Exercises PHY981 Spring 2015

The exercises are available at the beginning of the week and are to be handed in the week thereafter on **Wednesdays at noon**. This can be done electronically by sending your github link or by sending a scan of your notes, a pdf or postscript file, or ipython notebook or any format you prefer, by email to hjensen@nscl.msu.edu.

Exercise 5

This exercise serves to convince you about the relation between two different single-particle bases, where one could be our new Hartree-Fock basis and the other a harmonic oscillator basis.

a) Consider a Slater determinant built up of single-particle orbitals ψ_λ, with $\lambda = 1, 2, \ldots, A$.
   The unitary transformation
   $$\psi_a = \sum_\lambda C_{a\lambda}\phi_\lambda,$$
   brings us into the new basis. The new basis has quantum numbers $a = 1, 2, \ldots, A$. Show that the new basis is orthonormal. Show that the new Slater determinant constructed from the new single-particle wave functions can be written as the determinant based on the previous basis and the determinant of the matrix C. Show that the old and the new Slater determinants are equal up to a complex constant with absolute value unity. (Hint, C is a unitary matrix).

b) Starting with the second quantization representation of the Slater determinant
   $$\Phi_0 = \prod_{i=1}^{n} a^\dagger_{\alpha_i} |0\rangle ,$$
   use Wick's theorem to compute the normalization integral $< \Phi_0 | \Phi_0 >$.

Exercise 6

Calculate the matrix elements
$$\langle \alpha_1\alpha_2 | \hat{F} | \alpha_1\alpha_2 \rangle$$
and
$$\langle \alpha_1\alpha_2 | \hat{G} | \alpha_1\alpha_2 \rangle$$
with
$$|\alpha_1\alpha_2\rangle = a^\dagger_{\alpha_1} a^\dagger_{\alpha_2} |0\rangle ,$$
$$\hat{F} = \sum_{\alpha\beta} \langle \alpha | f | \beta \rangle a^\dagger_\alpha a_\beta,$$
$$\langle \alpha | f | \beta \rangle = \int \psi^*_\alpha(x) f(x) \psi_\beta(x) dx,$$
$$\hat{G} = \frac{1}{2} \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | g | \gamma\delta \rangle a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma,$$
and
$$\langle \alpha\beta | g | \gamma\delta \rangle = \int\int \psi^*_\alpha(x_1)\psi^*_\beta(x_2) g(x_1, x_2) \psi_\gamma(x_1)\psi_\delta(x_2) dx_1 dx_2$$

Compare these results with those from exercise 3c).

Exercise 7

Show that the onebody part of the Hamiltonian

$$\hat{H}_0 = \sum_{pq} \langle p| \hat{h}_0 |q\rangle a_p^\dagger a_q$$

can be written, using standard annihilation and creation operators, in normal-ordered form as

$$\begin{aligned}\hat{H}_0 &= \sum_{pq} \langle p| \hat{h}_0 |q\rangle a_p^\dagger a_q \\ &= \sum_{pq} \langle p| \hat{h}_0 |q\rangle \left\{a_p^\dagger a_q\right\} + \delta_{pq\in i} \sum_{pq} \langle p| \hat{h}_0 |q\rangle \\ &= \sum_{pq} \langle p| \hat{h}_0 |q\rangle \left\{a_p^\dagger a_q\right\} + \sum_{i} \langle i| \hat{h}_0 |i\rangle\end{aligned}$$

Explain the meaning of the various symbols. Which reference vacuum has been used?

Exercise 8

Show that the twobody part of the Hamiltonian

$$\hat{H}_I = \frac{1}{4} \sum_{pqrs} \langle pq| \hat{v} |rs\rangle a_p^\dagger a_q^\dagger a_s a_r$$

can be written, using standard annihilation and creation operators, in normal-ordered form as

$$\begin{aligned}\hat{H}_I &= \frac{1}{4} \sum_{pqrs} \langle pq| \hat{v} |rs\rangle a_p^\dagger a_q^\dagger a_s a_r \\ &= \frac{1}{4} \sum_{pqrs} \langle pq| \hat{v} |rs\rangle \left\{a_p^\dagger a_q^\dagger a_s a_r\right\} + \sum_{pqi} \langle pi| \hat{v} |qi\rangle \left\{a_p^\dagger a_q\right\} + \frac{1}{2} \sum_{ij} \langle ij| \hat{v} |ij\rangle\end{aligned}$$

Explain again the meaning of the various symbols.

This exercise is optional: Derive the normal-ordered form of the threebody part of the Hamiltonian.

$$\hat{H}_3 = \frac{1}{36} \sum_{\substack{pqr \\ stu}} \langle pqr| \hat{v}_3 |stu\rangle a_p^\dagger a_q^\dagger a_r^\dagger a_u a_t a_s$$

and specify the contributions to the twobody, onebody and the scalar part.