Prof. Stephan Fritzsche — 28. November 2016
TPI and HI Jena — Winter Term
— Advanced Quantum Theory —

Home Work (6)

Task 1: Tensor Product (3 Points)

a) Let

$$|\phi_1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |\phi_2\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

Calculate

$$|\phi_1\rangle \otimes |\phi_1\rangle, \; |\phi_1\rangle \otimes |\phi_2\rangle, \; |\phi_2\rangle \otimes |\phi_1\rangle, \; |\phi_2\rangle \otimes |\phi_2\rangle .$$

b) Consider the Pauli matrices

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Find $\sigma_x \otimes \sigma_z$ and $\sigma_z \otimes \sigma_x$.

c) Consider the state

$$|\psi\rangle = \frac{1}{2}\left(|0\rangle \otimes |0\rangle + |0\rangle \otimes |1\rangle + |1\rangle \otimes |0\rangle + |1\rangle \otimes |1\rangle\right) .$$

Can this state be written as a product state?

d) Let A be an $m \times m$ matrix and B be an $n \times n$ matrix. Let I_m, I_n be the $m \times m$ and $n \times n$ unit matrix, respectively. Show that

$$\mathrm{tr}\,(A \otimes B) = \mathrm{tr}\,(A)\,\mathrm{tr}\,(B)$$

and

$$\mathrm{tr}\,(A \otimes I_n + I_m \otimes B) = n\,\mathrm{tr}\,(A) + m\,\mathrm{tr}\,(B) .$$

Task 2: Commutators (3 Points)

Prove that

$$[H, \boldsymbol{L}] = 0 ,$$

where the many-particle Schrödinger Hamiltonian is given by

$$H = \sum_k \left(-\frac{1}{2}\nabla_k^2 - \frac{Z}{r_k}\right) + \sum_{k<i} \frac{1}{r_{ki}}$$

and $\boldsymbol{L} = \sum_k \boldsymbol{l}_k$ is the total angular momentum operator.

Task 3: Helium Wave Functions (2 Points)

Consider the wave functions for the $2\,^3S$ level of helium, which are given in the central field approximation by

$$\psi_c(2\,^3S) = \phi_-(r_1, r_2) \begin{cases} |\uparrow\uparrow\rangle & M_s = 1 \\ \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\right) & M_s = 0 \\ |\downarrow\downarrow\rangle & M_s = -1 \end{cases}$$

with

$$\phi_-(r_1, r_2) = \frac{1}{\sqrt{2}}\left(u_{1s}(r_1)u_{2s}(r_2) - u_{2s}(r_1)u_{1s}(r_2)\right)$$

Write the three functions $\psi_c(2\,^3S)$ in the form of (a sum of) Slater determinants constructed from the spin-orbitals

$$u_{1s\uparrow} = u_{1s}(r)\,|\uparrow\rangle \qquad u_{1s\downarrow} = u_{1s}(r)\,|\downarrow\rangle$$
$$u_{2s\uparrow} = u_{2s}(r)\,|\uparrow\rangle \qquad u_{2s\downarrow} = u_{2s}(r)\,|\downarrow\rangle$$

Task 4: Normalization and Matrix Elements of Slater Determinants (4 Points)

a) Show that a Slater determinant

$$\Psi\left(1, \ldots, N\right) = \frac{1}{\sqrt{N!}} \sum_P \left(-1\right)^P \phi_{\alpha_1}\left(\boldsymbol{x}_{P(1)}\right) \ldots \phi_{\alpha_N}\left(\boldsymbol{x}_{P(N)}\right) ,$$

where $\boldsymbol{x} = (\boldsymbol{r}_i, \sigma)$ is a combined spatial and spin coordinate, is properly normalized

$$\langle \Psi \,|\, \Psi \rangle = 1$$

b) Consider a one-particle operator $F = \sum_i F(\boldsymbol{x}_i)$. Show that the matrix elements of a Slater determinant fulfill

$$\langle \Psi' | F | \Psi \rangle = \begin{cases} \sum_i \langle i \,|\, f \,|\, i \rangle & \text{if } \Psi' = \Psi \\ \langle a' \,|\, f \,|\, a \rangle & \text{if } a \neq a' \\ 0 & \text{if more than one orbital differs} \end{cases}$$

$\langle a' \,|\, f \,|\, a \rangle$ denotes the one-electron matrix elements of orbital a in the operator f.

c) Consider a symmetric two-particle operator $G = \sum_{i<j} g\left(\boldsymbol{x}_i, \boldsymbol{x}_j\right)$. Show that the matrix elements are then given by

$$\left\langle \Psi' \,\middle|\, G \,\middle|\, \Psi \right\rangle = \begin{cases} \sum_{i<j} \left(\langle ij \,|\, g \,|\, ij \rangle - \langle ij \,|\, g \,|\, ji \rangle\right) & \text{if } \Psi = \Psi' \\ \sum_i \left(\langle ia' \,|\, g \,|\, ia \rangle - \langle ia' \,|\, g \,|\, ai \rangle\right) & \text{if } a' \neq a \\ \langle a'b' \,|\, g \,|\, ab \rangle - \langle a'b' | g | ba \rangle & \text{if } a' \neq a, b' \neq b \\ 0 & \text{if more than two orbitals differ} \end{cases}$$