4. Quantum exercise - Solution

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7. Daily commutator gymnastics

We use the following formulas to calculate x,x^2,x^3 and x^4 and the correspondent expectation values for the harmonic oscillator.

$a = \frac{1}{\sqrt{2}}(\frac{X}{x_0} + x_0 \frac{\partial}{\partial X})$, $a^\dagger = \frac{1}{\sqrt{2}}(\frac{X}{x_0} - x_0 \frac{\partial}{\partial X})$

$[a, a^\dagger]$=1, $[N, a]$=-a, $[N, a^\dagger]$=a†

Happy calculation leads to

$X = \frac{x_0}{\sqrt{2}}(a + a^\dagger)$

$X^2 = \frac{x_0^2}{2}((a)^2 + (a^\dagger)^2 + 2N + 1)$

$X^3 = \frac{x_0^3}{2^{3/2}}((a)^3 + (a^\dagger)^3 + 3aN + 3Na^\dagger)$

$X^4 = \frac{x_0^4}{4}((a^\dagger)^4 + (a)^4 + N(N-1) + (N+1)(N+2) + 4N + 4N^2 + 2(a^\dagger)^2 N + 2(a)^2 N + 2N(a^\dagger)^2 + 2N(a)^2 + 1)$

and finally the expectation values

$< X >= 0$

$< X^2 >= x_0^2(n + \frac{1}{2})$

$< X^3 >= 0$

$< X^4 >= \frac{3x_0^4}{2}(n^2 + n + \frac{1}{2})$

8. Lennard-Jones Potential

8a)

The Lennard-Jones Potential is defined as following:

$V(R) = V_0[(\frac{R_0}{R})^{12} - 2(\frac{R_0}{R})^6]$

Expansion around R_0 (to 3^{rd} order) leads to

$V(R) \approx -V_0 + \frac{1}{2}(R - R_0)^2 V_0 \frac{72}{R_0^2} - \frac{1}{6}(R - R_0)^3 V_0 \frac{1512}{R_0^3}$

In order to get Schrödinger's equation for the relative coordinate, one has to make a transformation to center of mass system (or to please our group members: CMS) and make a separation Ansatz for the CM and relative coordinate.

$R_{CM} = \frac{r_1+r_2}{2}$
$R = r_1 - r_2$

This leads to the following Schrödinger equation for the relative coordinate:

$(-\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial_R^2} + \frac{1}{2}(R - R_0)^2 \frac{72V_0}{R_0^2})\psi(R) = \epsilon\psi(R)$
where $\mu = \frac{m}{2}$ is the reduced mass and $\epsilon = E + V_0$

With $X = (R - R_0)$ and
$\omega^2 = \frac{72V_0}{\mu R_0^2}$
one arrives at the standard form for the harmonic oscillator

$(-\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial_X^2} + \frac{1}{2}\omega^2\mu X^2)\psi(R) = \epsilon\psi(R)$
with the known solution for the energy (already expressed with E instead of ϵ):

$E_n = -V_0 + \hbar\omega(n + \frac{1}{2})$

8b)

since this part is in some sense open for creative (but of course plausible) answers, I will only sketch here one possible way. In order to give the students a reason for why they should calculate x^3 and x^4 in Problem Set 7, one can calculate $< H >$ with the Potential expanded to 4th order and compare the $< x^2 >$ and $< x^4 >$ term in terms of the harmonic oscillator operators. There, the $< x^4 >$ term should be sufficiently

smaller than the $< x^2 >$ term.
Of course, this method in some sense is not really good, since we're still in the harmonic oscillator approximation. A more rigorous way would be of course perturbation theory for the $(R - R_0)^3$ term of the potential, where the matrix element for X^3 does not vanish in 2nd order perturbation theory.