Problem Sheet 4
FYS3110

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The hamiltonian of particle with mass m in a one-dimensional oscillator potetial having a characteristic frequency ω is

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

The ladder operators for the harmonic oscillator potential are

$$\hat{a} = \frac{1}{\sqrt{2\hbar m\omega}}(m\omega\hat{X} + i\hat{P}) \qquad \text{(lowering operator)} \tag{2}$$

$$\hat{a}^\dagger = \frac{1}{\sqrt{2\hbar m\omega}}(m\omega\hat{X} - i\hat{P}) \qquad \text{(raising operator)} \tag{3}$$

Problem 4.1

a)

I want to find an expression for $\hat{X}$ in terms of $\hat{a}_{nm}$ and $\hat{a}^\dagger_{nm}$. This can be done by first rewriting equation 2

$$\begin{aligned}\hat{a} = \frac{1}{\sqrt{2\hbar m\omega}}(m\omega\hat{X} + i\hat{P}) &= \sqrt{\frac{m\omega}{2\hbar}}\hat{X} + \frac{i}{\sqrt{2\hbar m\omega}}\hat{P} \\ &\to \hat{X} = \sqrt{\frac{2\hbar}{m\omega}}\hat{a} - \sqrt{\frac{2\hbar}{m\omega}}\frac{i}{\sqrt{2\hbar m\omega}}\hat{P},\end{aligned}$$

and then equation 3

$$\begin{aligned}\hat{a}^\dagger = \frac{1}{\sqrt{2\hbar m\omega}}(m\omega\hat{X} - i\hat{P}) &= \sqrt{\frac{2\hbar}{m\omega}}\hat{X} + \frac{i}{2\hbar m\omega}\hat{P} \\ &\to \hat{P} = \frac{2\hbar m\omega}{i}\sqrt{\frac{m\omega}{2\hbar}}\hat{X} - \frac{2\hbar m\omega}{i}\hat{a}^\dagger.\end{aligned}$$

Now putting the latter equation into the former yields

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

which simplifies to

$$
\hat{X} = \sqrt{\frac{\hbar}{2m\omega}}(\hat{a} + \hat{a}^\dagger) \tag{4}
$$

It will be necessary to know what $[\hat{a}, \hat{H}]$ is. This is easiest to compute if one knows how $\hat{a}$ and $\hat{a}^\dagger$ is related to $\hat{H}$. By looking at the expressions for $\hat{a}$ and $\hat{a}^\dagger$ one is tempted to compute the following

$$
\hat{a}\hat{a}^\dagger = \frac{m\omega}{2\hbar}\hat{X}^2 + \frac{1}{2m\omega\hbar}\hat{P}^2 + \frac{i}{2\hbar}[\hat{X}, \hat{P}],
$$

where $[X, P] = i\hbar$, which follows from $\hat{X} \to x$ and $\hat{P} \to i\hbar(d/dx)$, but is independent of basis. So we see that

$$
\hat{H} = \hbar\omega(\hat{a}\hat{a}^\dagger + \frac{1}{2}), \tag{5}
$$

or alternatively that $\hat{a}\hat{a}^\dagger = \frac{\hat{H}}{\hbar\omega} - \frac{1}{2}$. This combined ladder operator can be referred to by a new name $\hat{a}\hat{a}^\dagger = \hat{N}$, so that equation 5 becomes

$$
\hat{H} = \hbar\omega(\hat{N} + \frac{1}{2}), \tag{6}
$$

Thus, we have the energy eigenbasis which satisfy

$$
\hat{H}\left|n\right\rangle = \hbar\omega(n - \frac{1}{2})\left|n\right\rangle, \text{ for } i \in 0, 1, 2 \ldots \tag{7}
$$

We now get

$$
\hat{a}\left|n\right\rangle = C_n\left|n\right\rangle, \tag{8}
$$

where C_n is a constant which can be found the following way

$$
\begin{aligned}
\left\langle n\right| \hat{a}^\dagger\hat{a}\left|n\right\rangle =& \left|C_n\right|^2 \left\langle n-1|n-1\right\rangle \\
\to& \left|C_n\right| = \sqrt{n} = C_n,
\end{aligned}
$$

by choosing the phase to be zero[1]. We land at

$$
\hat{a}\left|n\right\rangle = \sqrt{n}\left|n-1\right\rangle \tag{9}
$$

Similarly for $\hat{a}^\dagger$

$$
\hat{a}^\dagger\left|n\right\rangle = D_n\left|n+1\right\rangle \tag{10}
$$

[1] Actually, $C_n = \sqrt{n}e^{i\phi}$ where ϕ is arbitrary, but is is conventional to set $\phi = 0$.

$$\begin{aligned}\langle n|\,\hat{a}\hat{a}^\dagger\,|n\rangle =& |D_n|^2\,\langle n+1|n+1\rangle \\ \rightarrow& |D_n| = \sqrt{n+1} = D_n\end{aligned}$$

$$\hat{a}^\dagger\,|n\rangle = \sqrt{n+1}\,|n+1\rangle \tag{11}$$

Now to compute the matrix elements for $\hat{a}$ and $\hat{a}^\dagger$

$$\langle m|\,\hat{a}\,|n\rangle = \sqrt{n}\,\langle m|n-1\rangle = \sqrt{n}\delta_{m,n-1} \tag{12}$$

$$\langle m|\,\hat{a}^\dagger\,|n\rangle = \sqrt{n-1}\,\langle m|n+1\rangle = \sqrt{n-1}\delta_{m,n+1}. \tag{13}$$

The actual matrices for these particular operators will look something like this[2]

$$a \leftrightarrow \begin{bmatrix} 0 & \sqrt{1} & 0 & 0 & \dots \\ 0 & 0 & \sqrt{2} & 0 & \\ 0 & 0 & 0 & \sqrt{3} & \\ \vdots & & & & \ddots \end{bmatrix} \tag{14}$$

$$a^\dagger \leftrightarrow \begin{bmatrix} 0 & 0 & 0 & \dots \\ \sqrt{1} & 0 & 0 & \\ 0 & \sqrt{2} & 0 & \\ 0 & 0 & \sqrt{3} & \\ \vdots & & & \ddots \end{bmatrix}. \tag{15}$$

Finding the matrix representation of $\hat{X}$ is now an easy matter of employing equation 4

$$X \leftrightarrow \sqrt{\frac{\hbar}{2m\omega}} \begin{bmatrix} 0 & \sqrt{1} & 0 & 0 & \dots \\ \sqrt{1} & 0 & \sqrt{2} & 0 & \\ 0 & \sqrt{2} & 0 & \sqrt{3} & \\ 0 & 0 & \sqrt{3} & 0 & \\ \vdots & & & & \ddots \end{bmatrix}, \tag{16}$$

while an algebraic expression will be (also employing equation 4)

$$\begin{aligned}\langle m|\,X\,|n\rangle &= \sqrt{\frac{\hbar}{2m\omega}}(\sqrt{n+1}\,\langle m|n+1\rangle + \sqrt{n}\,\langle m|n-1\rangle) \\ &= \sqrt{\frac{\hbar}{2m\omega}}(\sqrt{n+1}\delta_{m,n+1} - \sqrt{n}\delta_{m,n-1}).\end{aligned} \tag{17}$$

[2] I am perfectly aware that $\sqrt{1} = 1$ but I will keep the root symbol here in order to underline the symmetry.

b)

Let $|\psi(0)\rangle = \sum_{x=0}^{n} c_n |n\rangle$. It follows that

$$\begin{aligned}\langle\psi(0)|\psi(0)\rangle &= \sum_n |c_n|^2 \langle n|n\rangle + 2\sum_{n\neq n'} c_n c_{n'} \langle n|n'\rangle \\ &= \sum_n |c_n|^2 \delta_{n,n} + 2\sum_{n\neq n'} c_n c_{n'} \delta_{n,n'},\end{aligned}$$

where the first Kronecker delta will always be 1 and the second Kronecker delta will always be 0. The condition on the c_n's for $|\psi(0)\rangle$ to have unit norm is therefore

$$\sum_n |c_n|^2 = 1 \tag{18}$$

Letting the lowering operator work on the ground state outputs the ground state energy, $\hat{a}|0\rangle = 0$, here arbitrarily set to zero. Letting, $|0\rangle \mapsto \psi_0(x)$ and $\hat{a} \mapsto \frac{1}{\sqrt{2\hbar m\omega}}(m\omega\hat{X} + i\hat{P})$, one can expand upon this idea to find an expression for the ground state

$$\begin{aligned}\hat{a}|0\rangle &= \frac{1}{\sqrt{2\hbar m\omega}}(m\omega\hat{X} + i\hat{P})\psi_0(x) = \frac{1}{\sqrt{2\hbar m\omega}}(m\omega x + i\frac{\hbar}{i}\frac{d}{dx})\psi_0(x) = 0 \\ &\to \left(m\omega x + \hbar\frac{d}{dx}\right)\psi_0(x) = 0 \to \frac{d}{dx} = -\frac{m\omega x}{\hbar}\psi_0(x) \\ &\to \frac{d\psi_0(x)}{\psi_0} = -\frac{m\omega x}{\hbar}dx \to \psi_0(x) = C_0 e^{-m\omega x^2/2\hbar}\end{aligned}$$

Normalizing, denoting $\alpha = \frac{m\omega}{\hbar}$

$$\langle\psi_0(x)|\psi_0(x)\rangle = |C_0|^2 \int_{-\infty}^{\infty} e^{-\alpha x^2} dx = |C_0|^2 \sqrt{\frac{\pi}{\alpha}} = 1,$$

which gives

$$C_0 = \left(\frac{\pi\hbar}{m\omega}\right)^{\frac{1}{4}} \tag{19}$$

The full wave equation, $\Psi(x, y)$, is a product of two parts, the time-independent equation, $\psi(x)$, and the time-dependent equation $\phi(t) = ce^{-i\ E_n t/\hbar}$

$$\Psi(x, t) = \sum_{n=1}^{\infty} c_n \psi_n(x) e^{i\ E_n t/\hbar} \tag{20}$$

Alternatively, one can express the wave function with Dirac notation using $\psi_n = \langle x|n\rangle$

$$\psi_1(x) = \langle x| \hat{a}^\dagger |0\rangle \tag{21}$$

For a general expression one needs some general function for the eigenstates $|n\rangle$. These can be expressed as in terms of the ground state $|0\rangle$

$$\hat{a}^\dagger |n\rangle = \sqrt{n+1}\,|n+1\rangle \to |n\rangle = \frac{\hat{a}^\dagger}{\sqrt{n}}|n-1\rangle = \frac{(\hat{a}^\dagger)^2}{\sqrt{n(n-1)}}|n-1\rangle \ldots$$

thus giving the expression

$$|n\rangle = \frac{(\hat{a}^\dagger)^n}{\sqrt{n!}} |0\rangle \tag{22}$$

All the ingredients are there to write down the complete time-dependent wave function

$$\Psi_n(x,t) = \langle x| \phi_n(t) |n\rangle = \langle x| e^{-\frac{iE_n}{\hbar}t} \frac{(\hat{a}^\dagger)^n}{\sqrt{n!}} |0\rangle \tag{23}$$

c)

When computing the expected values of a harmonic oscillator Schrödinger wave function the time-dependency parts will equate to one, given normality.

$$\psi * (t)\psi(t) = e^{\frac{iE_n t}{\hbar}} e^{-\frac{iE_n t}{\hbar}} = e^0 = 1$$

Now the computation of the expected values are fairly straight-forward

$$\begin{aligned}
\left\langle \hat{X} \right\rangle_{nm} &= \langle \psi_n| \hat{X} |\psi_m\rangle = \sqrt{\frac{\hbar}{2m\omega}} \langle \psi_n| (\hat{a} + \hat{a}^\dagger) |\psi_m\rangle \\
&= \sqrt{\frac{\hbar}{2m\omega}} (\langle \psi_n| \sqrt{m} |\psi_{m-1}\rangle + \langle \psi_n| \sqrt{m+1} |\psi_{m+1}\rangle) \\
&= \sqrt{\frac{\hbar}{2m\omega}} (\sqrt{m} \langle \psi_n|\psi_{m-1}\rangle + \sqrt{m+1} \langle \psi_n|\psi_{m+1}\rangle) \\
&= \sqrt{\frac{\hbar}{2m\omega}} (\sqrt{m}\delta_{n,m-1} + \sqrt{m+1}\delta_{n,m+1}) = \begin{cases} \sqrt{\frac{\hbar(m+1)}{2m\omega}}, & n = m+1 \\ \sqrt{\frac{\hbar m}{2m\omega}}, & n = m-1 \\ 0, & \text{otherwise} \end{cases}
\end{aligned}$$

which has a similar symmetry to the matrix elements in equations 16 and 17. In fact, it is the exact same thing.

$$\begin{aligned}
\left\langle \hat{H} \right\rangle_{nm} &= \langle \psi_n| \hat{H} |\psi_m\rangle = \langle \psi_n| \hbar\omega \left(\hat{a}\hat{a}^\dagger + \frac{1}{2} \right) |\psi_m\rangle \\
&= \hbar\omega \langle \psi_n| \hat{a}\hat{a}^\dagger |\psi_m\rangle + \frac{\hbar\omega}{2} \langle \psi_n|\psi_m\rangle \\
&= \hbar\omega m \langle \psi_n|\psi_m\rangle + \frac{\hbar\omega}{2} \langle \psi_n|\psi_m\rangle = \hbar\omega \left(m + \frac{1}{2} \right) \delta_{n,m}
\end{aligned}$$

4.2

In three dimensions the Schrödinger equation for the harmonic oscillator using cartesian coordinates is

$$-\frac{\hbar}{2m} \nabla^2\psi + \frac{1}{2}(x^2 + y^2 + z^2)\psi = E\psi \tag{24}$$