Kwantummechanica 2021-2022 Eindtoets (Toets B) NS202B
4 Februari 2022
Grading model

The regular time for this test is **180** minutes. This test has **24** questions on **4** pages, for a total of **37** points.

Motivate all your answers, using words, calculations or drawings. Stating only the final answer without motivation will not be awarded points. You may answer in Dutch or English. Unclear and unreadable answers will be considered wrong.

1 Fermions and bosons (5 points)

We consider the problem of a particle in a box. The energy levels E_n are labeled by $n = 1, 2, ...$ with $n = 1$ being the lowest energy. The corresponding single particle wavefunctions read $\psi_n(x)$. In the following we consider a number of multiparticle states. First we consider fermions without spin (or if you wish, all in the spin-up state) and only concentrate on the spatial part. The following wavefunctions belong to either two bosons or two fermions. Indicate which is which and for each give a short argument or calculation to motivate your answer.

a. (1 point) $\Psi(x_1, x_2) = 1/\sqrt{2}\,(\psi_1(x_1)\psi_2(x_2) - \psi_1(x_2)\psi_2(x_1))$. it is an antisymmetric function valid for fermions point is given for mentioning or demonstrating antisymmetry

b. (1 point) $\Psi(x_1, x_2) = 1/\sqrt{2}\,(\psi_1(x_1)\psi_2(x_2) + \psi_1(x_2)\psi_2(x_1))$ it is a symmetric function valid for bosons. point is given for mentioning or demonstrating symmetry

c. (1 point) $\Psi(x_1, x_2) = \psi_1(x_1)\psi_1(x_2)$. it is a symmetric function valid for bosons. point is given for mentioning or demonstrating symmetry. Mentioning the Pauli principle in this specific question is also worth the point. . While it is not the answer we intended, the wavefunction is also good for distinguishable particles (in the question we did not say indistinguishable). However failure to mention two indistinguishable bosons gives only half a point.

From now on we consider electrons which have spin. The following wavefunctions describe spatial and spin part of a two-particle wavefunction. Which one(s) of the following describes two electrons with spin? For each, give a short argument or calculation why it can(not) be the correct wavefunction.

d. (1 point) $\Psi(x_1, x_2) = 1/2\,(\psi_1(x_1)\psi_2(x_2) - \psi_1(x_2)\psi_2(x_1))\,(|\uparrow_1\downarrow_2\rangle - |\downarrow_1\uparrow_2\rangle)$. Both the spatial part and the spin part are antisymmetric. That makes the full wavefunction symmetric, which is not suitable for fermions

e. (1 point) $\Psi(x_1, x_2) = 1/2\,(\psi_2(x_1)\psi_3(x_2) + \psi_2(x_2)\psi_3(x_1))\,(|\uparrow_1\downarrow_2\rangle - |\downarrow_1\uparrow_2\rangle)$ the spatial part is symmetric and the spin part is antisymmetric. That makes the full wavefunction antisymmetric, which is suitable for fermions

Take a new sheet of answer paper and proceed to the next page

2 One dimensional harmonic oscillator (8 points) Please use a new sheet

We consider a spinless particle in the 1-dimensional harmonic oscillator

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2 x^2 \,. \tag{1}$$

A way to solve this is to introduce the so-called ladder operators according to

$$\begin{aligned} \hat{a} &= \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} + \frac{i}{m\omega}\hat{p}_x\right) \\ \hat{a}^\dagger &= \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} - \frac{i}{m\omega}\hat{p}_x\right) \end{aligned} \tag{2}$$

a. (2 points) Show that the Hamiltonian can be rewritten as $\hat{H} = \hbar\omega\left(\hat{a}^\dagger\hat{a} + 1/2\right)$ Filling in the expressions for the operators we get

$$\begin{aligned} \hat{H} &= \hbar\omega\left(\hat{a}^\dagger\hat{a} + 1/2\right) \\ &= \hbar\omega\left(\frac{m\omega}{2\hbar}\left(\hat{x} - \frac{i}{m\omega}\hat{p}_x\right)\left(\hat{x} + \frac{i}{m\omega}\hat{p}_x\right) + 1/2\right) \\ &= \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2 x^2 + \hbar\omega\left(\frac{i}{2\hbar}[p,x] - \frac{1}{2}\right) \\ &= \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2 x^2 \,. \end{aligned}$$

where we have used $[p,x] = -[x,p] = -i\hbar$. It is also possible to express p and x in the ladder operators and work the other way. 1 point is for the general derivation, 1 point is specifically for using a commutator. (or directly expressing p in derivative operators although that is way more work).

b. (2 points) Show that $[\hat{a}, \hat{a}^\dagger] = 1$.

$$[\hat{a}, \hat{a}^\dagger] = \frac{m\omega}{2\hbar}\left[\left(\hat{x} + \frac{i}{m\omega}\hat{p}_x\right)\left(\hat{x} - \frac{i}{m\omega}\hat{p}_x\right) - \left(\hat{x} - \frac{i}{m\omega}\hat{p}_x\right)\left(\hat{x} + \frac{i}{m\omega}\hat{p}_x\right)\right]$$

Note that the terms with the squares of operators cancel and only the cross terms remain.

$$\begin{aligned} &= \frac{m\omega}{2\hbar}\frac{i}{m\omega}(px - xp + px - xp) \\ &= \frac{-i}{hbar}[x,p] = \frac{-i}{hbar}i\hbar = 1 \end{aligned}$$

We can label the eigenstates according to $|n\rangle$ ($n = 0, 1, \ldots$) with $\hat{H}|n\rangle = \hbar\omega(n + 1/2)|n\rangle$. We initialize a state $|\psi(t=0)\rangle = 1/\sqrt{2}\left(|0\rangle + |2\rangle\right)$.

c. (2 points) Determine $|\psi(t)\rangle$ for arbitrary t. Every energy eigenfunction evolves with $e^{iEt/\hbar}$, so that

$$\begin{aligned} |\psi(t)\rangle &= \frac{1}{\sqrt{2}}[e^{-iE_0 t/\hbar}|0\rangle + e^{-iE_2 t/\hbar}|2\rangle] \\ &= \frac{1}{\sqrt{2}}[e^{-i\omega t/2}|0\rangle + e^{-5i\omega t/2}|2\rangle] \end{aligned}$$

d. (2 points) Calculate the expectation value $\langle\psi(t)|x|\psi(t)\rangle$ as a function of t. (If you have no answer from the previous question, indicate that you assume that $|\psi(t)\rangle = \frac{1}{\sqrt{2}}(|0\rangle + e^{\frac{3}{2}i\omega t}|2\rangle)$, which is not the correct result)

$$\langle\psi(t)|x|\psi(t)\rangle = \frac{1}{2}[\langle 0|x|0\rangle + \langle 2|x|2\rangle + e^{-4i\omega t/2}\langle 0|x|2\rangle + e^{4i\omega t/2}\langle 2|x|0\rangle]$$

All the matrix elements are zero, as the wavefunctions are all even, and x is odd. We can also calculate them explicitly by expressing the operator x in the ladder operators. The result is of course the same, hence $\langle x(t)\rangle = 0$.

Take a new sheet of answer paper and proceed to the next page

3 Two dimensional harmonic oscillator (15 points) Please use a new sheet

We consider a spinless particle in the 2-dimensional harmonic oscillator. In the first part of the question, we work in purely 2-dimensional space, so the z-coordinate is not there. The Hamiltonian is

$$H = \frac{\hat{p}_x^2}{2m} + \frac{1}{2}m\omega^2 x^2 + \frac{\hat{p}_y^2}{2m} + \frac{1}{2}m\omega^2 y^2. \tag{3}$$

a. (3 points) Use a separation ansatz, $\psi(x, y) = X(x)Y(y)$ to show that we find two equations

$$\begin{aligned} \frac{\hat{p}_x^2}{2m}X(x) + \frac{1}{2}m\omega^2 x^2 X(x) = \hat{H}_x X(x) &= E_x X(x) \\ \frac{\hat{p}_y^2}{2m}Y(y) + \frac{1}{2}m\omega^2 y^2 Y(y) = \hat{H}_y Y(y) &= E_y Y(y) \end{aligned} \tag{4}$$

with $E = E_x + E_y$. We see that both H_z and H_y are harmonic oscillator hamiltonians for which all eigenvalues are positive. Since H_x contains neither y nor y-derivatives it commutes with $Y(y)$. Similar for H_y and $X(x)$. So we can write

$$EX(x)Y(y) = Y(y)H_x X(x) + X(x)H_y Y(y)$$

Now for this equation to be fulfilled $X(x)$ and $Y(y)$ must be eigenfunctions of their respective Hamiltonians. There are many ways to show this. For instance since $Y(y)$ must be normalized, we can take $\int dy Y^\dagger(y)(.)$ on both sides, yielding

$$EX(x) = H_x X(x) + X(x)\int dy Y^\dagger(y)H_y Y(y) = H_x X(x) + X(x)\langle H_y\rangle$$

$$(E - \langle H_y\rangle)X(x) = H_x X(x)$$

which is an eigenvalue equation ofr $X(x)$. (Also valid way: Take a point where X and Y are both nonzero and divide by the product XY to obtain the sum of two terms, one which only contains x and one which only contains y; these can sum to a constant only if they are both constant, we name the constants E_x, E_y.)

points given for:

1 for - correct insight that the operators for different variables commute.

1.0 for - Showing that the equation is fulfilled if both X and Y are eigenfunctions

0.5 for - Showing that they both need to be eigenfunctions.

We can now turn to solve the problem in x-direction. We introduce two operators $\hat{a}_x = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} + \frac{i}{m\omega}\hat{p}_x\right)$ and $\hat{a}_x^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} - \frac{i}{m\omega}\hat{p}_x\right)$. Following this we can rewrite $\hat{H}_x$ as $\hat{H}_x = \hbar\omega\left(\hat{a}_x^\dagger\hat{a}_x + 1/2\right)$. The same applies to the y-direction.

b. (3 points) Use that information to argue that the ground state energy is given by $E_0 = \hbar\omega$. In each coordinate we have a harmonic oscillator with eigenenergies $(n_{x,y} + 1/2)\hbar\omega$. Here $n = 0$ is the ground state. Now the lowest energy state occurs when both are in the ground state of energy $E_x = E_y = \hbar\omega/2$.

points given for:

1 for the insight that the X equation is a regular 1d harmonic osdcillator.

1 for the insight that the same applies to Y

1 for the correcyt calcualtion of the groiund state energies

NB these are relatively easy points as the harmonic oscillator was already present in the previous question and it is not necessary to prove that $n = 0$ is the ground state to gain full points.

c. (1 point) Calculate the energy of the **second** excited state E_2. Determine its degeneracy.
The easiest way is to make a table like this:

n_x	n_y	$E/\hbar\omega$	Energy level number	Degeneracy
0	0	1	0	1
0	1	2	1	2
1	0	2	1	2
1	1	3	2	3
2	0	3	2	3
0	2	3	2	3

The second excited state has energy $E_2 = 3\hbar\omega$ and degeneracy 3. Half a point if degeneracy wrong. Half a point if calculated E_1 instead of E_2. (Full points if E_0, E_1 are not in the table).

We now consider the case of a 2D harmonic oscillator in 3D space, so the z axis is present now. The Hamiltonian now includes an extra term,

$$H = \frac{\hat{p}_x^2}{2m} + \frac{1}{2}m\omega^2 x^2 + \frac{\hat{p}_y^2}{2m} + \frac{1}{2}m\omega^2 y^2 + \frac{\hat{p}_z^2}{2m}. \tag{5}$$

d. (2 points) Show that the hamiltonian is invariant under translations along the z axis and under rotations around that same axis. We can show that it commutes with the translation operator, which is $T_z(a) = exp(-iap_z/\hbar)$. This is true because in the Taylor series of the exponential there are only powers of p and the hamiltonian commutes with p as we show in the next question. As a result $T^\dagger HT = H$. Alternatively, for full points, we can simply say that nothing changes as $z->z+deltaz$, because z does not appear and $\partial/\partial z$ does not change under that transformation. For L_z, the differential operators do not depend on phi

e. (1 point) Show that H commutes with p_z. p_z commutes with itself and there is no z in H, so it must commute

f. (1 point) Show that H commutes with L_z. (a) L_z commutes with the Laplacian and therefore with the kinetic energy term. or (b) from the fact that H commutes with the rotation operator which can be expressed as a series in L_z

g. (2 points) Show that it follows that the operators p_z and L_z represent conserved quantities. From the generalized Ehrenfest theorem in the front flap it folows that if an operator does not depend explicitly on time and commutes with H, the time derivative of its expectation valueis always zero.

h. (2 points) Do you expect the other components of **L** and **p** to also be conserved? Why (not)? (Points are awarded for the motivation, not for a yes/no answer). Full points for any reasonable answer, such as: there is no translational invariance in the x, y directions, so $p_{x,y}$ are not conserved, and there is no rotational symmetry around the x, y axes so $L_{x,y}$ are not conserved. No need to demonstrate the absence of the rotational/translational symmetry.

Take a new sheet of answer paper and proceed to the next page

4 Perturbation theory (9 points) Please use a new sheet

We consider a spin $S = 1/2$ system with a Hamiltonian $H_0 = -\mu B S_z$ $(B > 0)$ where

$$S_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} . \tag{6}$$

and $\mu > 0$ is the magnetic moment associated with the spin.

a. (1 point) Verify that $\chi_+ = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $\chi_- = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ are normalized eigenvectors of H_0 and determine the corresponding eigenvalues. Multiply the matrix with the vectors......, find $E_\pm = \mp\mu B\hbar/2$. NB. E_+ is the ground state (not asked to identify the ground state so full points for only the energies).

The other components of the spin algebra are given by

$$S_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \text{and} \qquad S_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \tag{7}$$

b. (1 point) Determine the eigenvectors of S_x and the corresponding eigenvalues. One way is: The matrix is traceless so $\lambda_1 + \lambda_2 = 0$; the determinant is $-\frac{\hbar^2}{4}$ and is equal to $\lambda_1\lambda_2$; so we find $\lambda_1 = -\lambda_2 = \frac{\hbar}{2}$.

$$\frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix} a \\ b \end{pmatrix}$$

$$a = b$$

Normalizing the solution we find $\chi_1 = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$. The other solution has $a = -b$ so must be $\chi_2 = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}$. Note that eigenvectors may be chosen with a different phase. Only stating the solution is zero points, there must be some indication of the method used to find the eigenvectors.

c. (1 point) Determine the commutator $[S_x, S_z]$ through explicit calculation. Do the matrix multiplication, you find indeed $\sigma_x\sigma_z = -i\sigma_y$ and $\sigma_z\sigma_x = i\sigma_y$, leading to $[S_x, S_z] = -i\hbar S_y$. Full points if apparently the student misread the s, y subscripts and calculated e.g. $[S_x, S_y]$.

We introduce a perturbation $H_1 = -\alpha\mu B S_x$ where $0 < \alpha \ll 1$.

d. (1 point) Show that the first order correction to the ground state energy is zero.

$$\langle H_1\rangle = -\alpha\mu B\langle S_x\rangle$$

We see that due to the minus sign in H_0, χ_+ must be the ground state . As can be found by matrix multiplication,

$$\langle\chi_+|S_x|\chi_+\rangle = 0$$

e. (2 points) What is the correction to the ground state energy to second order? Here we use the second order formula [6.15 in 2nd Ed] for $n = 0$, which means that $m = 1$.

$$E_0^{(2)} = \frac{|\langle\chi_-|H_1|\chi_+\rangle|^2}{E_0 - E_1}$$

Now, $E_0 - E_1 = -\mu B\hbar/2 - \mu B\hbar/2 = -\mu B\hbar$, and the numerator is found

$$\langle\chi_-|H_1|\chi_-\rangle = -\alpha\mu B\hbar/2$$

yielding

$$E_0^{(2)} = (\alpha\mu B\hbar/2)^2/(-\mu B\hbar) = \frac{-1}{4}\alpha^2\mu B\hbar$$

Trivial calculation errors -0.5 point.

f. (1 point) What is the corresponding first order correction to the ground state spin wave-function? Here we use the formula [6.13 in 2nd Ed] for $n = 0$, which means that $m = 1$, and we re-use all the matrix elements that we have already calculated,

$$\chi_0^{(1)} = \frac{|\langle\chi_-|H_1|\chi_+\rangle|}{E_0 - E_1}\chi_-$$

$$= (-\alpha\mu B\hbar/2)(-\mu B\hbar)\chi_- = \frac{\alpha}{2}\chi_-$$

Now consider the full Hamiltonian $H = H_0 + H_1$.

g. (2 points) Determine the exact eigenvalues. How does it compare to the perturbative result? Here, we could write the full hamiltonian in matrix form and diagonalize the 2x2 matrix,

$$H = \frac{-\mu B\hbar}{2}\begin{pmatrix} 1 & \alpha \\ \alpha & -1 \end{pmatrix}.$$

Equivalently, we can see that if B represents a magnetic field in the z direction initially, the full hamiltoniam has a component in the x direction of αB so the total field strength is the length of the vector $(\alpha B, 0, B)$ which is $B\sqrt{1+\alpha^2}$. The exact groundstate is the ground state of a spin 1/2 along the quantization axis given by B, so it is $-\mu B\sqrt{1+\alpha^2}\hbar/2 \approx -\mu B\hbar/2 - \mu B\alpha^2\hbar/4$. Of course the matrix method gives the same result. Trivial calculation errors -0.5 point.

This is the end of the test. Please verify that all your answer sheets are marked with your name and student number, and return your answer sheets and this exam sheet to the proctor.

- xx Sofie