

# Problemas do Capítulo 18

## Problems

1. The Hamiltonian of a rigid rotator in a magnetic field perpendicular to the  $x$  axis is of the form  $AL^2 + BL_z + CL_y$ , if the term that is quadratic in the field is neglected. Obtain the exact energy eigenvalues and eigenfunctions of the Hamiltonian. Then, assuming  $B \gg C$ , use second-order perturbation theory to get approximate eigenvalues and compare these with the exact answers.
2. A charged particle is constrained to move on a spherical shell in a weak uniform electric field. Obtain the energy spectrum to second order in the field strength.
3. Apply perturbation theory to the elastically coupled harmonic oscillators of Problems 6 and 7 in Chapter 15, assuming that the interaction between the two particles is weak, and compare with the rigorous solutions.
4. Use second-order perturbation theory to calculate the change in energy of a linear harmonic oscillator when a constant force is added, and compare with the exact result.
5. A slightly anisotropic three-dimensional harmonic oscillator has  $\omega_z \approx \omega_x = \omega_y$ . A charged particle moves in a field of this oscillator and is at the same time exposed to a uniform magnetic field in the  $x$  direction. Assuming that the Zeeman splitting is comparable to the splitting produced by the anisotropy, but small compared to  $\hbar\omega$ , calculate to first order the energies of the components of the first excited state. Discuss various limiting cases.
6. Prove that if  $\psi_0 = e^{-\varphi_0}$  is a positive bounded function satisfying appropriate boundary conditions, it represents the ground state for a particle moving in a potential

$$V = \frac{\hbar^2}{2m} [(\nabla\varphi_0)^2 - \nabla^2\varphi_0] + E_0$$

and the corresponding energy is  $E_0$ . Verify the theorem for (a) the isotropic harmonic oscillator and (b) the hydrogen atom.

7. Apply the theorem proven in Problem 6 to a particle of mass  $m$  in one dimension, with the assumed ground state,

$$\psi_0(x) = \frac{C}{\cosh \kappa x}$$

and a corresponding energy eigenvalue  $E_0 = -\hbar^2\kappa^2/2m$ . Plot the resulting potential.

8. Prove that the trace of the direct product of two matrices equals the product of the traces of the matrices. Apply this result to show that the "center of gravity" of a multiplet split by the spin-orbit interaction is at the position of the unperturbed energy level.

9. Obtain the relativistic correction  $\propto p^4$  to the nonrelativistic kinetic energy of an electron, and, using first-order perturbation theory, evaluate the energy shift that it produces in the ground state of hydrogen.
10. Using the Hamiltonian for an atomic electron in a magnetic field, determine, for a state of zero angular momentum, the energy change to order  $B^2$ , if the system is in a uniform magnetic field represented by the vector potential  $\mathbf{A} = \mathbf{B} \times \mathbf{r}/2$ .  
Defining the atomic diamagnetic susceptibility  $\chi$  by  $E = -\chi B^2/2$ , calculate  $\chi$  for a helium atom in the ground state and compare the result with the measured value.
11. Apply second-order perturbation theory to a one-dimensional periodic perturbing potential

$$V(x) = \sum_{n=-\infty}^{+\infty} V_n e^{2\pi i n x / \xi}$$

with period  $\xi$ . To enforce closely spaced discrete energies, assume that the entire "crystal" has length  $L = N\xi$  and use the periodic boundary condition  $\Psi(x + L/2) = \Psi(x - L/2)$ , where  $N$  is a large even number. Assume that the zero-order Hamiltonian is that of a free particle subject to these boundary conditions. Show that nondegenerate perturbation theory breaks down at the band edges and that the forbidden energy gaps are proportional to the Fourier coefficients of the potential.

Show that in the limit  $L \rightarrow \infty$ , carried out as in Section 1 of the Appendix, the unperturbed (unnormalized) energy eigenfunctions are plane waves,  $e^{ikx}$ , and derive the second-order approximation to the dispersion function  $E(k)$ .

12. Assuming that the zero-order free particle energy is large compared with  $g/\xi$ , apply the results of Problem 11 to the special example of a Kronig-Penney potential with attractive  $\delta$ -functions of strength  $g$ . In the middle of the valence band at  $k\xi = \pi/2$ , verify the result of perturbation theory by expanding the exact eigenvalue condition (see Exercise 8.29).
13. Let  $\psi$  be a variational trial function for the ground state  $\psi_0$  of a system with nondegenerate energy eigenvalues. Assume that  $\psi$  and  $\psi_0$  are real, normalized to unity, and that  $\int \psi \psi_0 d^3r$  is positive. Show that

$$\frac{1}{2} \int (\psi - \psi_0)^2 d^3r \leq 1 - \left(1 - \frac{\langle H \rangle - E_0}{E_1 - E_0}\right)^{1/2} \approx \frac{1}{2} \frac{\langle H \rangle - E_0}{E_1 - E_0}$$

where  $E_0$  and  $E_1$  are the exact energies of the ground and first excited states, and  $\langle H \rangle$  is the expectation value of the Hamiltonian in the state  $\psi$ . Estimate the accuracy of the trial functions used in Section 17.8 for the ground state of the helium atom.

14. A rotator whose orientation is specified by the angular coordinates  $\theta$  and  $\varphi$  performs a hindered rotation described by the Hamiltonian

$$H = AL^2 + B\hbar^2 \cos 2\varphi$$

with  $A \gg B$ . Calculate the  $S$ ,  $P$ , and  $D$  energy levels of this system in first-order perturbation theory, and work out the corresponding unperturbed energy eigenfunctions.