TFY 4250 / FY 2045

QUM 1

Final Exam 2014

– Solutions –

1) a) Adding a_+ and a_-, we obtain

$$a_+ + a_- = \frac{1}{\sqrt{2}}\, 2 \left(\frac{m\omega}{\hbar}\right)^{1/2} x = \left(\frac{2m\omega}{\hbar}\right)^{1/2} x$$

$$\Rightarrow \boxed{x = \left(\frac{\hbar}{2m\omega}\right)^{1/2} (a_+ + a_-)}$$

b) We compute the expectation value as follows:

$$\langle 0 | x^4 | 0 \rangle = \frac{\hbar^2}{4m^2\omega^2} \langle 0 | (a_+ + a_-)^4 | 0 \rangle$$

$$= \frac{\hbar^2}{4m^2\omega^2} \langle 0 | a_+^4 + a_+^3 a_- + a_+^2 a_- a_+ + a_+^2 a_-^2 + a_+ a_- a_+^2 + a_+ a_- a_+ a_- + a_+ a_-^2 a_+ + a_+ a_-^3 + a_- a_+^3 + a_- a_+^2 a_- + a_- a_+ a_- a_+ + a_- a_+ a_-^2 + a_-^2 a_+^2 + a_-^2 a_+ a_- + a_-^3 a_+ + a_-^4 | 0 \rangle$$

Now, we use $a_- |0\rangle = 0$ and $\langle 0 | a_+ = \langle 0 | a_-^\dagger = \langle a_- 0 | = 0$:

$$\rightsquigarrow \langle 0 | x^4 | 0 \rangle = \frac{\hbar^2}{4m^2\omega^2} \langle 0 | a_- a_+^3 + a_- a_+ a_- a_+ + a_-^2 a_+^2 + a_-^3 a_+ | 0 \rangle$$

Next, we use $\langle 0 | a_- a_+^3 | 0 \rangle = 0$ and $\langle 0 | a_-^3 a_+ | 0 \rangle = 0$, see hint.

$$\Rightarrow \langle 0 | x^4 | 0 \rangle = \frac{\hbar^2}{4m^2\omega^2} \langle 0 | a_- a_+ a_- a_+ + a_-^2 a_+^2 | 0 \rangle$$

$$= \frac{\hbar^2}{4m^2\omega^2} \left[\langle 0 | a_- a_+ a_- a_+ | 0 \rangle + \langle 0 | a_-^2 a_+^2 | 0 \rangle \right]$$

see hint

$$= \frac{\hbar^2}{4m^2\omega^2} \left[\langle 0 | 0 \rangle + 2 \langle 0 | 0 \rangle \right]$$

$$= \frac{3\hbar^2}{4m^2\omega^2}.$$

Answer: $\boxed{\langle 0 | x^4 | 0 \rangle = \frac{3\hbar^2}{4m^2\omega^2}}$

2) a) i) For symmetry reasons, the probability p_x^{up} must be $p_x^{up} = 1/2$.

ii) ——— " ———, $\langle S_x \rangle$ must be $\langle S_x \rangle = 0$.

iii) After the measurement of the spin relative to the x-axis, it is either in the spin up or in the spin down state relative to the x-axis. Again for symmetry reasons, a subsequent measurement of the spin relative to the z-axis must yield $p_z^{up} = 1/2$.

<u>Note</u>: By "symmetry", we mean that space is assumed to be isotropic.

b) Let us denote

$\uparrow_z = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $\downarrow_z = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ as the spin eigenvectors of S_z, and $\uparrow_x = \begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix}$ and $\downarrow_x = \begin{pmatrix} 1/\sqrt{2} \\ -1/\sqrt{2} \end{pmatrix}$ as the spin eigenvectors of S_x. The latter can be seen easily by inspection. Then, we find:

i) $$p_x^{up} = \left[\begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} \cdot \begin{pmatrix} 1 \\ 0 \end{pmatrix}\right]^2 = \left(\frac{1}{\sqrt{2}}\right)^2 = \frac{1}{2}$$

ii) $$\langle S_x \rangle = \begin{pmatrix} 1 & 0 \end{pmatrix} S_x \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \end{pmatrix} \left[\frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\right] \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$
$$= 0$$

iii) Either
$$p_z^{up} = \left[\begin{pmatrix} 1 & 0 \end{pmatrix} \begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix}\right]^2 = \frac{1}{2}$$
or
$$p_z^{up} = \left[\begin{pmatrix} 1 & 0 \end{pmatrix} \begin{pmatrix} 1/\sqrt{2} \\ -1/\sqrt{2} \end{pmatrix}\right]^2 = \frac{1}{2}.$$
The answer is the same.

3) a) We write for the particle density ρ:

$$\rho = \frac{N}{V} = \frac{1}{2\pi^2}\int_0^\infty \frac{k^2}{e^{[\hbar^2k^2/2m-\mu]/k_BT}-1}\,dk\,, \qquad \underline{\mu=0.}$$

Now, we make the following substitutions:

$$x = \frac{\hbar^2k^2}{2mk_BT} \rightsquigarrow k = \frac{\sqrt{2mk_BT}}{\hbar}\sqrt{x}$$

$$\rightsquigarrow dk = \frac{\sqrt{2mk_BT}}{2\hbar}\frac{1}{\sqrt{x}}\,dx$$

This yields

$$\rho = \frac{1}{2\pi^2}\left(\frac{2mk_BT}{\hbar^2}\right)^{3/2}\frac{1}{2}\int_0^\infty \frac{\sqrt{x}}{e^x-1}\,dx$$

$$= \frac{1}{4\pi^2}\left(\frac{2mk_BT}{\hbar^2}\right)^{3/2}\underbrace{\int_0^\infty \frac{x^{\frac{3}{2}-1}}{e^x-1}\,dx}$$

$$\Rightarrow \boxed{\rho = \frac{1}{4\pi^2}\left(\frac{2mk_BT}{\hbar^2}\right)^{3/2}\cdot\Gamma\left(\tfrac{3}{2}\right)\cdot\zeta\left(\tfrac{3}{2}\right)}$$

$$\left(= \frac{1}{4\pi^2}\left(\frac{2mk_BT}{\hbar^2}\right)^{3/2}\cdot\frac{\sqrt{\pi}}{2}\cdot 2.612\right)$$

$$\left(= 2.612\cdot\left(\frac{mk_BT}{2\pi\hbar^2}\right)^{3/2}\right)$$

b) Solving the above expression for $T=T_c$ gives:

$$T_c = \frac{\hbar^2}{2mk_B}\cdot\left(\frac{4\pi^2\rho}{\Gamma(\frac{3}{2})\cdot\zeta(\frac{3}{2})}\right)^{2/3} \Rightarrow \boxed{T_c \sim \rho^{2/3}}$$

$$\left(T_c = \frac{2\pi\hbar^2}{mk_B}\cdot\left(\frac{\rho}{2.612}\right)^{2/3}\right)$$

4) a) The condition $V(x) = \infty$ for $x \leq 0$ requires that $\psi(0) = 0$. This means that for $x \geq 0$, the wave functions are simply described by those of the 1-D harmonic oscillator and $\psi(0) = 0$. Hence, the eigenfunctions are the "odd" $(n = 1, 3, 5, \ldots)$ eigenfunctions of the 1-D harmonic oscillator and the ground state $(n=1)$ gives

$$E_0 = \left(n + \tfrac{1}{2}\right)\hbar\omega = \tfrac{3}{2}\hbar\omega.$$

b) The expectation value of the energy is given by

$$\langle H \rangle = \frac{\langle \varphi | H | \varphi \rangle}{\langle \varphi | \varphi \rangle}.$$ In what follows, the constant c will cancel out. We find

$$\langle H \rangle = \frac{\int_0^\infty dx\, x e^{-\alpha x}\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2\right) x e^{-\alpha x}}{\int_0^\infty dx\, x^2 e^{-2\alpha x}}$$

In the first integral, we need to compute

$$\frac{d^2}{dx^2}\left(x e^{-\alpha x}\right) = \left(-2\alpha + \alpha^2 x\right) e^{-\alpha x}$$

$$\Rightarrow \langle H \rangle = \frac{\int_0^\infty dx\, e^{-2\alpha x}\left[\frac{\hbar^2}{2m}\left(2\alpha x - \alpha^2 x^2\right) + \frac{1}{2}m\omega^2 x^4\right)}{\int_0^\infty dx\, x^2 e^{-2\alpha x}}$$

The integrals are of the form

$$\int_0^\infty dx\, x^n e^{-2\alpha x}.$$

They can be solved by use of a formula collection, integration by parts or parametric differentiation.

We obtain

$$\langle H \rangle = \frac{\frac{\hbar^2}{2m}\left(2\alpha \frac{1!}{(2\alpha)^2} - \alpha^2 \frac{2!}{(2\alpha)^3}\right) + \frac{1}{2} m\omega^2 \frac{4!}{(2\alpha)^5}}{\frac{2!}{(2\alpha)^3}}$$

$$= \frac{\hbar^2}{2m}\alpha^2 + \frac{3}{2} m\omega^2 \frac{1}{\alpha^2} \qquad (*)$$

To find the minimum, we differentiate:

$$0 \stackrel{!}{=} \frac{d}{d\alpha}\langle H \rangle = \frac{\hbar^2}{m}\alpha - 3m\omega^2 \frac{1}{\alpha^3}$$

$$\Rightarrow \quad (\alpha^*)^4 = 3\frac{m^2\omega^2}{\hbar^2}$$

Substitution into (*) yields:

$$\langle H \rangle = \frac{\hbar^2}{2m}\sqrt{3}\frac{m\omega}{\hbar} + \frac{3}{2} m\omega^2 \frac{\hbar}{\sqrt{3}\, m\omega}$$

$$\Rightarrow \boxed{\langle H \rangle = \sqrt{3}\,\hbar\omega \approx 1{,}732\,\hbar\omega > 1.5\,\hbar\omega.}$$

$\boxed{\text{The approximation is reasonable but not great.}}$

5) ii) The Schrödinger equation (TE) reads

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\,\psi = E\psi .$$

Substituting $\psi(x) = A\cdot e^{\frac{i}{\hbar}S(x)}$, $A \neq 0$,

into it yields

$$\left(\psi' = A\frac{i}{\hbar}S' e^{i/\hbar\, S},\ \psi'' = \left(\frac{i}{\hbar}AS'' - \frac{A}{\hbar^2}(S')^2\right)e^{\frac{i}{\hbar}S}\right)$$

dash denotes derivative

$$\boxed{-\frac{i\hbar}{2m}S'' + \frac{1}{2m}(S')^2 + V(x) - E = 0} \quad (*)$$

iii) Next, we expand $S(x)$ in a power series and substitute it into $(*)$. We are only interested in order $\hbar^0$ and $\hbar^1$. Hence:

$$-\frac{i\hbar}{2m}\left(S_0'' + \hbar S_1''\right) + \frac{1}{2m}\left(S_0'^2 + 2\hbar S_0' S_1' + \hbar^2 S_1'^2\right) + V(x) - E = 0.$$

At each order, we find:

$$\hbar^0: \underbrace{\boxed{\frac{1}{2m}S_0'^2 + V(x) - E = 0}}_{(**)}, \qquad \hbar^1: \underbrace{\boxed{S_0' S_1' - \frac{i}{2}S_0'' = 0}}_{(***)}$$

iv) By inspection, we see that

$$S_0(x) = \pm\int^x p(x')\,dx'$$

and

$$S_1(x) = \frac{i}{2}\ln p(x)$$

are solutions.

$$(**): \frac{1}{2m}p^2(x) + V(x) - E = 0 \Rightarrow p(x) = \sqrt{2m(E - V(x))}. \ ✓$$

$$(***): p(x)\cdot\frac{i}{2}\frac{p'(x)}{p(x)} - \frac{i}{2}p'(x) = 0. \ ✓$$

Finally, we find the approximate wave function to be

$$\psi(x) = A \cdot e^{\frac{i}{\hbar} S(x)} = A \cdot e^{\frac{i}{\hbar}(S_0 + \hbar S_1)}$$

$$= A \cdot e^{\frac{i}{\hbar} S_0(x)} \cdot e^{i S_1(x)}$$

$$= A \cdot e^{\pm \frac{i}{\hbar} \int^x p(x')\,dx'} \cdot e^{-\frac{1}{2} \ln p(x)}$$

$$= A \cdot e^{\ln (p(x))^{-1/2}} \cdot e^{\pm \frac{i}{\hbar} \int^x p(x')\,dx'}$$

$$\Rightarrow \boxed{\psi(x) \simeq \frac{A}{\sqrt{p(x)}} \cdot e^{\pm \frac{i}{\hbar} \int^x p(x')\,dx'}}$$

6) i) To find ψ_{n-1}, we simply replace Δx by $-\Delta x$:

$$\boxed{\psi_{n-1} = \psi_n - \Delta x\, \psi_n' + \frac{(\Delta x)^2}{2}\psi_n'' - \frac{(\Delta x)^3}{6}\psi_n^{(3)} + \frac{(\Delta x)^4}{24}\psi_n^{(4)} - \frac{(\Delta x)^5}{120}\psi_n^{(5)}}$$

ii) Adding ψ_{n+1} and ψ_{n-1} gives

$$\boxed{\psi_{n+1} + \psi_{n-1} = 2\psi_n + (\Delta x)^2 \psi_n'' + \frac{(\Delta x)^4}{12}\psi_n^{(4)}} \quad (*)$$

iii) In $(*)$, we replace $\psi_n^{(4)}$ by

$$\psi_n^{(4)} = \frac{\psi_{n+1}'' + \psi_{n-1}'' - 2\psi_n''}{(\Delta x)^2}$$

and $\psi_n'' = -K_n\psi_n$ etc.

$$\rightsquigarrow \psi_n^{(4)} = \frac{-K_{n+1}\psi_{n+1} - K_{n-1}\psi_{n-1} + 2K_n\psi_n}{(\Delta x)^2}$$

Substitution into $(*)$ and rearranging yields the desired recursive equation for ψ_{n+1} in terms of ψ_n and ψ_{n-1}:

$$\psi_{n+1} + \psi_{n-1} = 2\psi_n + (\Delta x)^2(-K_n\psi_n) + \frac{(\Delta x)^2}{12}\left(-K_{n+1}\psi_{n+1} - K_{n-1}\psi_{n-1} + 2K_n\psi_n\right)$$

$$\Rightarrow \boxed{\left(1 + \frac{(\Delta x)^2}{12}K_{n+1}\right)\psi_{n+1} = \left(2 - \frac{5}{6}(\Delta x)^2 K_n\right)\psi_n - \left(1 + \frac{(\Delta x)^2}{12}K_{n-1}\right)\psi_{n-1}}$$

– end –