Many-body perturbation theory

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We assume here that we are only interested in the ground state of the system and expand the exact wave function in term of a series of Slater determinants

$$|\Psi_0\rangle = |\Phi_0\rangle + \sum_{m=1}^{\infty} C_m |\Phi_m\rangle,$$

where we have assumed that the true ground state is dominated by the solution of the unperturbed problem, that is

$$\hat{H}_0 |\Phi_0\rangle = W_0 |\Phi_0\rangle.$$

The state $|\Psi_0\rangle$ is not normalized, rather we have used an intermediate normalization $\langle\Phi_0|\Psi_0\rangle = 1$ since we have $\langle\Phi_0|\Phi_0\rangle = 1$.

The Schroedinger equation is

$$\hat{H} |\Psi_0\rangle = E |\Psi_0\rangle,$$

and multiplying the latter from the left with $\langle\Phi_0|$ gives

$$\langle\Phi_0|\hat{H}|\Psi_0\rangle = E\langle\Phi_0|\Psi_0\rangle = E,$$

and subtracting from this equation

$$\langle\Psi_0|\hat{H}_0|\Phi_0\rangle = W_0\langle\Psi_0|\Phi_0\rangle = W_0,$$

and using the fact that the both operators $\hat{H}$ and $\hat{H}_0$ are hermitian results in

$$\Delta E = E - W_0 = \langle\Phi_0|\hat{H}_I|\Psi_0\rangle,$$

which is an exact result. We call this quantity the correlation energy.

This equation forms the starting point for all perturbative derivations. However, as it stands it represents nothing but a mere formal rewriting of Schroedinger's equation and is not of much practical use. The exact wave function $|\Psi_0\rangle$ is unknown. In order to obtain a perturbative expansion, we need to expand the exact wave function in terms of the interaction $\hat{H}_I$.

Here we have assumed that our model space defined by the operator $\hat{P}$ is one-dimensional, meaning that

$$\hat{P} = |\Phi_0\rangle\langle\Phi_0|,$$

and

$$\hat{Q} = \sum_{m=1}^{\infty} |\Phi_m\rangle\langle\Phi_m|.$$

We can thus rewrite the exact wave function as

$$|\Psi_0\rangle = (\hat{P} + \hat{Q})|\Psi_0\rangle = |\Phi_0\rangle + \hat{Q}|\Psi_0\rangle.$$

Going back to the Schrödinger equation, we can rewrite it as, adding and a subtracting a term $\omega|\Psi_0\rangle$ as

$$\left(\omega - \hat{H}_0\right)|\Psi_0\rangle = \left(\omega - E + \hat{H}_I\right)|\Psi_0\rangle,$$

where ω is an energy variable to be specified later.

We assume also that the resolvent of $\left(\omega - \hat{H}_0\right)$ exits, that is it has an inverse which defined the unperturbed Green's function as

$$\left(\omega - \hat{H}_0\right)^{-1} = \frac{1}{\left(\omega - \hat{H}_0\right)}.$$

We can rewrite Schroedinger's equation as

$$|\Psi_0\rangle = \frac{1}{\omega - \hat{H}_0}\left(\omega - E + \hat{H}_I\right)|\Psi_0\rangle,$$

and multiplying from the left with $\hat{Q}$ results in

$$\hat{Q}|\Psi_0\rangle = \frac{\hat{Q}}{\omega - \hat{H}_0}\left(\omega - E + \hat{H}_I\right)|\Psi_0\rangle,$$

which is possible since we have defined the operator $\hat{Q}$ in terms of the eigenfunctions of $\hat{H}$.

These operators commute meaning that

$$\hat{Q}\frac{1}{\left(\omega - \hat{H}_0\right)}\hat{Q} = \hat{Q}\frac{1}{\left(\omega - \hat{H}_0\right)} = \frac{\hat{Q}}{\left(\omega - \hat{H}_0\right)}.$$

With these definitions we can in turn define the wave function as

$$|\Psi_0\rangle = |\Phi_0\rangle + \frac{\hat{Q}}{\omega - \hat{H}_0}\left(\omega - E + \hat{H}_I\right)|\Psi_0\rangle.$$

This equation is again nothing but a formal rewrite of Schrödinger's equation and does not represent a practical calculational scheme. It is a non-linear equation in two unknown quantities, the energy E and the exact wave function $|\Psi_0\rangle$. We can however start with a guess for $|\Psi_0\rangle$ on the right hand side of the last equation.

The most common choice is to start with the function which is expected to exhibit the largest overlap with the wave function we are searching after, namely $|\Phi_0\rangle$. This can again be inserted in the solution for $|\Psi_0\rangle$ in an iterative fashion and if we continue along these lines we end up with

$$|\Psi_0\rangle = \sum_{i=0}^{\infty}\left\{\frac{\hat{Q}}{\omega - \hat{H}_0}\left(\omega - E + \hat{H}_I\right)\right\}^i|\Phi_0\rangle,$$

for the wave function and

$$\Delta E = \sum_{i=0}^{\infty}\langle\Phi_0|\hat{H}_I\left\{\frac{\hat{Q}}{\omega - \hat{H}_0}\left(\omega - E + \hat{H}_I\right)\right\}^i|\Phi_0\rangle,$$

which is now a perturbative expansion of the exact energy in terms of the interaction $\hat{H}_I$ and the unperturbed wave function $|\Psi_0\rangle$.

In our equations for $|\Psi_0\rangle$ and ΔE in terms of the unperturbed solutions $|\Phi_i\rangle$ we have still an undetermined parameter ω and a dependecy on the exact energy E. Not much has been gained thus from a practical computational point of view.

In Brilluoin-Wigner perturbation theory it is customary to set $\omega = E$. This results in the following perturbative expansion for the energy ΔE

$$\Delta E = \sum_{i=0}^{\infty}\langle\Phi_0|\hat{H}_I\left\{\frac{\hat{Q}}{\omega - \hat{H}_0}\left(\omega - E + \hat{H}_I\right)\right\}^i|\Phi_0\rangle =$$

$$\langle\Phi_0|\left(\hat{H}_I + \hat{H}_I\frac{\hat{Q}}{E - \hat{H}_0}\hat{H}_I + \hat{H}_I\frac{\hat{Q}}{E - \hat{H}_0}\hat{H}_I\frac{\hat{Q}}{E - \hat{H}_0}\hat{H}_I + \ldots\right)|\Phi_0\rangle.$$

$$\Delta E = \sum_{i=0}^{\infty}\langle\Phi_0|\hat{H}_I\left\{\frac{\hat{Q}}{\omega - \hat{H}_0}\left(\omega - E + \hat{H}_I\right)\right\}^i|\Phi_0\rangle =$$

$$\langle\Phi_0|\left(\hat{H}_I + \hat{H}_I\frac{\hat{Q}}{E - \hat{H}_0}\hat{H}_I + \hat{H}_I\frac{\hat{Q}}{E - \hat{H}_0}\hat{H}_I\frac{\hat{Q}}{E - \hat{H}_0}\hat{H}_I + \ldots\right)|\Phi_0\rangle.$$

This expression depends however on the exact energy E and is again not very convenient from a practical point of view. It can obviously be solved iteratively, by starting with a guess for E and then solve till some kind of self-consistency criterion has been reached.

Actually, the above expression is nothing but a rewrite again of the full Schrödinger equation.

Defining $e = E - \hat{H}_0$ and recalling that $\hat{H}_0$ commutes with $\hat{Q}$ by construction and that $\hat{Q}$ is an idempotent operator $\hat{Q}^2 = \hat{Q}$. Using this equation in the above expansion for ΔE we can write the denominator

$$\hat{Q}\frac{1}{\hat{e} - \hat{Q}\hat{H}_I\hat{Q}} =$$

$$\hat{Q}\left[\frac{1}{\hat{e}} + \frac{1}{\hat{e}}\hat{Q}\hat{H}_I\hat{Q}\frac{1}{\hat{e}} + \frac{1}{\hat{e}}\hat{Q}\hat{H}_I\hat{Q}\frac{1}{\hat{e}}\hat{Q}\hat{H}_I\hat{Q}\frac{1}{\hat{e}} + \dots\right]\hat{Q}.$$

Inserted in the expression for ΔE leads to

$$\Delta E = \langle\Phi_0|\hat{H}_I + \hat{H}_I\hat{Q}\frac{1}{E - \hat{H}_0 - \hat{Q}\hat{H}_I\hat{Q}}\hat{Q}\hat{H}_I|\Phi_0\rangle.$$

In RS perturbation theory we set $\omega = W_0$ and obtain the following expression for the energy difference

$$\Delta E = \sum_{i=0}^{\infty}\langle\Phi_0|\hat{H}_I\left\{\frac{\hat{Q}}{W_0 - \hat{H}_0}\left(\hat{H}_I - \Delta E\right)\right\}^i|\Phi_0\rangle =$$

$$\langle\Phi_0|\left(\hat{H}_I + \hat{H}_I\frac{\hat{Q}}{W_0 - \hat{H}_0}(\hat{H}_I - \Delta E) + \hat{H}_I\frac{\hat{Q}}{W_0 - \hat{H}_0}(\hat{H}_I - \Delta E)\frac{\hat{Q}}{W_0 - \hat{H}_0}(\hat{H}_I - \Delta E) + \dots\right)|\Phi_0\rangle.$$

Recalling that $\hat{Q}$ commutes with $\hat{H}_0$ and since ΔE is a constant we obtain that

$$\hat{Q}\Delta E|\Phi_0\rangle = \hat{Q}\Delta E|\hat{Q}\Phi_0\rangle = 0.$$

Inserting this results in the expression for the energy results in

$$\Delta E = \langle\Phi_0|\left(\hat{H}_I + \hat{H}_I\frac{\hat{Q}}{W_0 - \hat{H}_0}\hat{H}_I + \hat{H}_I\frac{\hat{Q}}{W_0 - \hat{H}_0}(\hat{H}_I - \Delta E)\frac{\hat{Q}}{W_0 - \hat{H}_0}\hat{H}_I + \dots\right)|\Phi_0\rangle.$$

We can now this expression in terms of a perturbative expression in terms of $\hat{H}_I$ where we iterate the last expression in terms of ΔE

$$\Delta E = \sum_{i=1}^{\infty}\Delta E^{(i)}.$$

We get the following expression for $\Delta E^{(i)}$

$$\Delta E^{(1)} = \langle\Phi_0|\hat{H}_I|\Phi_0\rangle,$$

which is just the contribution to first order in perturbation theory,

$$\Delta E^{(2)} = \langle\Phi_0|\hat{H}_I\frac{\hat{Q}}{W_0 - \hat{H}_0}\hat{H}_I|\Phi_0\rangle,$$

which is the contribution to second order.

$$\Delta E^{(3)} = \langle\Phi_0|\hat{H}_I \frac{\hat{Q}}{W_0 - \hat{H}_0} \hat{H}_I \frac{\hat{Q}}{W_0 - \hat{H}_0} \hat{H}_I \Phi_0\rangle - \langle\Phi_0|\hat{H}_I \frac{\hat{Q}}{W_0 - \hat{H}_0} \langle\Phi_0|\hat{H}_I|\Phi_0\rangle \frac{\hat{Q}}{W_0 - \hat{H}_0} \hat{H}_I|\Phi_0\rangle,$$

being the third-order contribution.