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Soluton to final exam
FY2045 Quantum Mechanics I

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Problem 1 Multiple choice problems

a) The rule for addition two angular momenta with quantum numbers j_1 and j_2 is that the total angular momentum quantum number j can take the values

$$j = j_1 + j_2, j_1 + j_2 - 1, \ldots, |j_1 - j_2|.$$

With $j_1 = 5$ and $j_2 = 2$, we therefore get

$$j = 3, 4, 5, 6, 7.$$

Hence, alternative **C** is the correct answer.

b) Alternative **A** and **D** are eigenspinors of S_z, and therefore cannot be the eigenspinors of S_x. We check the remaining three options:

$$\frac{1}{\sqrt{2}}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\begin{pmatrix}1\\ \pm 1\end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix}\pm 1\\ 1\end{pmatrix} = \pm\frac{1}{\sqrt{2}}\begin{pmatrix}1\\ \pm 1\end{pmatrix},$$
$$\frac{1}{\sqrt{2}}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\begin{pmatrix}1\\ -i\end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix}-i\\ 1\end{pmatrix} = -\frac{i}{\sqrt{2}}\begin{pmatrix}1\\ i\end{pmatrix}.$$

We see that the spinor $\frac{1}{\sqrt{2}}\begin{pmatrix}1\\ 1\end{pmatrix}$ is the only eigenspinor of σ_x with eigenvalue $+1$, and is therefore an eigenspinor of S_x with eigenvalue $+\frac{\hbar}{2}$, meaning that alternative **E** is the correct answer.

c) The probability of measuring $+\hbar/2$ along the x direction for a given state χ is

$$P_{x+} = |\chi_{x+}^\dagger \chi|^2,$$

where

$$\chi_{x+} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix},$$

the eigenvector found in **c)**. Calculating the amplitudes for the different options, we get

$$\begin{aligned}
\mathbf{A} \quad & P_{x+} = \frac{1}{2} \left| \begin{pmatrix} 1 & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \right|^2 = 0.5 \\
\mathbf{B} \quad & P_{x+} = \frac{1}{10} \left| \begin{pmatrix} 1 & 1 \end{pmatrix} \begin{pmatrix} 2 \\ 1 \end{pmatrix} \right|^2 = \frac{3^2}{10} = 0.9 \\
\mathbf{C} \quad & P_{x+} = \frac{1}{10} \left| \begin{pmatrix} 1 & 1 \end{pmatrix} \begin{pmatrix} 2 \\ -i \end{pmatrix} \right|^2 = \frac{|2-i|^2}{10} = 0.5 \\
\mathbf{D} \quad & P_{x+} = \frac{1}{20} \left| \begin{pmatrix} 1 & 1 \end{pmatrix} \begin{pmatrix} 3 \\ 1 \end{pmatrix} \right|^2 = \frac{4^2}{20} = 0.8 \\
\mathbf{E} \quad & P_{x+} = \frac{1}{4} \left| \begin{pmatrix} 1 & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \right|^2 = 1.
\end{aligned}$$

Alternative **B** is the correct answer.

d) Since the Hamiltonian is diagonal, we directly read off the energy eigenvalues as $E_\pm = \pm\hbar\omega$, with corresponding eigenspinors

$$\chi_+ = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \chi_- = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

A general solution to the Schödinger equation is therefore $\chi = a_+\chi_+ e^{-E_+ t/\hbar} + a_-\chi_- e^{-iE_- t/\hbar}$. At $t = 0$, the given state can be written as a superposition of the two energy eigenstates with coefficients $a_\pm = 1/\sqrt{2}$, meaning that at times $t > 0$ we have

$$\chi(t) = \frac{1}{\sqrt{2}}\chi_+ e^{-iE_+ t/\hbar} + \frac{1}{\sqrt{2}}\chi_- e^{-iE_- t/\hbar} = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{-i\omega t} \\ e^{i\omega t} \end{pmatrix}. \tag{1}$$

Alternative **D** is the correct answer.

e) We consider each statement.

A: Even though the particle is in the eigenstate of S_x with eigenvalue $\hbar/2$ at $t = 0$, S_x and H do not commute, making the expectation value of S_x time-dependent. We will therefore not always measure $S_x = \hbar/2$. This is clear also from the answer in **e)**, where

the spin state is proportional to the eigenspinor of S_x with eigenvalue $+\hbar/2$ only at certain times. **Not true.**

B: We insert $t = \frac{\pi}{2\omega}$ into the time-dependent state found in **e)**, Eq. (1),

$$\chi\left(\frac{\pi}{2\omega}\right) = \frac{e^{-i\pi/2}}{\sqrt{2}}\begin{pmatrix}1\\ e^{i\pi}\end{pmatrix} = \frac{e^{-i\pi/2}}{\sqrt{2}}\begin{pmatrix}1\\ -1\end{pmatrix}, \tag{2}$$

which is not an eigenstate of S_y. **Not true.**

C: At certain times the state in Eq. (1) will be an eigenstate of S_y, e.g. at $t = \pi/4\omega$. If we measure at exactly these times, we will know the outcome of a measurement of the spin along the y direction. **Not true.**

D: Taking a second look at Eq. (2), we see that this actually is an eigenvector of S_x with eigenvalue $-\hbar/2$. If we measured S_x at exactly the given time, we would therefore be guaranteed to measure $S_x = -\hbar/2$. Hence this statement is **true**.

E: The energy eigenstates are simultaneous eigenstates of H and S_z, and a measurement of the energy would therefore also determine the component of the spin along z. Hence we do not lose all information about the spin state when measuring the energy. **Not true.**

Option **D** is the correct answer.

f) The momentum eigenstates are delta-function normalized,

$$\langle p_2|p_1\rangle = \delta(p_2 - p_1).$$

Hence, we get

$$\langle p_2|\hat{p}|p_1\rangle = p_1\langle p_2|p_1\rangle = p_1\delta(p_2 - p_1) = p_2\delta(p_2 - p_1),$$

where we can move p_1 outside the bracket since it is a number, not an operator. Hence, the correct answer is alternative **A**.

g) The easiest way to solve this problem is through dimensional analysis. $|\Phi|^2$ is a probability density in momentum space, and should therefore have dimension of inverse momentum, i.e. $[|\Phi|^2] = \mathrm{kg}^{-1}\,\mathrm{m}^{-1}\,\mathrm{s}$. From Eq. (2) we see that $\phi(k)$ has dimension $\sqrt{\text{length}}$, $[\phi(k)] = \mathrm{m}^{1/2}$, meaning that $\phi^2(k)/\hbar$ has the correct dimension, $[\phi^2(k)/\hbar] = \mathrm{m\,J}^{-1}\,\mathrm{s}^{-1} = \mathrm{kg}^{-1}\,\mathrm{m}^{-1}\,\mathrm{s}$. The only option with the correct dimension is therefore alternative **B**.

We can also calculate it directly. We insert a completeness relation into the expression for $\Psi(x,t)$,

$$\Psi(x,t) = \langle x|\Psi\rangle = \int_{-\infty}^{\infty} dp\ \langle x|p\rangle\langle p|\Psi\rangle = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} dp\ e^{ipx/\hbar}\Phi(p,t).$$

Using $p = \hbar k$, we get

$$\Psi(x,t) = \sqrt{\frac{\hbar}{2\pi}}\int_{-\infty}^{\infty} dk\ e^{ikx}\Phi(p,t) = \int_{-\infty}^{\infty} dk\ e^{ikx}\phi(k)e^{-i\omega(k)t},$$

where in the last equality we have inserted the expression from the problem set. Comparing the two sides of the equality, we find

$$\Phi(p,t) = \sqrt{\frac{2\pi}{\hbar}}\phi(p/\hbar)e^{-ip^2t/(2m\hbar)},$$

which is option **B**.

h) The probabilities of measuring E_1 and E_2 are given by the (absolute value) squared of the expansion coefficients, $P_1 = 2/6$ and $P_2 = 4/6$, respectively. Hence, we get

$$\langle E\rangle = P_1E_1 + P_2E_2 = \hbar\omega\frac{2+8}{6} = \frac{5\hbar\omega}{3},$$

making alternative **E** the correct answer.

i) The general rule is that the dual of $a|v\rangle$ is $a^*\langle v|$. Using this rule for the given state vector, we therefore get

$$\langle\psi| = \frac{1}{\sqrt{6}}\left[(2+i)^*\langle 1| + (i)^*\langle 2|\right] = \frac{1}{\sqrt{6}}\left[(2-i)\langle 1| - i\langle 2|\right],$$

meaning that the correct answer is option **C**. Since it is stated that the vector is normalized, we could also have calculated $\langle\psi|\psi\rangle$ for each alternative, which would have given $\langle\psi|\psi\rangle = 1$ only for option **C**.

Problem 2 Short answer questions

a) Bosons states must be symmetric under exchange of identical particles, which allows many identical bosons to occupy the same single-particle state. Fermion states must be completely antisymmetric under exchange of identical particles, which means that identical fermions cannot occupy the same single-particle state (Pauli exclusion principle). In three dimensions bosons have integer spin, while fermions have half-integer spin.

b) The Pauli principle states that identical fermions within a system cannot occupy the same single-particle state at the same time. A fermionic state has to be completely antisymmetric upon interchange of identical particles, resulting in the state 0 if two identical particles are in the same single-particle state. Hence, such a state cannot exist.

c) Physical observables should be real quantities, and must therefore be represented by Hermitian operators which have real eigenvalues.

Problem 3

a) The stationary state wavefunctions should be eigenfunctions of the time-independent Schrödinger equation, $\hat{H}\psi = E\psi$, where E is the eigenenergy. Inside the box, the potential is zero, and we therefore require

$$\begin{aligned}
-\frac{\hbar^2}{2m}\nabla^2\psi_{n_xn_yn_z} &= -\frac{\hbar^2}{2m}\sum_{i=x,y,z}\partial_i^2 A\sin\frac{\pi x n_x}{L_x}\sin\frac{\pi y n_y}{L_y}\sin\frac{\pi z n_z}{L_z} \\
&= \frac{\hbar^2}{2m}\left[\left(\frac{\pi n_x}{L_x}\right)^2+\left(\frac{\pi n_y}{L_y}\right)^2+\left(\frac{\pi n_z}{L_z}\right)^2\right]A\sin\frac{\pi x n_x}{L_x}\sin\frac{\pi y n_y}{L_y}\sin\frac{\pi z n_z}{L_z} \\
&= \frac{\hbar^2\pi^2}{2m}\left(\frac{n_x^2}{L_x^2}+\frac{n_y^2}{L_y^2}+\frac{n_z^2}{L_z^2}\right)\psi_{n_xn_yn_z} = E\psi_{n_xn_yn_z}. \qquad (3)
\end{aligned}$$

Setting $L_x = L_y = L$, we see that the wavefunctions are energy eigenfunctions with the eigenenergies given in the problem, and thus solutions to the Schrödinger equation inside the box. The final requirement is that the wavefunctions should be zero at the boundaries, since the potential is infinite there. Inserting $x = 0, L$, $y = 0, L$ and $z = 0, L_z$ we get zero in all cases when n_x, n_y, n_z are positive integers, making this a valid solution satisfying both the time-independent Schrödinger equation and the boundary conditions.

b) Since the particles have spin $\frac{1}{2}$, two particles can occupy each energy eigenstate by being in the spin-singlet state. We therefore need to find the quantum numbers n_x, n_y, n_z corresponding to the 11 lowest energies when $L_z = 0.1L$,

$$E_{n_xn_yn_z} = \frac{\hbar^2\pi^2}{2mL^2}\left(n_x^2+n_y^2+100n_z^2\right) \equiv E_0\left(n_x^2+n_y^2+100n_z^2\right). \qquad (4)$$

Since the last term has a prefactor of 100, increasing n_x and n_y leads to lower energy states than increasing n_z to 2 as long as $n_x, n_y \leq 20$. Hence the 11 lowest energy states are

$$\begin{aligned}
E_{111} &= 102E_0, \\
E_{211} = E_{121} &= 105E_0, \\
E_{221} &= 108E_0, \\
E_{311} = E_{131} &= 110E_0, \\
E_{321} = E_{231} &= 113E_0, \\
E_{411} = E_{141} &= 117E_0, \\
E_{331} &= 118E_0.
\end{aligned}$$

The maximal occupied one-particle energy is therefore $E_{331} = 118\frac{\hbar^2\pi^2}{2mL^2}$. With the given number of particles in the system, no particles have $n_z > 1$, making the system effectively two-dimensional.

c) In the macroscopic limit L is large, and the energy levels lie close together, and we treat the energy levels as a continuum. Defining $n = \sqrt{n_x^2 + n_y^2 + n_z^2}$, we write the energy as

$$E = \frac{\hbar^2 \pi^2}{2mL^2} n^2 \quad \Rightarrow \quad n = \frac{\sqrt{2mL^2 E}}{\hbar \pi}. \tag{5}$$

For a given maximal energy E, the total number of energy states is therefore given by the volume of the positive octant in n-space with radius n given by the above equation, giving the total number of single-particle states

$$N = 2 \cdot \frac{1}{8} \frac{4\pi n^3}{3} = \frac{\pi}{3} \left(\frac{2mL^2 E}{\hbar^2 \pi^2} \right)^{3/2} = \frac{V}{3\pi^2 \hbar^3} (2mE)^{3/2}, \tag{6}$$

where have multiplied with 2 to account for two spin states per energy level, and have defined $V = L^3$.

The density of states is then

$$g(E) = \frac{dN}{dE} = \frac{V}{2\pi^2} \left(\frac{2m}{\hbar^2} \right)^{3/2} \sqrt{E}. \tag{7}$$

Problem 4

Taking the time-derivative of the the expectation value, we get

$$\frac{d}{dt}\langle F \rangle = \left[\frac{\partial}{\partial t} \langle \psi | \right] \hat{F} |\psi\rangle + \langle \psi | \left[\frac{\partial}{\partial t} \hat{F} \right] |\psi\rangle + \langle \psi | \hat{F} \left[\frac{\partial}{\partial t} |\psi\rangle \right]. \tag{8}$$

The second term is the expectation value of the time-derivative of the operator. To simplify the remaining terms, we use the Schrödinger equation. For the vector $|\psi\rangle$, we have

$$i\hbar \frac{\partial}{\partial t} |\psi\rangle = \hat{H} |\psi\rangle \quad \Rightarrow \quad \frac{\partial}{\partial t} |\psi\rangle = -\frac{i}{\hbar} \hat{H} |\psi\rangle \tag{9}$$

Taking the adjoint or Hermitian conjugate, we get the Schrödinger equation for the dual vector,

$$-i\hbar \frac{\partial}{\partial t} \langle \psi | = [\hat{H} |\psi\rangle]^\dagger = \langle \psi | \hat{H} \quad \Rightarrow \quad \frac{\partial}{\partial t} \langle \psi | = \frac{i}{\hbar} \langle \psi | \hat{H}, \tag{10}$$

where we have used the fact that $\hat{H}$ is Hermitian. Hence, we get

$$\begin{aligned} \frac{d}{dt}\langle F \rangle &= \frac{i}{\hbar} \langle \psi | \hat{H}\hat{F} | \psi \rangle - \frac{i}{\hbar} \langle \psi | \hat{F}\hat{H} | \psi \rangle + \left\langle \frac{\partial \hat{F}}{\partial t} \right\rangle = \frac{i}{\hbar} \langle \psi | [\hat{H}, \hat{F}] | \psi \rangle + \left\langle \frac{\partial \hat{F}}{\partial t} \right\rangle \\ &= \frac{i}{\hbar} \langle [\hat{H}, \hat{F}] \rangle + \left\langle \frac{\partial \hat{F}}{\partial t} \right\rangle. \end{aligned} \tag{11}$$

Problem 5

a) The abstract ground state vector is defined by $a|0\rangle = 0$. We multiply with an adjoint position eigenvector from the left, and insert a completeness relation

$$0 = \langle x|a|0\rangle = \int dx' \ \langle x|a|x'\rangle\langle x'|0\rangle = \int dx'\langle x|a|x'\rangle\psi_0(x'). \tag{12}$$

We now insert the expression for a in terms of the position and momentum operators, and use the given formula for a bracket containing an operator,

$$\begin{aligned} 0 &= \sqrt{\frac{m\omega}{2\hbar}} \int dx' \langle x|\hat{x} + \frac{i}{m\omega}\hat{p}_x|x'\rangle\psi_0(x') = \sqrt{\frac{m\omega}{2\hbar}} \int dx' \ \left(x + \frac{\hbar}{m\omega}\frac{\partial}{\partial x}\right)\delta(x-x')\psi_0(x') \\ &= \sqrt{\frac{m\omega}{2\hbar}} \left[x\psi_0(x) + \frac{\hbar}{m\omega}\frac{\partial}{\partial x}\psi_0(x)\right]. \end{aligned} \tag{13}$$

We have to solve the differential equation

$$x\psi_0(x) + \frac{\hbar}{m\omega}\frac{\partial}{\partial x}\psi_0(x) = 0, \tag{14}$$

which we rewrite to

$$\begin{aligned} \frac{d\psi_0}{\psi_0} &= -\frac{m\omega x}{\hbar}dx \\ \Rightarrow \quad \ln\psi_0 &= -\frac{m\omega x^2}{2\hbar} + \text{const.} \end{aligned} \tag{15}$$

Hence, the ground state wavefunction is

$$\psi_0(x) = Ae^{-m\omega x^2/(2\hbar)}, \tag{16}$$

where A must be determined by normalization.

b) We determine A by requiring normalization,

$$1 = \int_{-\infty}^{\infty} dx \ |\psi_0(x)|^2 = |A|^2 \int_{-\infty}^{\infty} dx e^{-m\omega x^2/\hbar} = |A|^2\sqrt{\frac{\hbar\pi}{m\omega}}, \tag{17}$$

where we have used the Gaussian integration formulas given in the formula sheet. Choosing A real and positive, we get

$$A = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}, \tag{18}$$

and the normalized ground state wavefunction

$$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-m\omega x^2/(2\hbar)}. \tag{19}$$

c) We write the perturbation in terms of the raising and lowering operators using

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}[a + a^\dagger], \tag{20}$$

resulting in

$$\hat{V}_q = \frac{1}{4}q\hat{x}^4 = \frac{q}{4}\left(\frac{\hbar}{2m\omega}\right)^2 [a + a^\dagger]^4. \tag{21}$$

The first order correction is given by $\langle n|\hat{V}_q|n\rangle$, and we therefore need to calculate

$$\begin{aligned}\langle n|[a + a^\dagger]^4|n\rangle &= \langle n|[aa + aa^\dagger + a^\dagger a + a^\dagger a^\dagger]^2|n\rangle \\ &= \langle n|[aaa^\dagger a^\dagger + aa^\dagger aa^\dagger + a^\dagger aaa^\dagger + aa^\dagger a^\dagger a + a^\dagger aa^\dagger a + a^\dagger a^\dagger aa]|n\rangle,\end{aligned} \tag{22}$$

where we have neglected all terms with an unequal number of raising and lowering operators since the states are orthonormal, $\langle m|n\rangle = \delta_{mn}$. Using the given formulas for the effect of the raising and lowering operators, we get

$$\begin{aligned}\langle n|[a + a^\dagger]^4|n\rangle &= (n+1)(n+2) + (n+1)^2 + n(n+1) + n(n+1) + n^2 + n(n-1) \\ &= n^2 + 3n + 2 + n^2 + 2n + 1 + 2n^2 + 2n + n^2 + n^2 - n \\ &= 6n^2 + 6n + 3.\end{aligned} \tag{23}$$

Hence, the first order corrections are

$$E_n^{(1)} = \frac{3q}{16}\left(\frac{\hbar}{m\omega}\right)^2 \left[2n^2 + 2n + 1\right] = \frac{3q(\hbar\omega)^2}{16k^2}\left[2n^2 + 2n + 1\right], \tag{24}$$

which increase rapidly with increasing n. For higher n, the change in the potential due to the x^4-term becomes increasingly more important, and it is therefore reasonable that the correction should increase for larger n.

d) When $k < 0$, the potential no longer has a global minima at $x = 0$, but rather a local maxima, meaning that the Hamiltonian no longer describes a harmonic oscillator centered at $x = 0$. In fact, the frequency ω becomes imaginary for negative k, indicating that our analysis for $k > 0$ does not hold when $k < 0$. Hence, the given harmonic oscillator solutions ($|n\rangle$ and E_n) are not solutions of a solvable unperturbed Hamiltonian H_0 when $k < 0$, and we cannot use perturbation theory based on these solutions.

e) The expectation value is given by

$$\langle H\rangle = \frac{\langle\psi_c|\hat{H}|\psi_c\rangle}{\langle\psi_c|\psi_c\rangle} = \frac{\langle\psi_c|\frac{\hat{p}_x^2}{2m} + \frac{1}{2}k\hat{x}^2 + \frac{1}{4}q\hat{x}^4|\psi_c\rangle}{\langle\psi_c|\psi_c\rangle}, \tag{25}$$

where the denominator ensures normalization. We calculate the necessary quantities term by term in the position representation:[1]

$$\langle\psi_c|\psi_c\rangle = |C|^2 \int_{-\infty}^{\infty} dx\ e^{-m\Omega(x-x_0)^2/\hbar} = |C|^2\sqrt{\frac{\pi\hbar}{m\Omega}}, \tag{26}$$

$$\begin{aligned}\langle\psi_c|\frac{\hat{p}_x^2}{2m}|\psi_c\rangle &= \frac{1}{2m}\int_{-\infty}^{\infty} dx\ \psi_c^*(x)\hat{p}_x^2\psi_c(x) = \frac{1}{2m}\int_{-\infty}^{\infty} dx\ [\hat{p}_x\psi_c(x)]^*\hat{p}_x\psi_c(x)\\ &= \frac{\hbar^2}{2m}\int_{-\infty}^{\infty} dx\ \left|i\frac{m\Omega}{\hbar}(x-x_0)Ce^{-m\Omega(x-x_0)^2/2\hbar}\right|^2\\ &= |C|^2\frac{m\Omega^2}{2}\int_{-\infty}^{\infty} dy\ y^2e^{-m\Omega y^2/\hbar} = |C|^2\sqrt{\frac{\pi\hbar}{m\Omega}}\frac{\hbar\Omega}{4}\end{aligned} \tag{27}$$

$$\langle\psi_c|\frac{1}{2}k\hat{x}^2|\psi_c\rangle = \frac{k|C|^2}{2}\int_{-\infty}^{\infty} dy(y+x_0)^2e^{-m\Omega y^2/\hbar} = \frac{k|C|^2}{2}\sqrt{\frac{\pi\hbar}{m\Omega}}\left[\frac{\hbar}{2m\Omega}+x_0^2\right] \tag{28}$$

$$\langle\psi_c|\frac{1}{4}q\hat{x}^4|\psi_c\rangle = \frac{q|C|^2}{4}\int_{-\infty}^{\infty} dy(y+x_0)^4e^{-m\Omega y^2/\hbar} = \frac{q|C|^2}{4}\sqrt{\frac{\pi\hbar}{m\Omega}}\left[\frac{3}{4}\frac{\hbar^2}{m^2\Omega^2}+\frac{3\hbar}{m\Omega}x_0^2+x_0^4\right]. \tag{29}$$

[1] One elegant solution used by some was based on the special properties of Gaussian functions. From the probability density we can read off $\langle x\rangle = x_0$, $\langle p_x\rangle = 0$, and

$$\Delta x^2 = \langle x^2\rangle - \langle x\rangle^2 = \langle x^2\rangle - x_0^2 = \frac{\hbar}{2m\Omega}.$$

From this we directly get

$$\left\langle\frac{1}{2}kx^2\right\rangle = \frac{k}{2}\langle x^2\rangle = \frac{k}{2}\left[\frac{\hbar}{2m\Omega}+x_0^2\right].$$

Moreover, since the Gaussian wavefunction is a minimal uncertainty state, with $\Delta x\Delta p_x = \frac{\hbar}{2}$, we get

$$\left\langle\frac{\hat{p}_x^2}{2m}\right\rangle = \frac{\langle\hat{p}_x^2\rangle}{2m} = \frac{1}{2m}\frac{\hbar^2}{4\Delta x^2} = \frac{\hbar\Omega}{4}.$$

In principle one could also calculate $\langle x^4\rangle$ in a similar way by using the fact that all cumulants κ_n with $n > 2$ are zero for a Gaussian distribution. However, since that quickly becomes complicated (and would require a very good memory), it is probably easier to calculate the integral directly.

Here, we have defined $y = x - x_0$ and made use of the Gaussian integral formulas given in the formula sheet, resulting in the following solutions for the integrals,

$$\int_{-\infty}^{\infty} dy\ e^{-\alpha y^2} = \sqrt{\frac{\pi}{\alpha}},$$
$$\int_{-\infty}^{\infty} dy\ y^2 e^{-\alpha y^2} = -\frac{\partial}{\partial\alpha}\sqrt{\frac{\pi}{\alpha}} = \frac{1}{2}\sqrt{\frac{\pi}{\alpha}}\frac{1}{\alpha},$$
$$\int_{-\infty}^{\infty} dy\ y^4 e^{-\alpha y^2} = \frac{\partial^2}{\partial\alpha^2}\sqrt{\frac{\pi}{\alpha}} = \frac{3}{4}\sqrt{\frac{\pi}{\alpha}}\frac{1}{\alpha^2},$$

with $\alpha = m\Omega/\hbar$. All integrals with odd powers of y are zero.

Inserting Eqs. (26) to (29) into Eq. (25), we find the energy expectation value

$$\begin{aligned}\langle H\rangle = \frac{\langle\psi_c|\hat{H}|\psi_c\rangle}{\langle\psi_c|\psi_c\rangle} &= \frac{\hbar\Omega}{4} + \frac{k\hbar}{4m\Omega} + \frac{k}{2}x_0^2 + \frac{3q}{16}\frac{\hbar^2}{m^2\Omega^2} + \frac{3q}{4}\frac{\hbar}{m\Omega}x_0^2 + \frac{q}{4}x_0^4 \\ &= \frac{\hbar\Omega}{8} + \frac{3q\hbar^2\Omega^2}{64k^2} + \frac{k}{2}\left[1 - \frac{3q\hbar\Omega}{4k^2}\right]x_0^2 + \frac{q}{4}x_0^4 \equiv E(x_0),\end{aligned} \tag{30}$$

where we have used $\Omega = \sqrt{-2k/m}$ to simplify the result by eliminating the mass m from the expression.

f) According to the variational principle, we have the following inequality for the ground state energy E_0,

$$E_0 \leq \frac{\langle\psi_c|\hat{H}|\psi_c\rangle}{\langle\psi_c|\psi_c\rangle} = E(x_0). \tag{31}$$

To find an upper bound for the ground state energy we therefore minimize the expectation value with respect to the free parameter x_0,

$$0 = \frac{\partial E}{\partial x_0} = k\left(1 - \frac{3q\hbar\Omega}{4k^2}\right)x_0 + qx_0^3, \tag{32}$$

The solutions are $x_0 = 0$ and

$$x_0 = \pm\sqrt{-\frac{k}{q}}\sqrt{1 - \frac{3\hbar\Omega}{4}\frac{q}{k^2}} \equiv x_\pm. \tag{33}$$

Inserting the two solutions into $E(x_0)$, we get

$$E(0) = \frac{\hbar\Omega}{8} + \frac{3\hbar^2\Omega^2}{64}\frac{q}{k^2}, \tag{34}$$

and

$$E(x_\pm) = \frac{\hbar\Omega}{2} - \frac{k^2}{4q} - \frac{3\hbar^2\Omega^2}{32}\frac{q}{k^2}. \tag{35}$$

We see that $E(x_\pm)$ is lower than $E(0)$, which is consistent with the fact that the average potential energy of a particle is lowered if the position expectation value, $\langle x\rangle = x_0$, is in a region with negative potential energy.[2] The upper bound for the ground state energy is therefore

$$E_0 \leq \frac{\hbar\Omega}{2} - \frac{k^2}{4q} - \frac{3\hbar^2\Omega^2}{32}\frac{q}{k^2} \approx \frac{\hbar\Omega}{2} - \frac{k^2}{4q}, \tag{36}$$

when $\hbar\Omega q/k^2 \ll 1$. Hence the upper bound for the ground state energy takes the form of the regular harmonic oscillator ground state energy $\hbar\Omega/2$, but shifted towards negative energies by a constant term $-k^2/4q$ corresponding to the minima of the potential energy. This is consistent with the double well structure that appears when $k < 0$, which in the limit $\hbar\Omega q/k^2 \ll 1$ results in two approximately harmonic potentials with spring constant $2|k|$ centered at $x = x_\pm \approx \pm\sqrt{-k/q}$.[3]

[2] In fact, when $\hbar\Omega q/k^2 \ll 1$ the positions $x_\pm$ correspond to the two minima in the potential energy.

[3] *A comment for those interested:* Since the potential is symmetric, the actual wavefunctions of the system have to be either symmetric or antisymmetric about $x = 0$. Therefore,

$$\psi_\pm(x) = C_\pm\left[e^{-m\Omega(x-x_0)^2/2\hbar} \pm e^{-m\Omega(x+x_0)^2/2\hbar}\right]$$

would be better trial functions for this system, since they have the right symmetry properties. ψ_+ would be a good trial function for the ground state, which must be symmetric, and ψ_- for the first excited state. However, when $\hbar\Omega q/k^2 \ll 1$, the expectation values obtained using $\psi_\pm$ are close to identical due to a close to negligible overlap between the two terms in $\psi_\pm$ — the expectation value of the ground state and the first excited state are the same! The way to understand this is that the two potential wells have become so deep that they are decoupled from each other for the lowest energy states. The trial wavefunction ψ_c with x_0 set to the values $x_\pm \approx \pm\sqrt{-k/q} \equiv \pm x_{\min}$ found above correspond to superpositions of ψ_+ and ψ_-,

$$\psi_c(x)\big|_{x_0=x_{\min}} \propto [\psi_+(x) + \psi_-(x)]\Big|_{x_0=x_{\min}},$$
$$\psi_c(x)\big|_{x_0=-x_{\min}} \propto [\psi_+(x) - \psi_-(x)]\Big|_{x_0=x_{\min}},$$

resulting in two harmonic oscillator-like solutions located either in the right or left well.