PHY 341 HW Ch.2c

Do problems 2.18, 2.19*, 2.23; plus the following (* = optional bonus):

q2-8
Reduce the following commutators for the SHO to their simplest forms:
(a) $[a_-, a_- a_+]$
(b) $[a_+, a_- a_+]$
(c) $[x, \hat{H}]$
(d) $[p, \hat{H}]$

q2-9
Find the energies and wave functions of the half SHO potential
$V(x) = \begin{cases} \infty, & \text{if } x \le 0, \\ \frac{1}{2}m\omega^2 x^2, & \text{if } x > 0. \end{cases}$
Hint: Do it the eeezeee way by picking from the full SHO solutions those that happen to also satisfy the half-space boundary conditions, $\psi(0) = \psi(\infty) = 0$.

q2-10
The initial wave packet is given by a Gaussian $\Psi(x, 0) = A\exp(-ax^2)$. (a) Find the normalization constant A. (b) Find the momentum wave function $\phi(k)$. (c) Estimate Δx and $\Delta p = \hbar\Delta k$, and show $\Delta x \Delta p \ge \hbar/2$.

q2-11
The wave function of a particle is given by $\psi(x) = A\exp(-\alpha|x|)$. Let $\phi(p)$ be the wave function in momentum space, and Δp a measure of the "spread" of $\phi(p)$. As α is doubled, Δp will approximately
(A) double because $\Delta p \propto \alpha$
(B) stay the same because α is irrelevant to Δp
(C) be halved because $\Delta p \propto 1/\alpha$
(D) increase by four-fold because $\Delta p \propto \alpha^2$
(E) decrease by 1/4 because $\Delta p \propto 1/\alpha^2$

Useful integral (or just use sympy):
Let $I = \int_{-\infty}^{\infty} e^{-ax^2+bx}\,dx$. Make a variable substitution, $x = y + \frac{b}{2a}$, then

$$I = e^{b^2/4a} \int_{-\infty}^{\infty} e^{-ay^2}\,dy = \sqrt{\frac{\pi}{a}}\, e^{b^2/4a}$$

q2-12* Computational/recreational quantum mechanics.
In atomic units, the constants $m = \hbar = \omega = 1$, and the Schrödinger equation for the SHO may be written as

$$\psi''(x) = (x^2 - 2E)\psi(x). \quad (1)$$

Divide the space $[a, b]$ into a grid of size h, such that $x_j = a + jh$, $j = 0, 1, ..., N$, for some large N (so $h \sim 0.01$). Let $\psi(x_j) = \psi_j$. The ψ'' can be approximated by

$$\psi_j'' \simeq \frac{\psi_{j+1} - 2\psi_j + \psi_{j-1}}{h^2}. \tag{2}$$

Substituting ψ_j'' into Eq. (1) and rearranging a bit, we obtain the discretized Schrödinger equation

$$\psi_{j+1} = [2 + (x_j^2 - 2E)h^2]\psi_j - \psi_{j-1}. \tag{3}$$

Eq. (3) is a three-term recursion relation: knowing two seed values ψ_0 and ψ_1, we can obtain ψ_2, ψ_3, and so on. This way we obtain the numerical solutions. Of course, for the solution to be correct, it must vanish at infinity. And this does not happen for any E.

(a) Find the ground state energy of SHO by the shooting method using your favorite computing software. Let $h = 0.01$, and start from $x_0 = -5$, $\psi_0 = 0$, and $x_1 = -4.99$, $\psi_1 = 0.1$. First choose $E = 0.49$, and iterate Eq. (3) until $x = 5$. Plot ψ_j vs x_j. Note which way the wave function bends. Next, repeat the iteration but with $E = 0.51$. Again plot the wave function and note how it bends the other way.
Keep narrowing the energy range, and see how far out you can push the zero point of the wave function before it eventually blows up. What is the best energy you can find?

(b) Repeat the procedure for the first excited state.