Exercises FYS4480, week 44, October 31-November 4, 2022

Exercise 1

Show Thouless' theorem: An arbitrary Slater determinant $|c'\rangle$ which is not orthogonal to a determinant $|c\rangle = \prod_{i=1}^{n} a^\dagger_{\alpha_i}|0\rangle$, can be written as

$$|c'\rangle = exp\left\{\sum_{p=\alpha_{n+1}}^{\infty}\sum_{h=\alpha_1}^{\alpha_n} C_{ph} a_p^\dagger a_h\right\}|c\rangle$$

Exercise 2

Let $H = H_0 + V$ and $|\phi_n\rangle$ be the eigenstates of H_0 and that $|\psi_n\rangle$ are the corresponding ones for H. Assume that the ground states $|\phi_0\rangle$ and $|\psi_0\rangle$ are not degenerate. Show that

$$E_0 - \varepsilon_0 = \frac{\langle\phi_0| V |\psi_0\rangle}{\langle\phi_0|\psi_0\rangle},$$

with $H|\psi_0\rangle = E|\psi_0\rangle$ and $H_0|\phi_0\rangle = \varepsilon_0|\phi_0\rangle$.

a) Define the new operators $P = |\phi_0\rangle\langle\phi_0|$ and $Q = 1 - P$. Show that these operators are idempotent.

b) Show that for any z we have

$$|\psi_0\rangle = \langle\phi_0|\psi_0\rangle \sum_{n=0}^{\infty}\left(\frac{Q}{z - H_0}(z - E_0 + V)\right)^n |\phi_0\rangle,$$

and

$$E_0 = \varepsilon_0 + \sum_{n=0}^{\infty}\langle\phi_0| V\left(\frac{Q}{z - H_0}(z - E_0 + V)\right)^n |\phi_0\rangle.$$

c) Discuss these results for $z = E_0$ (Brillouin-Wigner perturbation theory) and $z = \varepsilon_0$ (Rayleigh-Schrödinger perturbation theory). Compare the first few terms in these expansions.

Exercise 3

Consider a system of two fermions spin $s = 1/2$ in the pair-orbitals $|m_0\rangle$ and $|-m_0\rangle$ in a single shell $j = l + s$ with $2j + 1 > 2$, where l is the orbital momentum with $l = 0, 1, 2, \ldots$. Assume that the matrix elements for the interaction between the particles takes the form

$$\langle m, -m| v |m', -m'\rangle = -G.$$

a) Show that the Brillouin-Wigner expansion from the previous exercise can be used to give

$$E_0 = -(j + 1/2)G.$$

b) Show thereafter by direct diagonalization of the Hamiltonian matrix that this is the exact energy. Use thereafter Rayleigh-Schrödinger perturbation theory and discuss the differences.