Supplementary Problems

13.13. Prove that the Pauli exclusion principle does not hold for bosons.

13.14. Show explicitly that the Slater determinant for three fermions is antisymmetric.

13.15. Show that any function on the real line is a sum of a symmetric and antisymmetric functions.

Ans. $f(x) = \dfrac{f(x)+f(-x)}{2} + \dfrac{f(x)-f(-x)}{2}$.

13.16. What happens to the Slater determinant if there is a linear dependency between $|\phi^{j_1}\rangle \cdots |\phi^{j_n}\rangle$?

Ans. It vanishes.

13.17. Three particles are confined within the potential

$$V(x, y) = \begin{cases} 0 & 0 \le x \le a \text{ and } 0 \le y \le b \\ \infty & \text{otherwise} \end{cases} \tag{13.17.1}$$

Find the ground state of the system when the particles are bosons.

Ans. $|\psi_0(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3)\rangle = |\phi_{1,1}(\mathbf{r}_1)\phi_{1,1}(\mathbf{r}_2)\phi_{1,1}(\mathbf{r}_3)\rangle$, where $\phi_{n_x, n_y}(x, y) = \sqrt{\dfrac{4}{ab}}\sin\left(\dfrac{n_x \pi x}{a}\right)\sin\left(\dfrac{n_y \pi y}{b}\right)$.

13.18. Refer to Problem 13.14 and find the ground state of the system when the particles are "spinless" fermions. (That is, use Pauli's exclusion principle, but neglect the additional degree of spin.)

Ans. $$|\psi_0(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3)\rangle = \frac{1}{\sqrt{3!}}\begin{vmatrix} |\phi_{11}(\mathbf{r}_1)\rangle & |\phi_{12}(\mathbf{r}_1)\rangle & |\phi_{21}(\mathbf{r}_1)\rangle \\ |\phi_{11}(\mathbf{r}_2)\rangle & |\phi_{12}(\mathbf{r}_2)\rangle & |\phi_{21}(\mathbf{r}_2)\rangle \\ |\phi_{11}(\mathbf{r}_3)\rangle & |\phi_{12}(\mathbf{r}_3)\rangle & |\phi_{21}(\mathbf{r}_3)\rangle \end{vmatrix}$$

13.19. Repeat to Problems 13.14 and 13.15, but now do not neglect the spin.

Ans. $$|\psi_0(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3)\rangle = \frac{1}{\sqrt{3!}}\begin{vmatrix} |\phi^+_{11}(\mathbf{r}_1)\rangle & |\phi^-_{11}(\mathbf{r}_1)\rangle & |\phi^-_{12}(\mathbf{r}_1)\rangle \\ |\phi^+_{11}(\mathbf{r}_2)\rangle & |\phi^-_{11}(\mathbf{r}_2)\rangle & |\phi^-_{12}(\mathbf{r}_2)\rangle \\ |\phi^+_{11}(\mathbf{r}_3)\rangle & |\phi^-_{11}(\mathbf{r}_3)\rangle & |\phi^-_{12}(\mathbf{r}_3)\rangle \end{vmatrix}$$ and three additional possible states by substituting ϕ^+_{12}, ϕ^-_{21}, and ϕ^+_{21} instead of ϕ^-_{12}.

13.20. Repeat Problem 13.10, but this time solve for two bosons.

Ans. $|\Phi(1, 2, \mathbf{r}_1, \mathbf{r}_2)\rangle = |\phi_1(\mathbf{r}_1); S_1\rangle|\phi_2(\mathbf{r}_2); S_2\rangle + |\phi_1(\mathbf{r}_2); S_1\rangle|\phi_2(\mathbf{r}_1); S_2\rangle$

$$\rho_{\text{two par.}}(\mathbf{r}_1, \mathbf{r}_2) = \begin{cases} |\phi_1(\mathbf{r}_1)|^2|\phi_2(\mathbf{r}_2)|^2 + |\phi_1(\mathbf{r}_2)|^2|\phi_2(\mathbf{r}_1)|^2 & S_1 \ne S_2 \\ |\phi_1(\mathbf{r}_1)\,\phi_2(\mathbf{r}_2) + \phi_1(\mathbf{r}_2)\phi_2(\mathbf{r}_1)|^2 & S_1 = S_2 \end{cases}$$

$$\rho_{\text{one par.}}(\mathbf{r}_1) = \int \rho_{\text{two}}(\mathbf{r}_1, \mathbf{r}_2)\, d^3 r_2 = |\phi_1(\mathbf{r}_1)|^2 + |\phi_2(\mathbf{r}_1)|^2$$

PROBLEMS

17–1. Two particles of mass m are placed in a rectangular box of sides $a \neq b \neq c$ in the lowest energy state of the system compatible with the conditions below. Assuming that the particles interact with each other according to the potential $V = V_0\,\delta(r_1 - r_2)$, use first-order perturbation theory to calculate the energy of the system under the following conditions: (a) Particles not identical. (b) Identical particles of spin zero. (c) Identical particles of spin one-half with spins parallel.

17–2. Calculate the cross section, including its spin dependence, for the scattering of thermal neutrons by neutrons. Assume that the interaction between neutrons is spin-independent and is of the form of a potential well of radius r_0 and depth V_0.

17–3. (a) State the Pauli exclusion principle and discuss its application. (b) Show in detail how with its aid one can order the elements in the periodic table according to their chemical properties. (c) Why do the rare-earth elements have similar chemical properties? (d) Why are the alkali metals similar?

17–4. Discuss the energy-level structure of the helium atom.

17–5. Calculate the differential scattering cross section for the mutual scattering of two identical hard spheres with spin one-half and radius $a \ll \lambda$. Include the effects of S-, P-, and D-waves but neglect higher partial waves.

17–6. (a) Show that the spin-exchange operator can be written as

$$\mathrm{S}_{12} = \frac{1}{\hbar^2}\,[\mathrm{S}_{1+}\mathrm{S}_{2-} + \mathrm{S}_{1-}\mathrm{S}_{2+} + (2\mathrm{S}_{1z}\mathrm{S}_{2z} + \tfrac{1}{2}\hbar^2)].$$

[*Hint:* Show that the first term in the brackets changes the spin state $-+$ into $+-$ and gives zero for the remaining three spin states of the form of Eq. (17–12). What operations do the remaining two terms in the brackets perform?] (b) Show that the above spin-exchange operator can be expressed as

$$\mathrm{S}_{12} = \frac{1}{\hbar^2}\,(2\mathbf{S}_1 \cdot \mathbf{S}_2 + \tfrac{1}{2}\hbar^2).$$

(c) Show that it can also be written as

$$\mathrm{S}_{12} = \frac{1}{\hbar^2}\,(\mathrm{S}^2 - \hbar^2).$$

Complement D_{XIV}

EXERCISES

1. Let h_0 be the Hamiltonian of a particle. Assume that the operator h_0 acts only on the orbital variables and has three equidistant levels of energies 0, $\hbar\omega_0$, $2\hbar\omega_0$ (where ω_0 is a real positive constant) which are non-degenerate in the orbital state space $\mathscr{E}_r$ (in the total state space, the degeneracy of each of these levels is equal to $2s + 1$, where s is the spin of the particle). From the point of view of the orbital variables, we are concerned only with the subspace of $\mathscr{E}_r$ spanned by the three corresponding eigenstates of h_0.

a. Consider a system of three independent electrons whose Hamiltonian can be written:

$$H = h_0(1) + h_0(2) + h_0(3)$$

Find the energy levels of H and their degrees of degeneracy.

b. Same question for a system of three identical bosons of spin 0.

2. Consider a system of two identical bosons of spin $s = 1$ placed in the same central potential $V(r)$. What are the spectral terms (*cf.* complement B_{XIV}, §2-b) corresponding to the $1s^2$, $1s2p$, $2p^2$ configurations?

3. Consider the state space of an electron, spanned by the two vectors $|\varphi_{p_x}\rangle$ and $|\varphi_{p_y}\rangle$ which represent two atomic orbitals, p_x and p_y, of wave functions $\varphi_{p_x}(\mathbf{r})$ and $\varphi_{p_y}(\mathbf{r})$ (*cf.* complement E_{VII}, §2-b):

$$\varphi_{p_x}(\mathbf{r}) = xf(r) = \sin\theta\cos\varphi\, rf(r)$$
$$\varphi_{p_y}(\mathbf{r}) = yf(r) = \sin\theta\sin\varphi\, rf(r)$$

a. Write, in terms of $|\varphi_{p_x}\rangle$ and $|\varphi_{p_y}\rangle$, the state $|\varphi_{p_\alpha}\rangle$ which represents the p_α orbital pointing in the direction of the xOy plane which makes an angle α with Ox.

b. Consider two electrons whose spins are both in the $|+\rangle$ state, the eigenstate of S_z of eigenvalue $+\hbar/2$.

Write the normalized state vector $|\psi\rangle$ which represents the system of two electrons, one of which is in the state $|\varphi_{p_x}\rangle$ and the other, in the state $|\varphi_{p_y}\rangle$.

c. Same question, with one of the electrons in the state $|\varphi_{p_\alpha}\rangle$ and the other one in the state $|\varphi_{p_\beta}\rangle$, where α and β are two arbitrary angles. Show that the state vector $|\psi\rangle$ obtained is the same.

d. The system is in the state $|\psi\rangle$ of question *b*. Calculate the probability density $\mathscr{P}(r, \theta, \varphi; r', \theta', \varphi')$ of finding one electron at (r, θ, φ) and the other one at (r', θ', φ'). Show that the electronic density $\rho(r, \theta, \varphi)$, [the probability density of finding any electron at (r, θ, φ)] is symmetrical with respect to revolution about the Oz axis. Determine the probability density of having $\varphi - \varphi' = \varphi_0$, where φ_0 is given. Discuss the variation of this probability density with respect to φ_0.

4. Collision between two identical particles

The notation used is that of §D-2-a-β of chapter XIV.

a. Consider two particles, (1) and (2), with the same mass m, assumed for the moment to have no spin and to be distinguishable. These two particles interact through a potential $V(r)$ which depends only on the distance between them, r. At the initial time t_0, the system is in the state $| 1 : p\mathbf{e}_z ; 2 : -p\mathbf{e}_z \rangle$. Let $U(t, t_0)$ be the evolution operator of the system. The probability amplitude of finding it in the state $| 1 : p\mathbf{n} ; 2 : -p\mathbf{n} \rangle$ at time t_1 is:

$$F(\mathbf{n}) = \langle 1 : p\mathbf{n} ; 2 : -p\mathbf{n} | U(t_1, t_0) | 1 : p\mathbf{e}_z ; 2 : -p\mathbf{e}_z \rangle$$

Let θ and φ be the polar angles of the unit vector $\mathbf{n}$ in a system of orthonormal axes $Oxyz$. Show that $F(\mathbf{n})$ does not depend on φ. Calculate in terms of $F(\mathbf{n})$ the probability of finding any one of the particles (without specifying which one) with the momentum $p\mathbf{n}$ and the other one with the momentum $-p\mathbf{n}$. What happens to this probability if θ is changed to $\pi - \theta$?

b. Consider the same problem [with the same spin-independent interaction potential $V(r)$], but now with two identical particles, one of which is initially in the state $| p\mathbf{e}_z, m_s \rangle$, and the other, in the state $| -p\mathbf{e}_z, m'_s \rangle$ (the quantum numbers m_s and m'_s refer to the eigenvalues $m_s\hbar$ and $m'_s\hbar$ of the spin component along Oz). Assume that $m_s \neq m'_s$. Express in terms of $F(\mathbf{n})$ the probability of finding, at time t_1, one particle with momentum $p\mathbf{n}$ and spin m_s and the other one with momentum $-p\mathbf{n}$ and spin m'_s. If the spins are not measured, what is the probability of finding one particle with momentum $p\mathbf{n}$ and the other one with momentum $-p\mathbf{n}$? What happens to these probabilities when θ is changed to $\pi - \theta$?

c. Treat problem *b* for the case $m_s = m'_s$. In particular, examine the $\theta = \pi/2$ direction, distinguishing between two possibilities, depending on whether the particles are bosons or fermions. Show that, again, the scattering probability is the same in the θ and $\pi - \theta$ directions.

5. Collision between two identical unpolarized particles

Consider two identical particles, of spin s, which collide. Assume that their initial spin states are not known: each of the two particles has the same probability of being in the $2s + 1$ possible orthogonal spin states. Show that, with the notation of the preceding exercise, the probability of observing scattering in the $\mathbf{n}$ direction is:

$$|F(\mathbf{n})|^2 + |F(-\mathbf{n})|^2 + \frac{\varepsilon}{2s+1}[F^*(\mathbf{n})F(-\mathbf{n}) + \text{c.c.}]$$

($\varepsilon = +1$ for bosons, -1 for fermions).

b. The two particles under consideration are now identical fermions of spin 1/2 (electrons or protons).

α. In the state space of the system, we first use the $\{ | \mathbf{r}_G, \mathbf{r}; S, M \rangle \}$ basis of common eigenstates of $\mathbf{R}_G$, $\mathbf{R}$, $\mathbf{S}^2$ and S_z, where $\mathbf{S} = \mathbf{S}_1 + \mathbf{S}_2$ is the total spin of the system (the kets $| S, M \rangle$ of the spin state space were determined in §B of chapter X). Show that:

$$P_{21} | \mathbf{r}_G, \mathbf{r}; S, M \rangle = (-1)^{S+1} | \mathbf{r}_G, -\mathbf{r}; S, M \rangle$$

β. We now go to the $\{ | \mathbf{p}_G; E_n, l, m; S, M \rangle \}$ basis of common eigenstates of $\mathbf{P}_G$, H_r, $\mathbf{L}^2$, L_z, $\mathbf{S}^2$ and S_z.

As in question *a* - β, show that:

$$P_{21} | \mathbf{p}_G; E_n, l, m; S, M \rangle = (-1)^{S+1}(-1)^l | \mathbf{p}_G; E_n, l, m; S, M \rangle$$

γ. Derive the values of l allowed by the symmetrization postulate for each of the values of S (triplet and singlet).

c. *(more difficult)*

Recall that the total scattering cross section in the center of mass system of two distinguishable particles interacting through the potential $V(r)$ can be written:

$$\sigma = \frac{4\pi}{k^2} \sum_{l=0}^{\infty} (2l + 1) \sin^2 \delta_l$$

where the δ_l are the phase shifts associated with $V(r)$ [*cf.* chap. VIII, formula (C-58)].

α. What happens if the measurement device is equally sensitive to both particles (the two particles have the same mass)?

β. Show that, in the case envisaged in question *a*, the expression for σ becomes:

$$\sigma = \frac{8\pi}{k^2} \sum_{l \text{ even}} (2l + 1) \sin^2 \delta_l$$

γ. For two unpolarized identical fermions of spin 1/2 (the case of question *b*), prove that:

$$\sigma = \frac{2\pi}{k^2} \left\{ \sum_{l \text{ even}} (2l + 1) \sin^2 \delta_l + 3 \sum_{l \text{ odd}} (2l + 1) \sin^2 \delta_l \right\}$$

7. Position probability densities for a system of two identical particles

Let $| \varphi \rangle$ and $| \chi \rangle$ be two normalized orthogonal states belonging to the orbital state space $\mathscr{E}_r$ of an electron, and let $| + \rangle$ and $| - \rangle$ be the two eigenvectors, in the spin state space $\mathscr{E}_s$, of the S_z component of its spin.

a. Consider a system of two electrons, one in the state $| \varphi, + \rangle$ and the other, in the state $| \chi, - \rangle$. Let $\rho_{II}(\mathbf{r}, \mathbf{r}')d^3r d^3r'$ be the probability of finding one of them in a volume d^3r centered at point $\mathbf{r}$, and the other in a volume d^3r' centered at $\mathbf{r}'$ (two-particle density function). Similarly, let $\rho_I(\mathbf{r})d^3r$ be the probability of finding one of the electrons in a volume d^3r centered at point $\mathbf{r}$ (one-particule density function). Show that:

$$\begin{aligned} \rho_{II}(\mathbf{r}, \mathbf{r}') &= |\varphi(\mathbf{r})|^2 \, |\chi(\mathbf{r}')|^2 + |\varphi(\mathbf{r}')|^2 \, |\chi(\mathbf{r})|^2 \\ \rho_I(\mathbf{r}) &= |\varphi(\mathbf{r})|^2 + |\chi(\mathbf{r})|^2 \end{aligned}$$

Show that these expressions remain valid even if $| \varphi \rangle$ and $| \chi \rangle$ are not orthogonal in $\mathscr{E}_{\mathbf{r}}$.

Calculate the integrals over all space of $\rho_I(\mathbf{r})$ and $\rho_{II}(\mathbf{r}, \mathbf{r}')$. Are they equal to 1 ?

Compare these results with those which would be obtained for a system of two distinguishable particles (both spin 1/2), one in the state $| \varphi, + \rangle$ and the other in the state $| \chi, - \rangle$; the device which measures their positions is assumed to be unable to distinguish between the two particles.

b. Now assume that one electron is in the state $| \varphi, + \rangle$ and the other one, in the state $| \chi, + \rangle$. Show that we then have:

$$\begin{aligned} \rho_{II}(\mathbf{r}, \mathbf{r}') &= |\varphi(\mathbf{r})\chi(\mathbf{r}') - \varphi(\mathbf{r}')\chi(\mathbf{r})|^2 \\ \rho_I(\mathbf{r}) &= |\varphi(\mathbf{r})|^2 + |\chi(\mathbf{r})|^2 \end{aligned}$$

Calculate the integrals over all space of $\rho_I(\mathbf{r})$ and $\rho_{II}(\mathbf{r}, \mathbf{r}')$.

What happens to ρ_I and ρ_{II} if $| \varphi \rangle$ and $| \chi \rangle$ are no longer orthogonal in $\mathscr{E}_{\mathbf{r}}$?

c. Same questions for two identical bosons, either in the same spin state or in two orthogonal spin states.

8. The aim of this exercise is to demonstrate the following point : once the state vector of a system of N identical bosons (or fermions) has been suitably symmetrized (or antisymmetrized), it is not indispensable, in order to calculate the probability of any measurement result, to perform another symmetrization (or antisymmetrization) of the kets associated with the measurement. More precisely, provided that the state vector belongs to $\mathscr{E}_S$ (or $\mathscr{E}_A$), the physical predictions can be calculated as if we were confronted with a system of distinguishable particles studied by imperfect measurement devices unable to distinguish between them.

Let $| \psi \rangle$ be the state vector of a system of N identical bosons (all of the following reasoning is equally valid for fermions). We have:

$$S \, | \psi \rangle = | \psi \rangle \tag{1}$$

I.

a. Let $| \chi \rangle$ be the normalized physical ket associated with a measurement in which the N bosons are found to be in the different and orthonormal individual states $| u_\alpha \rangle, | u_\beta \rangle, ..., | u_\nu \rangle$. Show that:

$$| \chi \rangle = \sqrt{N!} \, S \, | 1 : u_\alpha ; 2 : u_\beta ; ... ; N : u_\nu \rangle \tag{2}$$