CHEM 3410: PSET II Helpful Content

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Raising and Lowering Operators

Raising and lowering operators are incredibly useful for solving questions pertaining to the Harmonic Oscillator. Particularly, expectation value questions since they leverage the orthonormality of the eigenfunctions:

$$\int_{-\infty}^{\infty} dx \psi_m(x)\psi_n(x) = \delta_{nm}$$

That is, the integral is 1 if the states (i.e. the indices) match and 0 if they don't.

$$a\psi_n = \sqrt{n}\,\psi_{n-1} \tag{0.0.1}$$

$$a^\dagger\psi_n = \sqrt{n+1}\,\psi_{n+1} \tag{0.0.2}$$

Why are these relationships useful? The eigenfunctions are orthonormal! I'll list a few more useful relationships before giving an example. These are contingent on the definition from class for alpha: $\alpha = \sqrt{\frac{m\omega}{\hbar}}$

$$aa^\dagger - a^\dagger a = 1 \tag{0.0.3}$$

$$x = \frac{a + a^\dagger}{\alpha\sqrt{2}} \tag{0.0.4}$$

$$\frac{d}{dx} = \frac{\alpha(a - a^{\dagger)}}{\sqrt{2}} \tag{0.0.5}$$

$$a^\dagger a\,\psi_n = n\,\psi_n \longrightarrow a^\dagger a = n$$

To explicitly work the above relationship out:

$$a^\dagger \underbrace{a\,\psi_n}_{1st} = a^\dagger\,\sqrt{n}\psi_{n-1}$$

The index associated with ψ is now n-1, so $a^\dagger$ operating on it has the following result:

$$a^\dagger\,\sqrt{n}\psi_{n-1} = \sqrt{n}\sqrt{n}\psi_n = n\,\psi_n$$

Now, here's an example that you've already seen in class, but it will be useful to revisit:

$$\langle x\rangle = \int_{-\infty}^{\infty} dx\,\psi_n^*(x)\,x\,\psi_n(x)$$

we can re-write this using Eqn 0.0.4 as follows:

$$\langle x\rangle = \int_{-\infty}^{\infty} dx\,\psi_n^*(x)\,\frac{(a + a^\dagger)}{\alpha\sqrt{2}}\,\psi_n(x)$$

recall that operators act on whatever lies to the right of them:

$$\langle x\rangle = \frac{1}{\alpha\sqrt{2}}\int_{-\infty}^{\infty} dx\,\psi_n^*(x)\,\left(a\,[\,\psi_n(x)] + a^\dagger\,[\,\psi_n(x)]\right)$$

$$\langle x \rangle = \frac{1}{\alpha\sqrt{2}} \int_{-\infty}^{\infty} dx\, \psi_n^*(x)\, \left(\sqrt{n}\,\psi_{n-1}(x) + \sqrt{n+1}\,\psi_{n+1}(x)\right)$$

$$\langle x \rangle = \frac{1}{\alpha\sqrt{2}} \int_{-\infty}^{\infty} dx\, \psi_n^*(x)\, \sqrt{n}\,\psi_{n-1}(x) + \psi_n^*(x)\sqrt{n+1}\,\psi_{n+1}(x)$$

separate the two integrals and factor out terms with no n-dependence

$$\langle x \rangle = \frac{\sqrt{n}}{\alpha\sqrt{2}} \int_{-\infty}^{\infty} dx\, \psi_n^*(x)\, \psi_{n-1}(x) \;+\; \frac{\sqrt{n+1}}{\alpha\sqrt{2}} \int_{-\infty}^{\infty} dx \psi_n^*(x)\, \psi_{n+1}(x)$$

Since the indices here don't match (i.e. $n \neq n-1, n+1$ the wavefunctions will be orthogonal to one another. This means that the integrals will both evaluate to 0. Had the indices matched, we use the fact of normality $\left(|\psi|^2 = 1\right)$ which would have left us with

$$\frac{\sqrt{n}}{\alpha\sqrt{2}} + \frac{\sqrt{n+1}}{\alpha\sqrt{2}}$$

The indices, however, don't match so we're left with

$$\langle x \rangle = 0$$

for all n.

Frankly, the raising and lowering operators are tiresome for $\langle x^4 \rangle$, so I would recommend using the following things:

$$\psi_0(x) = \left(\frac{\alpha}{\sqrt{\pi}}\right)^{1/2} e^{\frac{-\alpha^2 x^2}{2}} \tag{0.0.6}$$

$$\psi_1(x) = \left(\frac{\alpha}{2\sqrt{\pi}}\right)^{1/2} 2\alpha x\, e^{\frac{-\alpha^2 x^2}{2}} \tag{0.0.7}$$

The following pattern will prove useful:

$$\int_0^{\infty} x^n e^{-ax^2}\, dx = \frac{(n-1)\cdot(n-3)\cdot \ldots \cdot 3 \cdot 1}{2^{\left(\frac{n}{2}+1\right)} a^{\frac{n}{2}}} \sqrt{\frac{\pi}{a}}$$

For $\langle x^4 \rangle$:

$$\langle x^4 \rangle_{\psi_0} = \int_{-\infty}^{\infty} \psi_0^*(x)\, x^4\, \psi_0(x)\, dx$$

Substitute in 0.0.6, simplify, and factor out constants:

$$\langle x^4 \rangle_{\psi_0} = \frac{\alpha}{\sqrt{\pi}} \int_{-\infty}^{\infty} x^4\, e^{-a^2 x^2}\, dx$$

Lastly, change the bounds so they match the pattern by multiplying the integral by 2:

$$\langle x^4 \rangle_{\psi_0} = \frac{2\alpha}{\sqrt{\pi}} \int_{0}^{\infty} x^4\, e^{-a^2 x^2}\, dx$$

Here, n = 4 and a is α^2 which leaves us with the following:

$$\langle x^4 \rangle_{\psi_0} = \frac{2\alpha}{\sqrt{\pi}} \frac{(4-1)\cdot(4-3)}{2^{\left(\frac{4}{2}+1\right)} \alpha 2^{\frac{4}{2}}} \sqrt{\frac{\pi}{\alpha^2}}$$

Simplify:

$$\frac{2\alpha}{\sqrt{\pi}} \cdot \frac{3}{2^3 \alpha^4} \cdot \frac{\sqrt{\pi}}{\alpha} = \frac{3}{4\alpha^4}$$