Quantum Mechanics FKA081/FIM400

Final Exam October 23 2013

Next review time for the exam: Thursday November 21 between 12-13 in my room.
NB: If you want to come to the review you must collect your exam before at the "Kansli" in Origo 5th floor. (This info is also available on the course homepage.)

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Allowed material during the exam:

- The course textbook J.J. Sakurai and Jim Napolitano, Modern Quantum Mechanics Second Edition (2010).
  NB: The old red cover version: J.J. Sakurai, Modern Quantum Mechanics Revised Edition (1994) is *also* allowed.
- A Chalmers approved calculator.

Write the final answers clearly marked by Ans: ...
and underline them.

You may use without proof any formula in the book.

There is a total of 30 points in this test. The grades are assigned according to the table in the course homepage.

Problem 1

Consider the following observable ($\epsilon \ll 1$)

$$A = \begin{pmatrix} 1 & \epsilon & \epsilon \\ \epsilon & 2 & \epsilon \\ \epsilon & \epsilon & 3 \end{pmatrix} \tag{1}$$

Q1 (*1 points*) Compute the eigenvalues to first order in ϵ.
Q2 (*2 points*) Compute the eigenvalues to second order in ϵ.

Problem 2

Consider two identical spin-1/2 particles of mass M, moving in one dimension and interacting with a two-body potential of the form

$$V = \frac{k}{2}(x_1 - x_2)^2 + \alpha(x_1 - x_2)^4 \mathbf{S}_1 \cdot \mathbf{S}_2 \tag{2}$$

Q1 (*3 points*) Compute the energies and the degeneracies of the two lowest states in the center of mass frame for the case $\alpha = 0$.
Q2 (*4 points*) Compute the first order correction in α of the two lowest states.

Problem 3

Consider a system containing three spin-1 particles.
Q1 (*4 points*) Assuming that all three particles are *distinguishable*, write all possible values for the total spin of the system, including possible degeneracies. (You *do not* have to write down the states explicitly).
Q2 (*3 points*) Assuming that all three particles are *indistinguishable*, and that their orbital wave-function is totally antisymmetric, write the possible values for the total spin of the system and the corresponding state explicitly.

Problem 4

Consider a spinless particle in one dimension with a potential $\lambda\delta(x)$ ($\lambda > 0$).
Q1 (*3 points*) Compute the transmission and reflection coefficients.

Problem 5

Consider a spinless particle in a state of orbital angular momentum $l = 1$. (That is, $L_z|\pm\rangle = \pm|\pm\rangle$ and $L_z|0\rangle = 0$.)

The Hamiltonian for the so called quadrupole moment can be described by

$$H = \hbar\omega(L_x L_z + L_z L_x) \tag{3}$$

Q1 (*3 points*) Find the eigenvalues of the Hamiltonian.
Q2 (*4 points*) Assuming that at time $t = 0$ the particle is in the state

$$|\psi, t = 0\rangle = \frac{1}{\sqrt{2}}(|+\rangle - |-\rangle) \tag{4}$$

find the state at time $t > 0$.

Problem 6

Consider the one dimensional Hamiltonian ($k > 0$)

$$H = \frac{p^2}{2m} + k|x| \tag{5}$$

Q1 (*2 points*) Compute the ground state energy using two possible trial wave functions: ($a > 0$)

case 1	$\exp(-a\|x\|)$
case 2	$\exp(-ax^2/2)$

Q2 (*1 point*) Which of the two is better and why?

PROBLEM 1:

Unperturbed states: $|1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, |2\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, |3\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$

Q1: Let $A' = \begin{pmatrix} 0 & \epsilon & \epsilon \\ \epsilon & 0 & \epsilon \\ \epsilon & \epsilon & 0 \end{pmatrix} = \epsilon \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}$

First order: $\langle 1|A'|1\rangle = \langle 2|A'|2\rangle = \langle 3|A'|3\rangle$
$= 0$ for all.

Q2: First notice that
$A'_{ij} = \langle i|A'|j\rangle = \epsilon$ for $i \neq j$.

Then: $E_1^{(2)} = \sum_{k\neq 1} \frac{|A'_{1k}|^2}{1-k} = \frac{\epsilon^2}{-1} + \frac{\epsilon^2}{-2} = -\frac{3\epsilon^2}{2}$

$E_2^{(2)} = \sum_{k\neq 2} \frac{|A_{2k}|^2}{2-k} = \frac{\epsilon^2}{1} + \frac{\epsilon^2}{-1} = 0.$

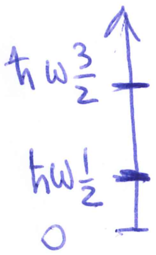
$E_3^{(2)} = \sum_{k\neq 3} \frac{|A_{3k}|^2}{3-k} = \frac{\epsilon^2}{2} + \frac{\epsilon^2}{1} = \frac{3\epsilon^2}{2}.$

PROBLEM 2

Set $x = x_1 - x_2$, $m = \frac{M}{2}$ (reduced mass).

Q1. For $\alpha = 0$ $\quad H_0 = \frac{p^2}{2m} + \frac{k}{2} x^2$

eigenvalues $E_n = \hbar\omega\left(n + \frac{1}{2}\right)$ $\quad \omega = \sqrt{\frac{k}{m}} = \sqrt{\frac{2k}{M}}$.



ORBITAL W.F. ANTISYMM. $\Rightarrow$ SPIN SYMM. ($S=1$)

ORBITAL W.f SYMMETRIC $\Rightarrow$ SPIN ANTISYMM ($S=0$).

thus: the grond state has energy $\frac{1}{2}\hbar\omega$ and $S=0$ $\Rightarrow$ no degeneracy (deg $=1$).

the Ist excited state $\frac{3}{2}\hbar\omega$ has $S=1$ $\Rightarrow$ 3 possible spin m_s (deg $=3$)

Q2: Write the states as

$|n\rangle \otimes \chi_{sm}$ where $|n\rangle$ refers to the harmonic oscillator and $\chi_{s,m}$ ($s = 0$ or 1) is the spin of the two particle system.

$$H' = \alpha (x_1 - x_2)^4 \, \vec{S}_1 \cdot \vec{S}_2 = \alpha x^4 \frac{\hbar^2}{2}\left(s(s+1) - \frac{3}{4} - \frac{3}{4}\right)$$

$$= \begin{cases} -\dfrac{3\alpha\hbar^2}{4} x^4 & \text{for } s=0 \text{ (ground state)} \\ +\dfrac{\alpha\hbar^2}{4} x^4 & \text{for } s=1 \text{ (1st excited st.)} \end{cases}$$

$$\langle 0|x^4|0\rangle = \left(\frac{\hbar}{2m\omega}\right)^2 \langle 0|(a+a^\dagger)^4|0\rangle = \frac{3\hbar^2}{4m^2\omega^2}$$

$$// \; \langle 0|(a+\cancel{a^\dagger})(a+a^\dagger)(a+a^\dagger)(\cancel{a}+a^\dagger)|0\rangle =$$

$$= \langle 0|a\,(\cancel{a^2} + a^\dagger a + a a^\dagger + \cancel{a^{\dagger 2}})\,a^\dagger|0\rangle =$$

$$= \langle 0|a a^\dagger a a^\dagger + a^2 a^{\dagger 2}|0\rangle = 1 + 2 = 3 \; //$$

$$\langle 1|x^4|1\rangle = \left(\frac{\hbar}{2m\omega}\right)^2 \langle 1|(a+a^\dagger)^4|1\rangle = \frac{15\hbar^2}{4m^2\omega^2}$$

$$// \; \langle 1|(a+a^\dagger)(a+a^\dagger)(a+a^\dagger)(a+a^\dagger)|1\rangle =$$

$$= \langle 0|a\,(a^2 a^{\dagger 2} + a a^\dagger a a^\dagger + a^\dagger a^2 a^\dagger + a a^{\dagger 2} a +$$

$$+ a^\dagger a a^\dagger a + \cancel{a^{\dagger 2}} a^2)\,a^\dagger|0\rangle =$$

$$6 + 2\cdot 2 + 2 + 2 + 1 = 15 \; //$$

Hence:

$$E_0^{(1)} = -\frac{3\alpha\hbar^2}{4} \times \frac{3\hbar^2}{4m^2\omega^2} = -\frac{9\alpha\hbar^4}{8MK}$$

$$E_1^{(1)} = +\frac{\alpha\hbar^2}{4} \cdot \frac{15\hbar^2}{4m^2\omega^2} = \frac{15\alpha\hbar^4}{8MK}$$

PROBLEM 3.

Let $\mathcal{H}^{(1)}_{S=1}$, $\mathcal{H}^{(2)}_{S=1}$ $\mathcal{H}^{(3)}_{S=1}$ be the part. 1, 2 and 3 Hilbert spaces.

Q1 Take the first 2 part's and combine them:

$$\mathcal{H}^{(1)}_{S=1} \otimes \mathcal{H}^{(2)}_{S=1} = \mathcal{H}^{(1,2)}_{S=0} \oplus \mathcal{H}^{(1,2)}_{S=1} \oplus \mathcal{H}^{(1,2)}_{S=2}$$

meaning that two $S=1$ part's combine to give $S=0$, 1 or 2.

Now take the third part and combine it with the previous ones

$$\mathcal{H}^{(3)}_{S=1} \otimes \mathcal{H}^{(1,2)}_{S=0} = \mathcal{H}^{(1,2,3)}_{S=1}$$

$$\mathcal{H}^{(3)}_{S=1} \otimes \mathcal{H}^{(1,2)}_{S=1} = \mathcal{H}^{(1,2,3)}_{S=0} \oplus \mathcal{H}^{(123)}_{S=1} \oplus \mathcal{H}^{(123)}_{S=2}$$

$$\mathcal{H}^{(3)}_{S=1} \otimes \mathcal{H}^{(1,2)}_{S=2} = \mathcal{H}^{(1,2,3)}_{S=1} \oplus \mathcal{H}^{(123)}_{S=2} \oplus \mathcal{H}^{(123)}_{S=3}.$$

where $\mathcal{H}^{(1,2,3)}_{S_{TOT}}$ is the total space.

All together:

		deg. (= how many indep. states)
S_{TOT} =	0	1 (means NO DEG).
	1	3
	2	2
	3	1

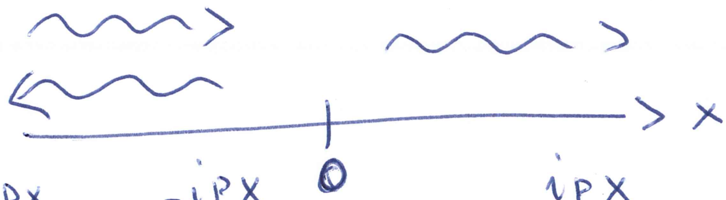
check: $1\times1 + 3\times3 + 2\times5 + 1\times7 = 27 = 3^3$.

Q2: They are BOSONS ⇒ TOTAL STATE must be symmetric ⇒ spin ANTISYMM.
⇒ no value of $m = 0, \pm1$ can be repeated.

$$\Rightarrow \chi^{spin} = \frac{1}{\sqrt{6}}\Big(|+\rangle|0\rangle|-\rangle - |+\rangle|-\rangle|0\rangle - |0\rangle|+\rangle|-\rangle + |0\rangle|-\rangle|+\rangle + |-\rangle|+\rangle|0\rangle - |-\rangle|0\rangle|+\rangle\Big)$$

the $\frac{1}{\sqrt{6}}$ is so that $\|\chi\|^2 = 1$ if the $|m\rangle$ states are properly normalized.

PROBLEM 4



$E = \frac{p^2}{2m}$.

$\underbrace{e^{ipx} + a e^{-ipx}}_{\psi_-(x)}$ $\qquad$ $\underbrace{b e^{ipx}}_{\psi_+(x)}$

set $\hbar = 1$ for convenience

continuity at $x=0$ $\Rightarrow$ $1+a=b$.

$$\int_{-\epsilon}^{+\epsilon}\left(-\frac{1}{2m}\psi''(x) + \lambda\delta(x)\psi(x)\right)dx = E\int_{-\epsilon}^{\epsilon}\psi(x)\,dx$$

$$\Downarrow$$

$$-\frac{1}{2m}\psi'(x)\Big]_{-\epsilon}^{+\epsilon} + \lambda\psi(0) = E\cdot\cancel{O(\epsilon)} \to 0$$

$$\Rightarrow -\frac{1}{2m}\left(ipb - ip + ipa\right) + \lambda(1+a) = 0.$$

$$\Rightarrow a = \frac{-\lambda}{\lambda - ip/m}, \qquad b = \frac{-ip/m}{\lambda - ip/m}$$

$$\Rightarrow R = |a|^2 = \frac{\lambda^2}{\lambda^2 + p^2/m^2} \qquad T = |b|^2 = \frac{p^2/m^2}{\lambda^2 + p^2/m^2} = 1 - R \ \checkmark$$

PROBLEM 5

Using $L_x = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$

$L_y = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & -i & 0 \\ i & 0 & i \\ 0 & i & 0 \end{pmatrix}$

$L_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$

(Can be obtained with $L_\pm$ if you forget).

$$H = \frac{\hbar\omega}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & -1 \\ 0 & -1 & 0 \end{pmatrix}$$

Q1: $\begin{vmatrix} -\lambda & 1 & 0 \\ 1 & -\lambda & -1 \\ 0 & -1 & -\lambda \end{vmatrix} = 0$ $\quad \lambda_1 = 0,\ \lambda_2 = \sqrt{2},\ \lambda_3 = -\sqrt{2}$

$\Rightarrow$ energies: $0, \pm\hbar\omega$.

Q2: Energy eigenstates:

$|E=0\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}$ $\quad |E=\hbar\omega\rangle = \frac{1}{2}\begin{pmatrix} 1 \\ \sqrt{2} \\ -1 \end{pmatrix}$.

$|E=-\hbar\omega\rangle = \frac{1}{2}\begin{pmatrix} -1 \\ \sqrt{2} \\ 1 \end{pmatrix}$

At $t=0$:

$$|\psi, t=0\rangle = \frac{1}{\sqrt{2}}\left(|+\rangle - |-\rangle\right) = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\\-1\end{pmatrix} \equiv |\psi_0\rangle =$$

$$= |E=0\rangle\langle E=0|\psi_0\rangle + |E=\hbar\omega\rangle\langle E=\hbar\omega|\psi_0\rangle +$$

$$+ |E=-\hbar\omega\rangle\langle E=-\hbar\omega|\psi_0\rangle =$$

$$= \frac{1}{\sqrt{2}}|E=+\hbar\omega\rangle - \frac{1}{\sqrt{2}}|E=-\hbar\omega\rangle$$

At time $t>0$:

$$|\psi, t\rangle = \frac{1}{\sqrt{2}}\left(e^{-i\omega t}|E=+\hbar\omega\rangle - e^{+i\omega t}|E=-\hbar\omega\rangle\right)$$

$$= \frac{1}{2\sqrt{2}}\begin{pmatrix} e^{-i\omega t} + e^{i\omega t} \\ \sqrt{2}\left(e^{-i\omega t} - e^{+i\omega t}\right) \\ -e^{-i\omega t} - e^{i\omega t}\end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix}\cos\omega t \\ -\sqrt{2}i\sin\omega t \\ -\cos\omega t\end{pmatrix}$$

PROBLEM 6 . set $\hbar=1$ for convenience.

Let $\varphi_1(x) = e^{-a|x|}$ $\varphi_2(x) = e^{-ax^2/2}$.

Q1: Be careful that φ_1'' has a $\delta(x)$ in it.

Better to write:

$$\int_{-\infty}^{+\infty} \varphi_1 \varphi_1'' dx = -\int_{-\infty}^{+\infty} \varphi_1'^2 dx = -2\int_0^{\infty} \varphi_1'^2 dx = -a$$

Also $\int_{-\infty}^{\infty} |x| \varphi_1^2 dx = 2\int_0^{\infty} x \varphi_1^2 dx = \frac{1}{2a^2}$.

and $\int_{-\infty}^{+\infty} \varphi_1^2 dx = 2\int_0^{\infty} \varphi_1^2 dx = \frac{1}{a}$.

$$\overline{H}_1 = \frac{-\frac{1}{2m}(-a) + k \cdot \frac{1}{2a^2}}{1/a} = \frac{a^2}{2m} + \frac{k}{2a}$$

minimum for $a = \left(\frac{km}{2}\right)^{1/3}$

$$\Rightarrow \overline{H}_{1\,\text{MIN}} = \left(\frac{2}{mk}\right)^{\frac{1}{3}} \cdot \frac{3}{4} k \cong 0.945 \times \left(\frac{k^2}{m}\right)^{\frac{1}{3}}.$$

Similarly:

$$\langle \psi_2 | \psi_2 \rangle = \int_{-\infty}^{+\infty} \psi_2^2 \, dx = \sqrt{\frac{\pi}{a}}$$

$$\int_{-\infty}^{+\infty} \psi_2 \psi_2'' \, dx = -\int_{-\infty}^{+\infty} \psi_2'^2 = -\frac{\sqrt{\pi a}}{2}$$

$$\int_{-\infty}^{+\infty} |x| \psi_2^2 \, dx = 2 \cdot \int_0^{\infty} x \psi_2^2 \, dx = \frac{1}{a}.$$

$$\Rightarrow \bar{H}_2 = \frac{\frac{\sqrt{\pi a}}{4m} + k/a}{\sqrt{\pi/a}} = \frac{a}{4m} + \frac{k}{\sqrt{\pi a}}$$

min for $a = \left(\frac{2km}{\sqrt{\pi}}\right)^{2/3}$.

$$\Rightarrow \bar{H}_{2\,min} = \frac{3}{2}\left(\frac{k^2}{2\pi m}\right)^{\frac{1}{3}} \simeq 0{,}813 \cdot \left(\frac{k^2}{m}\right)^{\frac{1}{3}}.$$

Q2: The second value is better because it is lower, and the variational approach always gives an upper bound.