Exercises Quantum Physics (GEMF) – Real world problems

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1. **Particles with elevated spin moments:** Elementary particles such as photons, gluons and W- and Z-bosons are integer spin particles (bosons) with $S = 1$. Composite particles such as the α-particle also have $S = 1$. Calculate the eigenvalues and eigenvectors of the $\hat{S}_x$ operator for these particles. Show that the commutator $[\hat{S}_x, \hat{S}_y] = i\hbar\hat{S}_z$. The matrix representation of the operators is

$$\hat{S}_x = \frac{\hbar}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \qquad \hat{S}_y = \frac{\hbar}{\sqrt{2}}\begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix} \qquad \hat{S}_z = \hbar\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

2. **Perturbation theory in matrix representation:** Given the following zeroth-order Hamiltonian $\hat{H}^{(0)}$ and perturbation operator $\hat{V}^{(0)}$

$$\hat{H}^{(0)} = \begin{pmatrix} 6 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad \hat{V}^{(0)} = \begin{pmatrix} 0 & 1 & 2 \\ 1 & 0 & 0 \\ 2 & 0 & 1 \end{pmatrix}$$

calculate the first and second order corrections to the energy and compare to the exact energies.

3. **Perturbation theory in position representation:** The ideal harmonic oscillator can be subject to different perturbations. Here we will study the effect of fatigue and of anharmonicity.

$$\text{Ideal: } F = -m\omega_0^2 x \quad \Rightarrow \quad V(x) = \frac{1}{2}m\omega_0^2 x^2 \quad \text{and} \quad E = \hbar\omega_0(n + \tfrac{1}{2})$$

$$\text{Fatigue: } F = -m\omega_0^2 x + \lambda x \quad \Rightarrow \quad V(x) = \frac{1}{2}m\omega^2 x^2 = \frac{1}{2}m\omega_0^2 x^2 - \frac{1}{2}\lambda x^2$$

   (a) Use the modified potential energy operator to express the new frequency ω in terms of the initial frequency ω_0 and the fatigue parameter λ

   (b) Use the approximation $\sqrt{1+x} \approx 1 + x/2$ for small x, to derive $\omega = \omega_0 - \frac{\lambda}{2m\omega_0^2}$

   (c) Substitute ω in the energy expression to check that the fatigue lowers the energy of the ground state by $\frac{\hbar\lambda}{4m\omega_0}$

   This "*exact*" result is now being compared to the outcomes of perturbation theory.

(d) Write down the Hamiltonian of the harmonic oscillator as sum of the unperturbed oscillator and the "*fatigue*" operator, which act as perturbation operator.

(e) Calculate the first-order correction to the energy of the ground state and compare to the "*exact*" result. The ground state wave function of the unperturbed harmonic oscillator is

$$\psi_0^{(0)} = \left(\frac{a}{\pi}\right)^{\frac{1}{4}} e^{-\frac{1}{2}ax^2} \qquad \text{with} \quad a = \frac{m\omega_0}{\hbar}$$

The following standard integral may be useful

$$\int_{-\infty}^{\infty} x^n e^{-bx^2} = b^{-\frac{1}{2}(n-1)} 2^{-n} \frac{n!}{(n/2)!} \sqrt{\pi}$$

Next, we focus attention to the effect of anharmonicity. The potential energy operator is extended with a cubic and a quartic term

$$V(x) = \frac{1}{2} m\omega^2 x + \alpha x^3 + \beta x^4$$

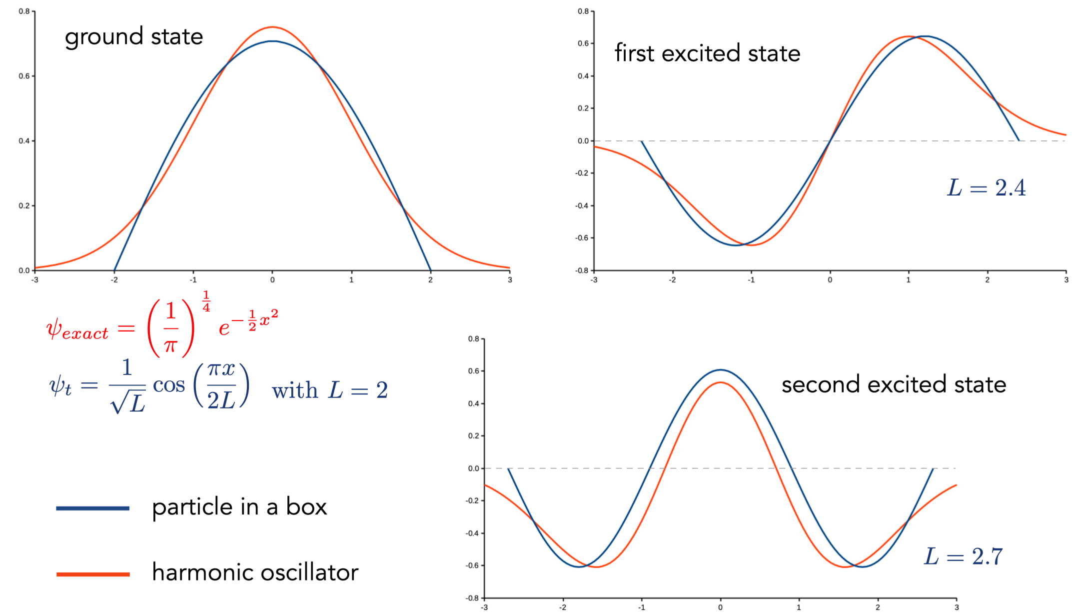
(f) Calculate the first-order correction to the energy due to the cubic and quartic perturbations of the harmonic oscillator.

4. **Variational method with one parameter:** The comparison of the lowest three eigenfunctions of a particle in box and the harmonic oscillator suggests that the eigenfunctions of the particle in a box can give a more or less accurate estimate of the latter provided L is chosen wisely. Use the variational method to determine the optimal L for the three lowest states of the harmonic oscillator. The L-values in the figure are not the optimal ones! They are just an educated guess to show that the optimal L will vary form level to level.

   Use the following standard integrals:

$$\int x^2 \cos^2 ax dx = \frac{x^3}{6} + \left(\frac{x^2}{4a} - \frac{1}{8a^3}\right) \sin 2ax + \frac{x}{4a^2} \cos 2ax$$
$$\int x^2 \sin^2 ax dx = \frac{x^3}{6} - \left(\frac{x^2}{4a} - \frac{1}{8a^3}\right) \sin 2ax - \frac{x}{4a^2} \cos 2ax$$

   Calculate the overlap between the different solutions. What does this imply for the wave function of the second excited state?



5. **Variational method with two parameters:** Determine the optimal values for c_1 and c_2 of the trial wave function $\psi_t = c_1\phi_1 + c_2\phi_2$ to describe the ground state of the H_2 molecule. ϕ_1 and ϕ_2 are the exact ground state wave functions of the hydrogen atom. Repeat the exercise for the HeH^+ molecule, where ϕ_2 is the exact ground state wave of the He^+ ion.

6. **Many-particle systems:** Consider three non-interacting particles in a box with $V(x) = 0$ for $0 \le x \le L$ and $V(x) = \infty$ everywhere else. Write down the energy and wave function of the ground state of the system when the particles are (i) spinless and have different mass: $m_1 < m_2 < m_3$; (ii) identical bosons and (iii) identical with spin $\frac{1}{2}$. Repeat the exercise for the first excited state.

7. **Ionization energies:** Calculate the ionization energies of the elements H, He^+, Li^{2+} and Be^{3+} and compare to the experimental values. Do the same for atoms He, Li^+ and Be^{2+}. Experimental ionization energies in eV:

Atom	first	second	third	fourth
H	13.6			
He	24.6	54.4		
Li	5.4	75.6	122.5	
Be	9.3	18.2	153.9	217.7