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Perturbation Theory for a Nondegenerate Level

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Le Bellac use $H = H_0 + \lambda W$

Replace $W \to H_1$

Le Bellac uses $|n, r\rangle$ for eigenstates of H_0, energy $E_0^{(n)}$, r labels different degenerate states in the same level.

Thus he writes

$$H_0 = \sum_n E_0^{(n)} P^{(n)} \qquad P^{(n)} = \sum_r |n, r\rangle\langle n, r|$$

However, Le Bellac in his (14.2) uses $|k\rangle$ in place of ~~the pair of labels~~ $|k, r\rangle$

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In the following notes we use

$$|n,r\rangle \longrightarrow |\varphi_0^\alpha\rangle \qquad \alpha \text{ replaces } n,r$$

so

$$H_0|\varphi_0^\alpha\rangle = E_0^\alpha|\varphi_0^\alpha\rangle$$

Write

$$H = H_0 + \lambda H_1$$

Fix a <u>particular</u> α, and in place of

$$H\,|\varphi^\alpha(\lambda)\rangle = E^\alpha(\lambda)|\varphi^\alpha(\lambda)\rangle$$

drop the superscript label

$$(H_0 + \lambda H_1)|\varphi(\lambda)\rangle = E(\lambda)|\varphi(\lambda)\rangle$$

$$|\varphi(\lambda=0)\rangle = |\varphi_0\rangle$$

One chooses $|\varphi(\lambda)\rangle$ such that

$$\langle\varphi_0|\varphi(\lambda)\rangle = 1 \qquad (14a)$$

a very important condition, which says $|\varphi(\lambda)\rangle$ is (in general) not normalized.

Then expand

$$|\varphi(\lambda)\rangle = |\varphi_0\rangle + \lambda|\varphi_1\rangle + \lambda^2|\varphi_2\rangle + \cdots$$

whence, by (14a)

$$\langle\varphi_0|\varphi_0\rangle = 1$$

$$\langle\varphi_0|\varphi_j\rangle = 0 \quad \text{for } j \geq 1$$

Also assume

$$E(\lambda) = E_0 + \lambda E_1 + \lambda^2 E_2 + \cdot$$

and write

$$[H - E(\lambda)]\,|\varphi(\lambda)\rangle$$

$$= [H_0 + \lambda H_1 - E_0 - \lambda E_1 - \lambda^2 E_2]\cdot[|\varphi_0\rangle + \lambda|\varphi_1\rangle + \lambda^2|\varphi_2\rangle + \cdot\ ] = 0$$

$$\downarrow$$

$$H_0 - E_0 + \lambda(H_1 - E_1) - \lambda^2 E_2 \cdots$$

and sort out the different terms by powers of λ

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$$(H_0 - E_0)|\varphi_0\rangle = 0$$

$$(H_0 - E_0)|\varphi_1\rangle + (H_1 - E_1)|\varphi_0\rangle = 0 \qquad (15a)$$

$$(H_0 - E_0)|\varphi_2\rangle + (H_1 - E_1)|\varphi_1\rangle - E_2|\varphi_0\rangle = 0$$

If we were to write this in the form $(H_2 - E_2)|\varphi_0\rangle$ it would look more "natural" and would be correct if
$H = H_0 + \lambda H_1 + \lambda^2 H_2 + \cdots$

We think about these equations by expanding them in the orbasis provided by eigenstates of H_0, say
$|\varphi_0\rangle = |\alpha_0\rangle$, $|\beta_0\rangle$ with $\beta \neq \alpha$, and so forth

To find expansion coefficients, take inner product of equations with these basis vectors

Start off with inner product with $|\varphi_0\rangle$

Then we get, using

$$\langle\varphi_0|(H_0-E_0)=0$$

the results

$$\langle\varphi_0|H_1-E_1|\varphi_0\rangle=0$$

$$\langle\varphi_0|H_1-E_1|\varphi_1\rangle+\langle\varphi_0|H_2-E_2|\varphi_0\rangle=0$$

$$\langle\varphi_0|H_1-E_1|\varphi_2\rangle+\langle\varphi_0|H_2-E_2|\varphi_1\rangle+\langle\varphi_0|H_3-E_3|\varphi_0\rangle=0$$

etc.

Then use $\langle\varphi_0|\varphi_0\rangle=1 \qquad \langle\varphi_0|\varphi_j\rangle=0$ for $j\geq 1$

to rewrite as

$$\langle\varphi_0|H_1|\varphi_0\rangle-E_1=0$$

$$\langle\varphi_0|H_1|\varphi_1\rangle+\langle\varphi_0|H_2|\varphi_0\rangle-E_2=0$$

that gives us

$$E_1=\langle\varphi_0|H_1|\varphi_0\rangle$$

$$E_2=\langle\varphi_0|H_1|\varphi_1\rangle+\langle\varphi_0|H_2|\varphi_0\rangle$$

$$E_3=\langle\varphi_0|H_1|\varphi_2\rangle+\langle\varphi_0|H_2|\varphi_1\rangle+\langle\varphi_0|H_3|\varphi_0\rangle$$

and so forth.

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Of course, if

$$H_2 = H_3 = \cdots 0$$

then we obtain just

$$E_1 = \langle \varphi_0 | H_1 | \varphi_0 \rangle$$

$$E_2 = \langle \varphi_0 | H_1 | \varphi_1 \rangle$$

$$E_3 = \langle \varphi_0 | H_1 | \varphi_2 \rangle$$

and so forth. Thus to get E_{j+1} we need to first find $|\varphi_j\rangle$

Next step: To determine $|\varphi_1\rangle$, etc.

use the previous set of equations, but expand in a general element of the orthonormal basis.

Begin by rewriting with $|\varphi_j\rangle \to |\alpha_j\rangle$ and placing superscripts on energies. One could also use $|\varphi_j^\alpha\rangle$

So

$$(H_0 - E_0^\alpha)|\varphi_0^\alpha\rangle = 0$$

$$(H_0 - E_0^\alpha)|\varphi_1^\alpha\rangle + (H_1 - E_1^\alpha)|\varphi_1^\alpha\rangle = 0$$

$$(H_0 - E_0^\alpha)|\varphi_2^\alpha\rangle + (H_1 - E_1^\alpha)|\varphi_1^\alpha\rangle + (H_2 - E_2^\alpha)|\varphi_0^\alpha\rangle = 0$$

and left multiply by $\langle\varphi_0^\beta|$ to get

$$(E_0^\beta - E_0^\alpha)\langle\varphi_0^\beta|\varphi_0^\alpha\rangle = 0$$

$$(E_0^\beta - E_0^\alpha)\langle\varphi_0^\beta|\varphi_1^\alpha\rangle + \langle\varphi_0^\beta|H_1 - E_1^\alpha|\varphi_0^\alpha\rangle = 0$$

$$= (E_0^\beta - E_0^\alpha)\langle\varphi_0^\beta|\varphi_1^\alpha\rangle + \langle\varphi_0^\beta|H_1|\varphi_0^\alpha\rangle = 0$$

Solve this equation for the coefficient $\langle\varphi_0^\beta|\varphi_1^\alpha\rangle$ one wants for the expansion of $|\varphi_1^\alpha\rangle$, and we have

$$\langle\varphi_0^\beta|\varphi_1^\alpha\rangle = \frac{\langle\varphi_0^\beta|H_1|\varphi_0^\alpha\rangle}{E_0^\alpha - E_0^\beta}$$

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Noting that $\langle \varphi_0^\alpha | \varphi_1^\alpha \rangle = 0$ by the normalization choice, we arrive at

$$|\varphi_1^\alpha\rangle = \sum_{\beta(\neq\alpha)} \frac{|\varphi_0^\beta\rangle\langle\varphi_0^\beta|H_1|\varphi_0^\alpha\rangle}{E_0^\alpha - E_0^\beta}$$

Comment: It is at this point we have made use of the assumed nondegeneracy of the state $|\alpha_0\rangle$. Obviously this expression would not make sense if we had $E_0^\beta = E_0^\alpha$ for some $\beta \neq \alpha$.

With this expression in hand, and assuming $H_2 = 0$, we arrive at

$$E_2^\alpha = \langle\varphi_0^\alpha|H_1|\varphi_1^\alpha\rangle = \sum_{\beta(\neq\alpha)} \frac{\langle\varphi_0^\alpha|H_1|\varphi_0^\beta\rangle\langle\varphi_0^\beta|H_1|\varphi_0^\alpha\rangle}{E_0^\alpha - E_0^\beta}$$

or

$$\boxed{E_2^\alpha = \sum_{\beta(\neq\alpha)} \frac{|\langle\varphi_0^\alpha|H_1|\varphi_0^\beta\rangle|^2}{E_0^\alpha - E_0^\beta}}$$

Mnemonic for order in the denominator.
Second order ground state (so $E_0^\beta > E_0^\alpha$) correction is always <u>negative</u>