Correlation Energy

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I. HAMILTONIAN WITH VARIABLE COUPLING CONSTANT

$$
\begin{aligned}
&H(\lambda) = H_0 + \lambda H_1 \\
&H(1) = H \qquad H(0) = H_0
\end{aligned} \tag{1}
$$

Suppose we know the eigenvalues and eigenfunctions of $H(\lambda)$, then

$$
\begin{aligned}
&H(\lambda)|\psi_0(\lambda)\rangle = E(\lambda)|\psi_0(\lambda)\rangle \\
&\text{where } \langle\psi_0(\lambda)|\psi_0(\lambda)\rangle = 1
\end{aligned} \tag{2}
$$

Therefore

$$
\begin{aligned}
&E(\lambda) = \langle\psi_0(\lambda)|H(\lambda)|\psi_0(\lambda)\rangle \\
\Rightarrow &\frac{dE(\lambda)}{d\lambda} = \langle\psi_0(\lambda)|H_1|\psi_0(\lambda)\rangle + E(\lambda)\frac{d}{d\lambda}\langle\psi_0(\lambda)|\psi_0(\lambda)\rangle \\
\Rightarrow &\frac{dE(\lambda)}{d\lambda} = \langle\psi_0(\lambda)|H_1|\psi_0(\lambda)\rangle
\end{aligned} \tag{3}
$$

Therefore upon integration

$$
\begin{aligned}
E - E_0 &= \int_0^1 d\lambda \, \langle\psi_0(\lambda)|H_1|\psi_0(\lambda)\rangle \\
&= \int_0^1 \frac{d\lambda}{\lambda} \, \langle\psi_0(\lambda)|\lambda H_1|\psi_0(\lambda)\rangle
\end{aligned} \tag{4}
$$

II. CORRELATION ENERGY

The energy due to Coulomb interaction is

$$
\langle V\rangle = \frac{1}{2}\sum_{k,k',q} V(q)\langle c^\dagger_{k+q}c^\dagger_{k'-q}c_{k'}c_k\rangle \tag{5}
$$

Thus the total energy of the system is

$$
E = E_{\text{kin}} + E_{\text{exc}} + E_{\text{corr}} \tag{6}
$$

where $E_{\text{corr}} = \langle V\rangle - E_{\text{exc}}$. Define

$$
\begin{aligned}
iD(q,\omega) &= \sum_{k,k'}\langle c^\dagger_{k+q}c^\dagger_{k'-q}c_{k'}c_k\rangle \\
iD_0(q,\omega) &= \sum_{k,k'}\langle c^\dagger_{k+q}c^\dagger_{k'-q}c_{k'}c_k\rangle_0
\end{aligned} \tag{7}
$$

where '$\langle ...\rangle$' is the average with respect to the interacting ground state while '$\langle ...\rangle_0$' is the average with respect to the non-interacting ground state. Therefore

$$
E_{\text{corr}} = \frac{1}{2}\sum_q \int_{-\infty}^{\infty}\frac{\hbar d\omega}{2\pi}V(q)\left[iD(q,\omega) - iD_0(q,\omega)\right] \tag{8}
$$

Assuming that the Coulomb interaction term can be tuned by a coupling constant λ,

$$E_{\rm corr} = \frac{i}{2}\int_0^1 \frac{d\lambda}{\lambda}\sum_q \int_{-\infty}^{\infty}\frac{\hbar d\omega}{2\pi}\lambda V(q)\left[D_\lambda(q,\omega) - D_0(q,\omega)\right] \tag{9}$$

The perturbative expansion of the average '$\langle ...\rangle$' is done

$$\begin{aligned} V(q)D(q,\omega) &= U(q,\omega)D^*(q,\omega) \\ &= \left[V + VD^*V + ...\right]D^*(q,\omega) \\ &= \frac{V(q)D^*(q,\omega)}{1 - V(q)D^*(q,\omega)} \end{aligned} \tag{10}$$

where $D^*(q,\omega)$ is the proper polarization. [If only the polarization bubble is included as proper polarization, then we get the contribution of all the ring diagrams]. The dielectric constant is then defined as

$$\varepsilon(q,\omega) = 1 - V(q)D^*(q,\omega) \Rightarrow V(q)D(q,\omega) = \frac{1}{\varepsilon(q,\omega)} - 1 \tag{11}$$

Define

$$\begin{aligned} \lambda V(q)D_0(q,\omega) &= \Pi_{0,\lambda}(q,\omega) \\ \lambda V(q)D_\lambda(q,\omega) &= \frac{1}{\varepsilon_\lambda(q,\omega)} - 1 \end{aligned} \tag{12}$$

Thus, the correlation energy can be expressed as

$$\begin{aligned} E_{\rm corr} &= \frac{i}{2}\int_0^1 \frac{d\lambda}{\lambda}\sum_q \int_{-\infty}^{\infty}\frac{\hbar d\omega}{2\pi}\lambda V(q)\left[D_\lambda(q,\omega) - D_0(q,\omega)\right] \\ &= i\int_0^1 \frac{d\lambda}{\lambda}\sum_q \int_0^{\infty}\frac{\hbar d\omega}{2\pi}\left[\frac{1}{\varepsilon_\lambda(q,\omega)} - 1 - \Pi_{0,\lambda}(q,\omega)\right] \end{aligned} \tag{13}$$

Since energy is real, and in general ε and Π are complex. We can pick the appropriate components such the the correlation energy is real.

$$E_{\rm corr} = -\int_0^1 \frac{d\lambda}{\lambda}\sum_q \int_0^{\infty}\frac{\hbar d\omega}{2\pi}\left[{\rm Im}\left(\frac{1}{\varepsilon_\lambda(q,\omega)}\right) - {\rm Im}\left(\Pi_{0,\lambda}(q,\omega)\right)\right] \tag{14}$$

III. ELECTRON ONE-COMPONENT SYSTEM

$$E_{\rm corr} = -\int_0^1 \frac{d\lambda}{\lambda}\sum_q \int_0^{\infty}\frac{\hbar d\omega}{2\pi}\left[{\rm Im}\left(\frac{1}{\varepsilon_\lambda(q,\omega)}\right) - {\rm Im}\left(\Pi_{0,\lambda}(q,\omega)\right)\right] \tag{15}$$

where the dielectric constant is the sum of the electron polarization $\varepsilon = 1 - \Pi^H_{e,\lambda}$ and $\Pi_{0,\lambda} = \Pi_{e,\lambda}$. The superscript '$H$' in the dielectric constant corresponds to the Hubbard correction.

$$\Pi^H_{e,\lambda} = \frac{\Pi_{e,\lambda}}{1 + f\Pi_{e,\lambda}} \tag{16}$$

For the case of electrons,

$$\begin{aligned} \Pi_{e,\lambda} &= A_\lambda + i\Sigma_\lambda \\ \Pi^H_{e,\lambda} &= \frac{\Pi_{e,\lambda}}{1 + f\Pi_{e,\lambda}} \\ \frac{1}{\varepsilon_\lambda} &= \frac{1 + f\Pi_{e,\lambda}}{1 - (1-f)\Pi_{e,\lambda}} = \frac{1 + fA_\lambda + if\Sigma_\lambda}{1 - A'_\lambda - i\Sigma'_\lambda} \end{aligned} \tag{17}$$

where $A'_\lambda = (1-f)A_\lambda$ and $\Sigma'_\lambda = (1-f)\Sigma_\lambda$. The term $\Pi_{0,\lambda} = \Pi_{e,\lambda} = A_\lambda - i\Sigma_\lambda$.

$$\begin{aligned} \mathrm{Im}\left[\frac{1}{\varepsilon_\lambda}\right] &= \frac{\Sigma_\lambda}{(1-A'_\lambda)^2 + (\Sigma'_\lambda)^2} \\ \mathrm{Im}\left[\Pi_{0,\lambda}\right] &= \Sigma_\lambda \end{aligned} \tag{18}$$

Since $A_\lambda = \lambda A$ and $\Sigma_\lambda = \lambda\Sigma$,

$$\begin{aligned} E_{\mathrm{corr}} &= -\int_0^1 \frac{d\lambda}{\lambda} \sum_q \int_0^\infty \frac{\hbar d\omega}{2\pi} \left[\frac{\lambda\Sigma}{(1-\lambda A')^2 + \lambda^2(\Sigma')^2} - \lambda\Sigma\right] \\ &= \sum_q \int_0^\infty \frac{d\omega}{2\pi} \left[\frac{\Sigma}{\Sigma'} \tan^{-1}\left(\frac{-\Sigma'}{1-A'}\right) + \Sigma\right] \end{aligned} \tag{19}$$

Thus the correlation energy is

$$E_{\mathrm{corr}} = \sum_q \int_0^\infty \frac{\hbar d\omega}{2\pi} \left[\frac{1}{1-f} \tan^{-1}\left(\frac{-(1-f)\Sigma}{1-(1-f)A}\right) + \Sigma\right] \tag{20}$$

The Hubbard correction factor f is

$$f(q) = \begin{cases} \dfrac{1}{2}\dfrac{q^2}{q^2+k_F^2} & \text{3D} \\ \dfrac{1}{2}\dfrac{q}{q+k_F} & \text{2D} \end{cases}$$

The correlation energy per electron is

$$\varepsilon_{\mathrm{corr}} = \frac{1}{N} \sum_q \int_0^\infty \frac{\hbar d\omega}{2\pi} \left[\frac{1}{1-f} \tan^{-1}\left(\frac{-(1-f)\Sigma}{1-(1-f)A}\right) + \Sigma\right] \tag{21}$$

where N is the number of electrons.

IV. ELECTRON-HOLE TWO-COMPONENT SYSTEM

$$E_{\mathrm{corr}} = -\int_0^1 \frac{d\lambda}{\lambda} \sum_q \int_0^\infty \frac{\hbar d\omega}{2\pi} \left[\mathrm{Im}\left(\frac{1}{\varepsilon_\lambda(q,\omega)}\right) - \mathrm{Im}\left(\Pi_{0,\lambda}(q,\omega)\right)\right] \tag{22}$$

where the dielectric constant is the sum of the electron and hole polarization $\varepsilon = 1 - \left(\Pi^H_{e,\lambda} + \Pi^H_{h,\lambda}\right)$ and $\Pi_{0,\lambda} = \Pi_{e,\lambda} + \Pi_{h,\lambda}$. The superscript '$H$' in the dielectric constant corresponds to the Hubbard correction.

$$\Pi^H_{e/h,\lambda} = \frac{\Pi_{e/h,\lambda}}{1 + f\Pi_{e/h,\lambda}} \tag{23}$$

If the electrons and holes have the same mass,

$$\begin{aligned} \Pi_{e,\lambda} &= \Pi_{h,\lambda} = \Pi_\lambda = A_\lambda + i\Sigma_\lambda \\ \Pi^H_{e,\lambda} + \Pi^H_{h,\lambda} &= \frac{2\Pi_\lambda}{1+f\Pi_\lambda} \\ \frac{1}{\varepsilon_\lambda} &= \frac{1+f\Pi_\lambda}{1-(2-f)\Pi_\lambda} = \frac{1+fA_\lambda + if\Sigma_\lambda}{1-A'_\lambda - i\Sigma'_\lambda} \end{aligned} \tag{24}$$

where $A'_\lambda = (2-f)A_\lambda$ and $\Sigma'_\lambda = (2-f)\Sigma_\lambda$. The term $\Pi_{0,\lambda} = \Pi_{e,\lambda} + \Pi_{h,\lambda} = 2A_\lambda - i2\Sigma_\lambda$.

$$\begin{aligned} \mathrm{Im}\left[\frac{1}{\varepsilon_\lambda}\right] &= \frac{2\Sigma_\lambda}{(1-A'_\lambda)^2 + (\Sigma'_\lambda)^2} \\ \mathrm{Im}\left[\Pi_{0,\lambda}\right] &= 2\Sigma_\lambda \end{aligned} \tag{25}$$

Since $A_\lambda = \lambda A$ and $\Sigma_\lambda = \lambda\Sigma$,

$$\begin{aligned} E_{\text{corr}} &= -\int_0^1 \frac{d\lambda}{\lambda} \sum_q \int_0^\infty \frac{\hbar d\omega}{2\pi} \left[\frac{2\lambda\Sigma}{(1-\lambda A')^2 + \lambda^2(\Sigma')^2} - \lambda 2\Sigma \right] \\ &= \sum_q \int_0^\infty \frac{\hbar d\omega}{2\pi} \left[\frac{2\Sigma}{\Sigma'} \tan^{-1}\left(\frac{-\Sigma'}{1-A'} \right) + 2\Sigma \right] \end{aligned} \tag{26}$$

From this we can generalize to a situation where the electron and hole masses are different by making the following substitutions

$$\begin{aligned} &2\Sigma = \Sigma_e + \Sigma_h \\ &\Sigma' = (2-f)\Sigma = (1-f/2)(\Sigma_e + \Sigma_h) \\ &A' = (2-f)A = (1-f/2)(A_e + A_h) \end{aligned} \tag{27}$$

Thus the correlation energy is

$$E_{\text{corr}} = \sum_q \int_0^\infty \frac{\hbar d\omega}{2\pi} \left[\frac{1}{1-f/2} \tan^{-1}\left(\frac{-(1-f/2)(\Sigma_e+\Sigma_h)}{1-(1-f/2)(A_e+A_h)} \right) + (\Sigma_e+\Sigma_h) \right] \tag{28}$$

The Hubbard correction factor f is

$$f(q) = \begin{cases} \frac{1}{2}\frac{q^2}{q^2+k_F^2} & \text{3D} \\ \frac{1}{2}\frac{q}{q+k_F} & \text{2D} \end{cases}$$

The correlation energy per electron-hole pair is

$$\varepsilon_{\text{corr}} = \frac{1}{N} \sum_q \int_0^\infty \frac{\hbar d\omega}{2\pi} \left[\frac{1}{1-f/2} \tan^{-1}\left(\frac{-(1-f/2)(\Sigma_e+\Sigma_h)}{1-(1-f/2)(A_e+A_h)} \right) + (\Sigma_e+\Sigma_h) \right] \tag{29}$$

where N is the number of electron-hole pairs.