Prof. Stephan Fritzsche
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— Advanced Quantum Theory —

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Winter Term

Home Work (11)

Task 1: Interacting Fermions in Hartree–Fock Approximation (8 Points)

Again, we consider two interacting Fermions with the Hamiltonian

$$H = \frac{1}{2}\left(p_1^2 + p_2^2 + x_1^2 + x_2^2\right) + \frac{\lambda}{2}\left(x_1 - x_2\right)^2 .$$

with a positive coupling constant λ. Apply the Hartree–Fock method to find an approximate ground state wave function.

a) As an ansatz, we want to use the Slater determinant that is given by $\Psi\left(x_1, x_2\right) = \varphi(x_1)\varphi(x_2)\chi$ Show by variation of the energy expectation value $E\left[\varphi\right] = \langle\Psi\,|\,H\,|\,\Psi\rangle$ that the Hartree–Fock equations reduce to

$$\left(-\partial_x^2 + x^2 + \lambda\int \mathrm{d}y\,(x-y)^2\left|\varphi(y)\right|^2\right)\varphi = \epsilon\varphi(x)$$

b) Solve this equation iteratively. Start in lowest order approximation with the ground state wave function of the harmonic oscillator for $\varphi^{(1)}(x)$ and compute $\varphi^{(n)}$ and $\epsilon^{(n)}$ until the iteration converges. What are the solutions for $\epsilon^{(\infty)}$ and $\varphi^{(\infty)}$?

Task 2: Molecular Hydrogen (3 Points)

The hydrogen molecule H_2 is composed of two protons and two electrons. For this molecule, the electronic Hamiltonian is given by

$$H = -\frac{1}{2}\nabla^2_{\mathbf{r}_1} - \frac{1}{2}\nabla^2_{\mathbf{r}_2} - \frac{1}{r_{A1}} - \frac{1}{r_{A2}} - \frac{1}{r_{B1}} - \frac{1}{r_{B2}} + \frac{1}{r_{12}} + \frac{1}{R}$$

where i describes the electrons, while A and B corresponds to nuclei. The valence-bond wave functions are

$$\left|\Phi_g\right\rangle = \frac{1}{2}\left(\left|A1\right\rangle\left|B2\right\rangle + \left|A2\right\rangle\left|B1\right\rangle\right)\left|00\right\rangle ,$$
$$\left|\Phi_u\right\rangle = \frac{1}{2}\left(\left|A1\right\rangle\left|B2\right\rangle - \left|A2\right\rangle\left|B1\right\rangle\right)\left|1M_s\right\rangle .$$

Here $|A1\rangle = \psi_{1s}(r_{A1})$, $|A2\rangle = \psi_{1s}(r_{A2})$, $|B1\rangle = \psi_{1s}(r_{B1})$, and $|B2\rangle = \psi_{1s}(r_{B2})$, while $\psi_{1s}(r)$ is the normalised ground state wave function for atomic hydrogen. The spin wave function $|00\rangle$ describes the singlet case, and $|1M_s\rangle$ corresponds to the triplet case. Use $|\Phi_{g,u}\rangle$ as trial functions in the variational method to express the energy $E_{g,u}$ in terms of the integrals

$$I = \langle A1|B1\rangle ,$$
$$J = \langle A1, B2|\left(\frac{1}{r_{12}} - \frac{1}{r_{A2}} - \frac{1}{r_{B1}}\right)|A1, B2\rangle ,$$
$$K = \langle A1, B2|\left(\frac{1}{r_{12}} - \frac{1}{r_{A2}} - \frac{1}{r_{B1}}\right)|B1, A2\rangle .$$

Task 3: Number Operator (2 Points)

In analogy to the number operator defined in the lecture, consider the operator

$$W = \sum_{\alpha,\beta} a_\alpha^\dagger a_\beta^\dagger a_\beta a_\alpha$$

Show that for a state with a fixed particle number N the expectation value of this operator is given by $N^2 - N$ for both bosons and fermions.