7. PERTURBATION THEORY

Formal perturbation theory

Start with partitioning the Hamiltonian as

$$H = H_0 + H_1$$

unperturbed part — perturbation

One must choose H_0 such that the associated Schrödinger equation

$$H_0 |\Phi_k\rangle = E_k^{(0)} |\Phi_k\rangle$$

can be easily solvable.

⇒ In practice: H_0 = one-body operator

Eigenstates $|\Phi_k\rangle$ form a complete orthonormal basis of the many-body Hilbert space

$$\langle \Phi_k | \Phi_l \rangle = \delta_{kl} \qquad \text{and} \qquad \langle \Phi_0 | \Psi_0^A \rangle = 1$$

Ground-state of H_0 (= reference state) and exact wave function are adiabatically connected via H_1

Associated to the above partitioning one defines the projection operators

$$P \equiv |\Phi\rangle\langle\Phi|$$

$$Q \equiv 1 - P$$

→ now drop subscript for g.s. and write $|\Phi_0\rangle = |\Phi\rangle$, $|\Psi_0^A\rangle = |\Psi^A\rangle$

The operator Q can be written explicitly as

$$Q \equiv \sum_{k \neq 0} |\Phi_k\rangle\langle\Phi_k|$$

The exact ground state can now be written as

$$|\Psi^A\rangle = P|\Psi^A\rangle + Q|\Psi^A\rangle$$

$$= |\Phi\rangle\langle\Phi|\Psi^A\rangle + \sum_{k \neq 0} |\Phi_k\rangle\langle\Phi_k|\Psi^A\rangle$$

$$\equiv |\Phi\rangle \qquad + \quad |\chi\rangle$$

The exact energy reads

$$E^A = \langle\Phi|H|\Psi^A\rangle$$

projective formula for the energy (as opposed to expectation value $\langle\Psi^A|H|\Psi^A\rangle$)

$$= \langle\Phi|H|\Phi\rangle + \cancel{\langle\Phi|H_0|\chi\rangle} + \langle\Phi|H_1|\chi\rangle$$

$$\equiv E_{ref} + \Delta E$$

Let us now introduce the resolvent operator

$$R \equiv \sum_{k \neq 0} \frac{|\Phi_k\rangle\langle\Phi_k|}{E^{(0)} - E_k^{(0)}}$$

for which $R|\Phi\rangle = 0$. After a long derivation one obtains

$$|\chi\rangle = \sum_{k=1}^{\infty} (RH_1)^k |\Phi\rangle_c$$

$$\Delta E = \langle\Phi| H_1 \sum_{k=1}^{\infty} (RH_1)^k |\Phi\rangle_c$$

"connected"

One can then write

$$|\Psi^A\rangle = \sum_{p=0}^{\infty} |\Psi^{(p)}\rangle$$

$$E^A = \sum_{p=0}^{\infty} E^{(p)}$$

with $|\Psi^{(0)}\rangle = |\Phi\rangle$ and $E_{ref} = E^{(0)} + E^{(1)}$.

The first non-trivial correction to the energy appears at $p=2$

$$E^{(2)} = \langle\Phi| H_1 R H_1 |\Phi\rangle$$

$$= \sum_{k\neq 0} \frac{\langle\Phi| H_1 |\Phi_k\rangle\langle\Phi_k| H_1 |\Phi\rangle}{E^{(0)} - E_k^{(0)}}$$

Many-body perturbation theory

Let us take the Hartree-Fock Slater determinant $|\Phi\rangle = |\Phi^{HF}\rangle$ as reference state and apply Wick's theorem to the nuclear Hamiltonian with respect to $|\Phi\rangle$

$$H = \underbrace{E^{HF} + \sum_p h_{pp} :c_p^\dagger c_p:}_{= H_0} + \underbrace{\frac{1}{4}\sum_{pqrs} \bar{v}_{pqrs} :c_p^\dagger c_q^\dagger c_s c_r:}_{= H_1}$$

$|\Phi\rangle$ is the lowest-energy eigenstate of H_0, i.e.

$$H_0 |\Phi\rangle = E^{HF} |\Phi\rangle$$

All other eigenstates of H_0 can be obtained via

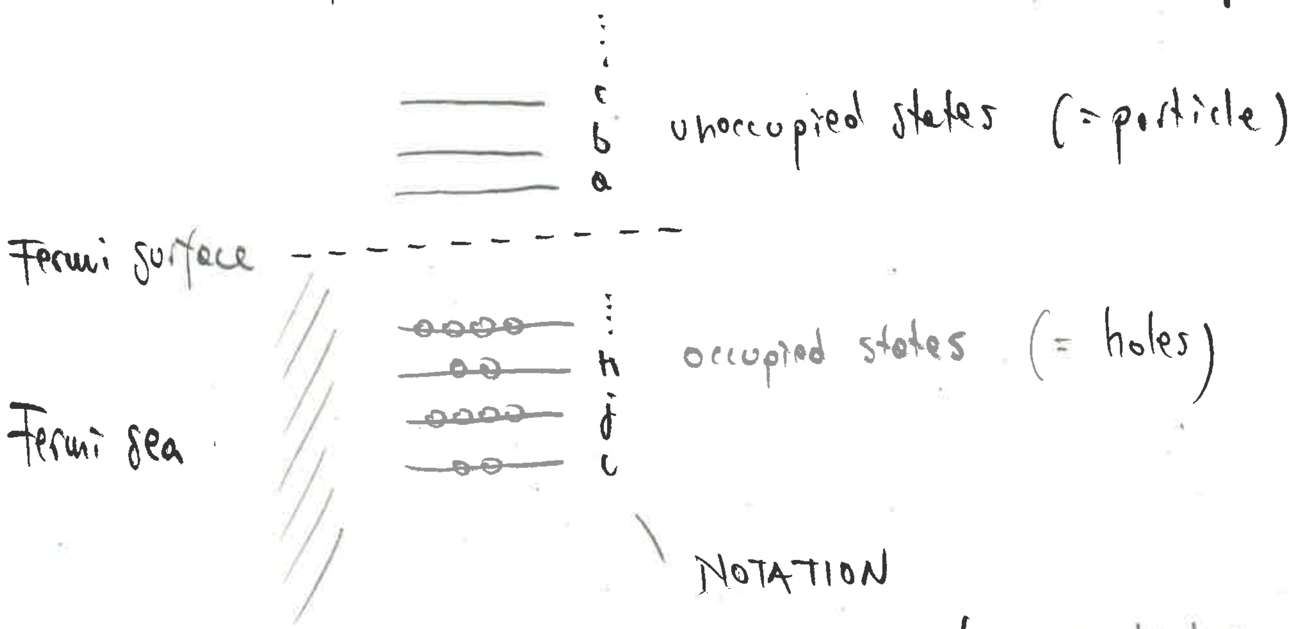
$$H_0 |\phi^{abc\ldots}_{ijk\ldots}\rangle = \left(E^{HF} + \mathcal{E}^{abc\ldots}_{ijk\ldots}\right) |\phi^{abc\ldots}_{ijk\ldots}\rangle$$

where

$$|\phi^{abc\ldots}_{ijk\ldots}\rangle \equiv c^{+}_{a} c^{+}_{b} c^{+}_{c} \ldots c_k c_j c_i |\phi\rangle$$

are Slater determinants obtained from $|\phi\rangle$ via n-particle - n-hole excitations and

$$\mathcal{E}^{abc\ldots}_{ijk\ldots} \equiv \underbrace{\left(e_a + e_b + e_c + \ldots\right)}_{\text{"particle" energies}} - \underbrace{\left(e_i + e_j + e_k + \ldots\right)}_{\text{"hole" energies}}$$



NOTATION

$a, b, c, \ldots$	for particles
$i, j, k, \ldots$	for holes
$p, q, r, s, \ldots$	for both = (when p/h character is not specified)

With these, the projection operator Q reads

$$Q = \sum_{ai} |\phi_i^a\rangle\langle\phi_i^a| + \sum_{abij} |\phi_{ij}^{ab}\rangle\langle\phi_{ij}^{ab}| + \underbrace{\cdots\cdots}_{\text{np-nh excitations with } n\geq 3}$$

and the resolvent

$$R = -\sum_{ai} \frac{|\phi_i^a\rangle\langle\phi_i^a|}{\varepsilon_i^a} - \left(\frac{1}{2!}\right)^2 \sum_{abij} \frac{|\phi_{ij}^{ab}\rangle\langle\phi_{ij}^{ab}|}{\varepsilon_{ij}^{ab}} + \cdots$$

Then, the second-order correction takes the form

$$E^{(2)} = -\frac{1}{4}\sum_{abij} \frac{\bar{V}_{abij}\,\bar{V}_{ijab}}{\varepsilon_{ij}^{ab}}$$

and similarly (but increasingly more complicated) for higher-order corrections.

Recall the expression for energy corrections

$$\Delta E = \langle\phi|\, H_1 \sum_{k=1}^{\infty} (RH_1)^k\, |\phi\rangle$$

To compute expectation values of products of operators, a "ladder" of tools exists

1) Work through canonical commutations of $a^\dagger$ and a
2) Wick's theorem (= way to capture the result of point 1 in a systematic and compact way)
3) Many-body diagrams (= way to handle graphically terms coming from Wick and collect equivalent contributions)
4) Automated generation of many-body diagrams