Advanced Quantum Mechanics

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Exercise sheet 6 **Due: Sunday May 14 at 24:00**

1 The swap again

In the lecture it was claimed[1] that

$$\tau = \frac{1}{2} \sum_{j=0,x,y,z} \sigma_j^{(1)} \sigma_j^{(2)} = \frac{1}{2}\hat{1} + \frac{1}{2}\vec{\sigma}^{(1)} \cdot \vec{\sigma}^{(2)}.$$

Show this relation.
Hint: You have kind of shown this half-way already in a previous exercise (although it might not be much of a difference to just start from scratch). Also, $\sigma_0 = \hat{1}$.

(3 points)

2 Two fermions in a one-dimensional box

This exercise is more or less an application of section 2.1.3 "The exchange interaction" in the lecture notes. We have just replaced the interaction Hamiltonian.

Two identical spin-$\frac{1}{2}$ fermions with mass m move in a one-dimensional box of length L. More precisely, they are affected by the potential

$$V(x) = \begin{cases} +\infty & \text{if} \quad x < 0, \\ 0 & \text{if} \quad 0 \leq x \leq 1, \\ +\infty & \text{if} \quad 1 < x. \end{cases}$$

Let us denote the *single-particle* eigenstates as $|\phi_n\rangle$, with $|\phi_1\rangle$ being the ground-state and $|\phi_2\rangle$ the first excited state. The corresponding wave-functions are $\phi_n(x) = \langle x|\phi_n\rangle = \sqrt{\frac{2}{L}}\sin(n\pi\frac{x}{L})$.

a) Assume for the moment that there is no interaction between the two fermions. *What is the ground state energy? Write down the corresponding ground state, in terms of the single-particle states $|\phi_1\rangle$, $|\phi_2\rangle$ as well as the spin states $|\uparrow\rangle$ and $|\downarrow\rangle$. What is the energy of the first excited state? What is the degeneracy of the first excited state? Write down the corresponding (orthonormal) first-excited states, in such a way that each of them is either a spin-singlet or a spin-triplet.*

Hint: Inside the box, the *single-particle* Hamiltonian acts like the differential operator $-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$. What are the *single-particle* eigenenergies?

(4 points)

Remark: Since the first-excited eigenspace is degenerate, one can of course choose any basis in that subspace. However, here we ask you to choose the particular egienbasis where we additionally have well defined spin singlets and triplets.

[1] Well, the factor $\frac{1}{2}$ was missing in the lecture.

b) Let us now assume that we turn on an interaction potential

$$h^{(1,2)}(x_1, x_2) = -a\delta(x_2 - x_1), \quad a > 0,$$

where δ denotes the delta-function. *Within first order perturbation theory, what is the energy difference between the first excited spin-singlet states and the first excited spin triplet states?* (Evaluate the integral.) *Which of them are higher in energy?* It is OK to apply the results in the lecture notes. You don't have to re-derive everything.

Hint: Recall that the first-order perturbed energies are $E_n^{(1)} = E_n^{(0)} + \langle \psi_n^{(0)} | h^{(1,2)} | \psi_n^{(0)} \rangle$, where $E_n^{(0)}$ are the unperturbed eigenenergies and $|\psi_n^{(0)}\rangle$ are the unperturbed eigenstates. You can use the following trigonometric relation

$$\sin^2(ax)\sin^2(2ax) = \frac{1}{4} - \frac{1}{2}\cos(2ax) - \frac{1}{4}\cos(4ax) + \frac{1}{2}\cos^3(2ax)$$

and it is OK to look up integrals.

(4 points)

c) Mini gold star exercise: In the lecture notes, as well as in b), it looks like we are using non-degenerate perturbation theory. One might object that since the first excited state is degenerate, one should use degenerate perturbation theory. That is indeed true, but as it so happens, the first excited spin-singlet and spin-triplet states are also eigenstates to the perturbation $h^{(1,2)}$ and thus diagonalizes it. Because of this, the end result is as above (and one can understand why we are so keen on the first excited spin singlet and triples in a)). *Check these things.*

(0 points)

3 Energy spectrum for identical particles

In the lecture we discussed how the anti-symmetry of fermionic states give rise to the exchange interaction. In this exercise we explore very closely related effects, where the symmetry and anti-symmetry affect the energy spectrum in a simple model.

Suppose that we have two identical particles of mass m on a line, and that these interact via a harmonic potential, such that the Hamiltonian is $H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_1^2} - \frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_2^2} + \frac{k}{2}(x_1 - x_2)^2$. As you may recall, it is useful to change to the center of mass coordinate $R = (mx_1 + mx_2)/(2m) = \frac{1}{2}(x_1 + x_2)$ and the relative coordinate $r = x_1 - x_2$. By separation of variables, the eigenfunctions of H can be written $\psi_{p,n}(R, r) = e^{ipR}\phi_n(r)$, where ϕ_n for $n = 0, 1, 2, \ldots$ are the solutions to the harmonic oscillator $H' = -\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} + \frac{k}{2}r^2$, with the reduced mass $\mu = m/2$.

a) *How does r and R transform under the exchange of particles?* **(1 point)**

b) *What can we conclude concerning the symmetry or anti-symmetry of the factor e^{ipR}? Argue that it is only $\phi_n(r)$ that determines whether $\psi_{p,n}(R, r)$ is symmetric or anti-symmetric under particle exchange.*

Hint: Recall that a function f is symmetric if $f(-x) = f(x)$, and it is anti-symmetric if $f(-x) = -f(x)$.

(2 points)

c) *For which $n = 0, 1, 2, \ldots$ does ϕ_n correspond to a solution that is symmetric under permutation of particles 1 and 2, and for which n are they anti-symmetric? If these particles have no additional degrees of freedom, what would be the spectrum be for two identical bosons, and what would it be for two identical fermions?* Ignore the center of mass motion, and express the spectrum in terms of m and k. **(2 points)**

d) Suppose now that the two particles in addition have a spin degree of freedom, and more precisely that they are spin-half fermions. *What is the spectrum, and what are the degeneracies?* (Do again ignore the center of mass motion.) *What is the lowest energy that the system can have if the total spin is restricted to be in a spin-singlet state? What is the lowest energy if it is restricted to a spin triplet?* **(4 points)**

Remark: In the lecture we discussed the effect of the anti-symmetry of the electrons on the spectrum of the Helium-atom. However, this does not apply only to electrons. For example, the proton is a spin-half fermion. If we consider a hydrogen molecule, H_2, the two protons can either be in a nuclear spin singlet state (parahydrogen) or in a nuclear spin triplet (orthohydrogen). Apart from the nuclear spin, the two protons can also orbit each other, and much analogous to this exercise, it turns out that the nuclear spin state affects the allowed orbital states, which leads to a different ground state energy for ortho- and parahydrogen. In the production of liquid hydrogen one often uses a catalyst to speed the conversion to the lowest energy state.