} \Big] \lambda^{\nu+1}. \right]\!\right] \tag{12}$$

This is now the Master Equation. It can be simplified, by the following steps:

Master Eqtn for Perturbation Theory as an Iteration

Simplifying Eq. (12)...

1. On the LHS, split off the $\mu=0$ term, and set $\sum_{\mu=1}^{\infty} = \sum_{\nu=0}^{\infty}$, with $\mu=\nu+1$. Then...

$$\left[\begin{matrix}\text{LHS of}\\ \text{Eq. (12)}\end{matrix}\right\} = (E_k^{(0)} - E_m^{(0)}) a_{mk}^{(0)} + \sum_{\nu=0}^{\infty} \Big[\underbrace{\sum_{\sigma=0}^{\nu+1} E_k^{(\nu+1-\sigma)} a_{mk}^{(\sigma)}}_{= E_k^{(0)} a_{mk}^{(\nu+1)} + \sum_{\sigma=0}^{\nu} E_k^{(\nu+1-\sigma)} a_{mk}^{(\sigma)}} - E_m^{(0)} a_{mk}^{(\nu+1)} \Big] \lambda^{\nu+1}; \quad (13)$$

Take entire RHS of (12), and put over to LHS. Then (12) becomes...

$$\rightarrow (E_k^{(0)} - E_m^{(0)}) a_{mk}^{(0)} + \sum_{\nu=0}^{\infty} \Big[(E_k^{(0)} - E_m^{(0)}) a_{mk}^{(\nu+1)} + \sum_{\sigma=0}^{\nu} E_k^{(\nu+1-\sigma)} a_{mk}^{(\sigma)} - \sum_n V_{mn} a_{nk}^{(\nu)} \Big] \lambda^{\nu+1} = 0. \quad (14)$$

This is the first simplification.

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2. Consider Eq. (14) as a <u>power series in λ</u> for $\lambda \neq 0$ ($0 < \lambda \leq 1$ is OK). Since λ is an independently variable parameter, the only way the power series can $=0$ is if every one of its coefficients vanish, i.e.

$$\left[\begin{aligned} &\text{I.}\ (E_k^{(0)} - E_m^{(0)}) a_{mk}^{(0)} = 0; && (15a)\\ &\text{II.}\ (E_k^{(0)} - E_m^{(0)}) a_{mk}^{(\nu+1)} + E_k^{(\nu+1)} a_{mk}^{(0)} = \sum_n V_{mn} a_{nk}^{(\nu)} - \sum_{\sigma=1}^{\nu} E_k^{(\nu+1-\sigma)} a_{mk}^{(\sigma)}. && (15b)\end{aligned}\right.$$

This extremely powerful simplification justifies the whole procedure of using power series in λ. Note that II is a recursion relation for $a_{mk}^{(\nu+1)} = \text{fcn}\ a_{mk}^{(\mu\leq\nu)}$.

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3. In Eq. (15a), $a_{mk}^{(0)} \equiv 0$ for $m \neq k$ (the $E_n^{(0)}$ are not degenerate). Then, for $m=k$ we need $a_{kk}^{(0)} = 1$, so that $\psi_k = \psi_k^{(0)}$ when V vanishes. So: $\boxed{a_{mk}^{(0)} = \delta_{mk}}$. Use of this in Eq. (15b), plus rewrite of last term RHS (let $\mu = \sigma - 1$) gives...

$$\boxed{(E_k^{(0)} - E_m^{(0)}) a_{mk}^{(\nu+1)} + E_k^{(\nu+1)} \delta_{mk} = \sum_n V_{mn} a_{nk}^{(\nu)} - \sum_{\mu=0}^{\nu-1} E_k^{(\nu-\mu)} a_{mk}^{(\mu+1)}}\ ; \ \nu = 0, 1, 2, \ldots \quad (16)$$

term contributes for $\nu \geq 1$ only.

This is the <u>new</u> version of our <u>Master Eq.</u> for perturbation. The order parameter $\nu = 0, 1, 2, \ldots$ corresponds to working on $O(\lambda)$, $O(\lambda^2)$, $O(\lambda^3)$ terms, i.e. to working on 1st, 2nd, 3rd order perturbative corrections.

SS Perturbation Theory: Iteration of Master Eq. (16).

4) Now we iterate the Master Eqtn to get the $a_{mk}^{(1)}$ from the already known $a_{mk}^{(0)}=\delta_{mk}$, the $a_{mk}^{(2)}$ from the $a_{mk}^{(1)}$ & $a_{mk}^{(0)}$, etc. Also the $E_k^{(1)}$ from the $E_k^{(0)}$, etc. Like this:

In Eq. (16), choose $\nu=0$ ($\Rightarrow$ working to $O(\lambda)$, 1st order perturbation theory).

So $\longrightarrow$ $$(E_k^{(0)}-E_m^{(0)})\,a_{mk}^{(1)}+E_k^{(1)}\delta_{mk}=\sum_n V_{mn}\overset{\delta_{nk}}{a_{nk}^{(0)}}+(\text{zero})=V_{mk}. \quad (17)$$

1. $m\neq k$, (17) $\Rightarrow$ $\boxed{a_{mk}^{(1)}=V_{mk}/(E_k^{(0)}-E_m^{(0)})}$. (17a)

So $$\psi_k=\psi_k^{(0)}+\underbrace{\sum_m a_{mk}^{(1)}\psi_m^{(0)}}_{\text{"small" correction only if}}+\cdots$$ $|a_{mk}^{(1)}|\ll 1$, or $|V_{mk}|\ll|E_k^{(0)}-E_m^{(0)}|$ (as advertised at top of p. SS 2).

2. $m=k$, (17) $\Rightarrow$ $(\text{zero})+E_k^{(1)}=V_{kk}+(\text{zero})$, i.e. $\boxed{E_k^{(1)}=V_{kk}}$. (17b)

So $$E_k=E_k^{(0)}+\underbrace{V_{kk}}_{\text{"small" only if}}+\cdots$$ $|V_{kk}|\ll|E_k^{(0)}|$, within state k. (as advertised on top of p. SS 2).

NOTE: the $m=k$ eqtn for $\nu=0$ gives no information on $a_{kk}^{(1)}$.

$\boxed{\text{ASIDE}}$: What value do we give $a_{kk}^{(1)}$? Assertion: we can set $a_{kk}^{(1)}=0$.

(1) We can defend the assertion on grounds that ψ_k should be normed: $\langle\psi_k|\psi_k\rangle=1$. The argument goes as follows. Write the wavefcn ψ_k as ...

$$\left[\begin{array}{l}\psi_k=\sum_n a_{nk}\psi_n^{(0)}=\sum_n\left(\sum_{\sigma=0}^{\infty}\lambda^\sigma a_{nk}^{(\sigma)}\right)\psi_n^{(0)}=\sum_{\sigma=0}^{\infty}\psi_k^{(\sigma)},\\ \text{w/}\quad \psi_k^{(\sigma)}=\lambda^\sigma\sum_n a_{nk}^{(\sigma)}\psi_n^{(0)}=\lambda^\sigma\left[a_{kk}^{(\sigma)}\psi_k^{(0)}+\sum_n{}' a_{nk}^{(\sigma)}\psi_n^{(0)}\right].\end{array}\right. \quad (18)$$

prime means $\sum_{n\neq k}$ (sum w/o $n=k$ term)

$\psi_k^{(\sigma)}$ is the σ^{th} order correction to $\psi_k^{(0)}$; note $\psi_k^{(\sigma)}|_{\sigma=0}=\psi_k^{(0)}$, as should be (here use $a_{nk}^{(0)}=\delta_{nk}$). Now we calculate the norm, $\langle\psi_k|\psi_k\rangle$, after splitting off $\psi_k^{(0)}$, i.e. put $\psi_k=\psi_k^{(0)}+\sum_{\sigma=1}^{\infty}\psi_k^{(\sigma)}$ and calculate ...

Normalization of perturbed wavefcn ψ_k.

$$\rightarrow \langle\psi_k|\psi_k\rangle = \langle \psi_k^{(0)} + \sum_{\sigma=1}^{\infty}\psi_k^{(\sigma)} \,|\, \psi_k^{(0)} + \sum_{\mu=1}^{\infty}\psi_k^{(\mu)}\rangle$$

$$= 1 + 2\,\mathrm{Re}\sum_{\sigma=1}^{\infty}\underbrace{\langle\psi_k^{(0)}|\psi_k^{(\sigma)}\rangle}_{1} + \sum_{\sigma,\mu=1}^{\infty}\underbrace{\langle\psi_k^{(\sigma)}|\psi_k^{(\mu)}\rangle}_{2} \qquad (19)$$

(2) Use $\psi_k^{(\sigma)}$ from Eq. (18) to evaluate the projections ① & ②. Thus...

$$① = \lambda^\sigma\langle\psi_k^{(0)}\,|\,a_{kk}^{(\sigma)}\psi_k^{(0)} + {\sum_n}' a_{nk}^{(\sigma)}\psi_n^{(0)}\rangle = \lambda^\sigma a_{kk}^{(\sigma)}; \qquad (20a)$$

only contrib^{n}

$$② = \lambda^{\sigma+\mu}\langle a_{kk}^{(\sigma)}\psi_k^{(0)} + {\sum_n}' a_{nk}^{(\sigma)}\psi_n^{(0)}\,|\,a_{kk}^{(\mu)}\psi_k^{(0)} + {\sum_m}' a_{mk}^{(\mu)}\psi_m^{(0)}\rangle$$

$$= \lambda^{\sigma+\mu}\Big\{a_{kk}^{(\sigma)*}a_{kk}^{(\mu)} + \sum_{n,m} a_{nk}^{(\sigma)*}a_{mk}^{(\mu)}\underbrace{\langle\psi_n^{(0)}|\psi_m^{(0)}\rangle}_{\delta_{nm},\text{ now sum over } m.}\Big\}. \qquad (20b)$$

Put results of Eqs. (20) into Eq. (19) to get the ψ_k norm as...

$$\boxed{\langle\psi_k|\psi_k\rangle = 1 + 2\,\mathrm{Re}\sum_{\sigma=1}^{\infty}\lambda^\sigma a_{kk}^{(\sigma)} + \sum_{\sigma,\mu=1}^{\infty}\lambda^{\sigma+\mu}\Big\{a_{kk}^{(\sigma)*}a_{kk}^{(\mu)} + {\sum_n}' a_{nk}^{(\sigma)*}a_{nk}^{(\mu)}\Big\}}. \qquad (21)$$

This expression is exact. Clearly $\langle\psi_k|\psi_k\rangle \neq 1$ in general (despite $\langle\psi_k^{(0)}|\psi_k^{(0)}\rangle = 1$).

(3) Now suppose we are working in the $\sigma = 1^{st}$ order of perturbation theory, as we did in Eqs. (17) on p. SS6. Eq. (21) prescribes (to $O(\lambda)$ and no higher)...

$$\rightarrow \langle\psi_k|\psi_k\rangle = 1 + 2\lambda\,\mathrm{Re}\,a_{kk}^{(1)} + \cancel{O(\lambda^2)}^{\,0},$$

so reqt. that $\langle\psi_k|\psi_k\rangle = 1 \Rightarrow \underline{\mathrm{Re}\,a_{kk}^{(1)} = 0}$, or $a_{kk}^{(1)} = i\,b_k^{(1)}$ ← $a_{kk}^{(1)}$ is pure imaginary

and $\psi_k \simeq \psi_k^{(0)} + \psi_k^{(1)} = [1 + \lambda a_{kk}^{(1)}]\psi_k^{(0)} + \left(\lambda {\sum_n}' a_{nk}^{(1)}\psi_n^{(0)}\right)$ ← this is $O(\lambda^2) \to 0$, by $a_{nk}^{(1)} = \dfrac{\lambda V_{nk}}{E_k^{(0)} - E_n^{(0)}}$.

$$\text{or } \psi_k \simeq [1 + i\lambda b_k^{(1)}]\psi_k^{(0)} \rightarrow [e^{i\lambda b_k^{(1)}}]\psi_k^{(0)}, \text{ to } O(\lambda). \qquad (22)$$

So the evanescent $a_{kk}^{(1)}$ enters 1st order theory at most as a phase factor, which is arbitrary. We can set $b_k^{(1)} \equiv 0$ w/o harm. So, as advertised, $\underline{a_{kk}^{(1)} = 0}$.

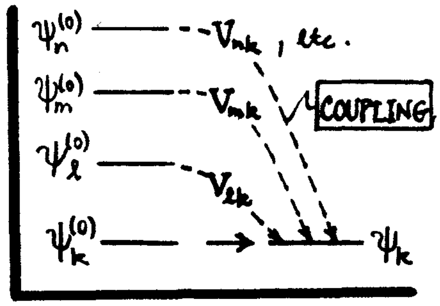
Form of theory when all phases $a_{kk}^{(\sigma)} \equiv 0$.

(4) Now we can claim with confidence that in 1st order theory...

$$\left[\begin{aligned} a_{mk}^{(1)} &= \begin{cases} V_{mk}/(E_k^{(0)} - E_m^{(0)}), & \text{for } m \neq k; \\ \underline{\underline{0}}, & \text{for } m = k; \end{cases} \\ \text{so}\quad \psi_k &\simeq \psi_k^{(0)} + \sum_n{}' \left(\frac{V_{nk}}{E_k^{(0)} - E_n^{(0)}}\right)\psi_n^{(0)} \end{aligned}\right] \tag{23}$$

← is 1st order perturbed wavefcn [prime on $\sum_n{}'$ ⇒ $n \neq k$ in sum]

This maneuver removes the possibility that $a_{kk}^{(1)} = \left(\frac{V_{nk}}{E_k^{(0)} - E_n^{(0)}}\right)\Big|_{n=k}$ diverges for $V_{kk} \neq 0$. Also, it ensures that $\langle \psi_k | \psi_k \rangle = 1 + \Theta(\lambda^2)$, i.e. that ψ_k is normed to 1 to within the order of approxn $[\Theta(\lambda)]$. Note that in 1st order theory, the mixed state ψ_k has a contribution from $\psi_n^{(0)}$ only if the "Coupling" $V_{nk} \neq 0$.



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(5) It is clear from the Master Eq. (16) that in general the $a_{kk}^{(\sigma)}$, $\sigma \geq 1$, are free constants (phase factors) because for $m = k$ the eqtn reads...

$$\rightarrow (E_k^{(0)} - \cancel{E_k^{(0)}})^{\,0}\, a_{kk}^{(\nu+1)} + E_k^{(\nu+1)} = \sum_n{}' V_{kn} a_{nk}^{(\nu)} + \left[V_{kk} a_{kk}^{(\nu)} - \sum_{\sigma=1}^{\nu} E_k^{(\nu+1-\sigma)} a_{kk}^{(\sigma)}\right]. \tag{24}$$

Since the first term LHS drops out, we get no restrictions on $a_{kk}^{(\nu+1)}$ from any of the previous iterations for $a_{nk}^{(\sigma)}$ & $E_k^{(\sigma)}$, $\sigma \leq \nu$. We thus have the freedom:

$$\underline{\underline{\text{Choose}: a_{kk}^{(\sigma)} \equiv 0, \text{ for all } \sigma \geq 1}} \tag{25}$$

So 1. $\langle \psi_k | \psi_k \rangle = 1 + \sum_n{}' \left(\sum_{\sigma,\mu=1}^{\infty} a_{nk}^{(\sigma)*} a_{nk}^{(\mu)} \lambda^{\sigma+\mu} \right)$, from Eq. (21); ← 1st term is $\Theta(\lambda^4)$ (usually negligible).

2. $\langle \psi_k^{(\sigma)} | \psi_k \rangle = \lambda^\sigma \sum_n{}' \left(\sum_{\mu=1}^{\infty} a_{nk}^{(\sigma)*} a_{nk}^{(\mu)} \lambda^\mu \right)$ ← the ( ) = $\Theta(\lambda^2)$ at least, so $\psi_k^{(\sigma)}$ is ⊥ ψ_k, negl. $\Theta(\lambda^{\sigma+2})$.

3. $\underline{E_k^{(\nu+1)} = \sum_n{}' V_{kn} a_{nk}^{(\nu)}}$, from Eq. (24). ← NICE SIMPLIFICATION!

END of ASIDE