Non-Degenerate Perturbation Theory

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Notation

$$V_{00} = \langle \psi_0 | V | \psi_0 \rangle$$

$$E_{0\alpha} = E_0 - E_\alpha$$

$$\Sigma_{x_1 x_2 \cdots x_n} = \sum_{\alpha_1, \alpha_2, \cdots \alpha_n \neq 0} \frac{V_{0\alpha_1} V_{\alpha_1 \alpha_2} \cdots V_{\alpha_n 0}}{E_{0\alpha_1}^{x_1} E_{0\alpha_2}^{x_2} \cdots E_{0\alpha_n}^{x_n}}$$

Examples

$$\Sigma_1 = \sum_{\alpha \neq 0} \frac{\left| V_{0\alpha} \right|^2}{E_{0\alpha}}$$

$$\Sigma_{12} = \sum_{\alpha_1, \alpha_2 \neq 0} \frac{V_{0\alpha_1} V_{\alpha_1 \alpha_2} V_{\alpha_2 0}}{E_{0\alpha_1} E_{0\alpha_2}^2}$$

Energy Corrections

$$\mathrm{Tr}[\Delta_1] = V_{00}$$

$$\mathrm{Tr}[\Delta_2] = \Sigma_1$$

$$\begin{aligned} \mathrm{Tr}[\Delta_3] = \Sigma_{11} \\ - V_{00} \Sigma_2 \end{aligned}$$

$$\begin{aligned} \mathrm{Tr}[\Delta_4] = \Sigma_{111} - \Sigma_2 \Sigma_1 \\ - V_{00} \left(\Sigma_{12} + \Sigma_{21} \right) \\ + V_{00}^2 \Sigma_3 \end{aligned}$$

$$
\begin{aligned}
\mathrm{Tr}[\Delta_5] = \Sigma_{1111} &- \Sigma_1\Sigma_{12} - \Sigma_1\Sigma_{21} - \Sigma_2\Sigma_{11} \\
&- V_{00}\left(\Sigma_{211} + \Sigma_{121} + \Sigma_{112} - \Sigma_2^2 - 2\Sigma_1\Sigma_3\right) \\
&+ V_{00}^2\left(\Sigma_{22} + \Sigma_{13} + \Sigma_{31}\right) \\
&- V_{00}^3\Sigma_4
\end{aligned}
$$

$$
\begin{aligned}
\mathrm{Tr}[\Delta_6] = \Sigma_{11111} &+ \Sigma_1^2\Sigma_3 + \Sigma_1\Sigma_2^2 - \Sigma_1\Sigma_{112} - \Sigma_1\Sigma_{121} - \Sigma_1\Sigma_{211} - \Sigma_{11}\Sigma_{12} - \Sigma_{11}\Sigma_{21} - \Sigma_2\Sigma_{111} \\
&+ V_{00}\left(2\Sigma_1\Sigma_{13} + 2\Sigma_1\Sigma_{31} + 2\Sigma_1\Sigma_{22} + 2\Sigma_3\Sigma_{11} - \Sigma_{1112} - \Sigma_{1121} - \Sigma_{1211} - \Sigma_{2111} + 2\Sigma_2\Sigma_{12} + 2\Sigma_2\Sigma_{21}\right) \\
&+ V_{00}^2\left(\Sigma_{113} + \Sigma_{131} + \Sigma_{311} + \Sigma_{221} + \Sigma_{212} + \Sigma_{122} - 3\Sigma_1\Sigma_4 - 3\Sigma_2\Sigma_3\right) \\
&- V_{00}^3\left(\Sigma_{14} + \Sigma_{41} + \Sigma_{23} + \Sigma_{32}\right) \\
&+ V_{00}^4\Sigma_5
\end{aligned}
$$