

Chapter 2

Systems of One or More Particles

Abstract A particle moving in an external field is an example of one-body system. The Schrödinger equation reduces to a single differential equation for central potential. The relative motion of a two-body system with mutual potential reduces to one-body Schrödinger equation. Symmetry of the wave function for identical particles is discussed. In this connection, spin and isospin and wave functions involving them are introduced. Next many-body wave equation is written down and the need for approximations and models stressed. Mean-field approximation and independent particle model are introduced.

2.1 One-Body System: A Particle in a Potential Field

We first consider the simplest system consisting of a single particle of mass m moving in an external time-independent potential $V(\vec{r})$. In the following, we review this topic, which can be found in standard texts in quantum mechanics, for example references [1–6]. The time-independent Schrödinger equation is

$$\left[-\frac{\hbar^2}{2m} \nabla^2 + V(\vec{r}) \right] \psi(\vec{r}) = E \psi(\vec{r}), \quad (2.1)$$

where \vec{r} is the position vector of the particle of mass m and the Laplacian is

$$\begin{aligned} \nabla^2 &= \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \\ &= \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \phi^2}, \end{aligned} \quad (2.2)$$

(x, y, z) and (r, θ, ϕ) being the Cartesian and spherical polar coordinates of \vec{r} . The Laplacian can also be expressed in terms of the orbital angular momentum operator \hat{L}^2

$$\nabla^2 = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) - \frac{\hat{L}^2}{r^2 \hbar^2}, \quad (2.3)$$

since \hat{L}^2 is given in spherical polar coordinates as

$$\hat{L}^2 = -\hbar^2 \left[\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right]. \quad (2.4)$$

The operator \hat{L}^2 satisfies an eigenvalue equation

$$\hat{L}^2 Y_{lm}(\theta, \phi) = \hbar^2 l(l+1) Y_{lm}(\theta, \phi), \quad (2.5)$$

with eigenvalue $\hbar^2 l(l+1)$ and the spherical harmonics $Y_{lm}(\theta, \phi)$ as the corresponding eigenfunction. Note that each component of $\hat{\mathbf{L}}$ commutes with \hat{L}^2 , but components of $\hat{\mathbf{L}}$ do not commute among themselves in pairs. Hence, *only one component* of $\hat{\mathbf{L}}$ and \hat{L}^2 can simultaneously be specified. Conventionally, this component is chosen as the z-component \hat{L}_z , with eigenvalue $m\hbar$. $Y_{lm}(\theta, \phi)$ is the simultaneous eigenfunction of \hat{L}^2 and \hat{L}_z .

If the potential is spherically symmetric, i.e., independent of the direction (θ, ϕ) , so that $V(\vec{r}) = V(r)$ (such a potential is called *central*, since then the force is always directed along the line joining the particle with the center), then the orbital angular momentum (l) and its projection (m) are good quantum numbers (since the Hamiltonian commutes with both \hat{L}^2 and \hat{L}_z) and the wave function has the form

$$\psi_{nlm}(\vec{r}) = \frac{R_{nl}(r)}{r} Y_{lm}(\theta, \phi). \quad (2.6)$$

The factor $\frac{1}{r}$ is included to remove the first derivative with respect to r . The radial Schrödinger equation satisfied by $R_{nl}(r)$ becomes

$$\left[-\frac{\hbar^2}{2m} \frac{d^2}{dr^2} + \frac{\hbar^2 l(l+1)}{2mr^2} + V(r) - E \right] R_{nl}(r) = 0. \quad (2.7)$$

This second-order ordinary differential equation can be solved, subject to appropriate boundary conditions to get the energy eigenvalue E and the radial wave function $R_{nl}(r)$. For a bound state, the probability of finding the particle must be finite only within a finite region of space and vanish at great distances from the center. Hence, $R_{nl}(r)$ must be square integrable and vanish for $r \rightarrow \infty$. From Eq. (2.7), we see that this requirement is satisfied if $E < V(\infty)$. Moreover, since ψ should be finite everywhere, Eq. (2.6) shows that $R_{nl}(r)$ must also vanish at the origin. Imposition of these boundary conditions at the origin and at $r \rightarrow \infty$ makes energy eigenvalue (E) *discrete* and less than $V(\infty)$ for the bound state. The *quantum number* n is usually associated with numbering the discrete energy eigenvalues consecutively with increasing energy, for a particular l . Taking $n = 0$ for the lowest energy state for a particular value of l , n is the number of nodes in the radial wave function $R_{nl}(r)$.

For the unbound scattering state, probability of finding the particle at a large distance is nonvanishing. Hence, $E > V(\infty)$ and energy eigenvalues form a *continuum* [7]. In this case, the discrete quantum number n is replaced by the energy eigenvalue E . The boundary conditions on the radial wave function are $R_{E,l}(r)$ vanishes at the origin, while it oscillates with a finite amplitude as $r \rightarrow \infty$.

If the potential has a simple form, like an infinite square well, a harmonic oscillator, or a Coulomb potential, the radial equation can be solved analytically, although for most other potentials, analytic solutions are not possible. What is the inherent reason that only some potentials admit exact analytic solutions? This can be understood from the concept of supersymmetric quantum mechanics. Using the technique of supersymmetric quantum mechanics [8], one can obtain a supersymmetric partner potential for any given potential. Then it can be shown that exact algebraic solutions can be obtained for a potential, if the potential and its supersymmetric partner have the same mathematical shape, but involves different parameters. Such a potential is called a *shape invariant potential*. It has been shown that only a few potentials belong to this category, the infinite square well, the harmonic oscillator, and the Coulomb potentials being some of them [8].

Unfortunately, most of the potentials appearing in physical problems do not permit any analytical solution. In such cases, we need to solve the Schrödinger equation numerically. Usually, the second-order differential equation (2.7) is written as a system of two coupled first-order differential equations, which are then solved by a standard technique, e.g., the Runge–Kutta algorithm [9]. Choosing an initial trial energy, the integration is done in two parts: outward from the origin to a suitably chosen match radius (r_M) and inward from a large enough value of r to r_M . Next the trial energy is changed until the log derivatives at $r = r_M$ obtained from the inward and outward integrations match (usually done by a root-finding algorithm [9]). This gives the eigen energy. The wave function obtained at this energy is then normalized to get the final normalized wave function. The method will be discussed in detail in Chap. 10.

2.2 Two-Body System with Mutual Interaction

We now consider the next more complex system, *viz.*, the two-body system interacting through mutual forces. In addition to solving the two-body Schrödinger equation, we have to worry about the symmetry of the wave function, if the particles are identical [1]. This brings the spin of the particle into consideration, even if the potential is spin independent. If, in addition, the mutual force depends on the spins of the particles, additional terms in the Hamiltonian coming from the spins are to be considered. Thus we see that the system already starts to be complicated, even when it contains only two particles. First, we discuss how the two-body Schrödinger equation in space variables can be solved in a suitable way.

2.2.1 Two Distinct Particles

For a system consisting of two particles of masses m_1 and m_2 with position vectors \vec{r}_1 and \vec{r}_2 and interacting through a mutual time-independent potential $V(\vec{r}_1 - \vec{r}_2)$, the Schrödinger equation is (for the moment we ignore spin variables)

$$\left[-\frac{\hbar^2}{2m_1} \nabla_1^2 - \frac{\hbar^2}{2m_2} \nabla_2^2 + V(\vec{r}_1 - \vec{r}_2) - E_T \right] \Psi(\vec{r}_1, \vec{r}_2) = 0, \quad (2.8)$$

E_T is the total energy of the system and

$$\begin{aligned} \nabla_i^2 &= \frac{\partial^2}{\partial x_i^2} + \frac{\partial^2}{\partial y_i^2} + \frac{\partial^2}{\partial z_i^2} \\ &= \frac{1}{r_i^2} \frac{\partial}{\partial r_i} \left(r_i^2 \frac{\partial}{\partial r_i} \right) + \frac{1}{r_i^2 \sin \theta_i} \frac{\partial}{\partial \theta_i} \left(\sin \theta_i \frac{\partial}{\partial \theta_i} \right) + \frac{1}{r_i^2 \sin^2 \theta_i} \frac{\partial^2}{\partial \phi_i^2}. \end{aligned} \quad (2.9)$$

where (x_i, y_i, z_i) are the Cartesian coordinates and (r_i, θ_i, ϕ_i) are the spherical polar coordinates of \vec{r}_i ($i = 1, 2$). In order to solve this equation, one can easily separate the relative motion from the center-of-mass motion, by introducing the relative vector [7]

$$\vec{r} = \vec{r}_1 - \vec{r}_2 \quad (2.10)$$

and the center-of-mass vector

$$\vec{R} = \frac{m_1 \vec{r}_1 + m_2 \vec{r}_2}{m_1 + m_2}. \quad (2.11)$$

By a straight forward evaluation of the partial derivatives, we can verify that

$$\frac{1}{m_1} \nabla_1^2 + \frac{1}{m_2} \nabla_2^2 = \frac{1}{\mu} \nabla_r^2 + \frac{1}{M} \nabla_R^2, \quad (2.12)$$

where ∇_r^2 and ∇_R^2 are the Laplacians with respect to \vec{r} and \vec{R} , respectively, $M = m_1 + m_2$ is the total mass and

$$\mu = \frac{m_1 m_2}{m_1 + m_2} \quad (2.13)$$

is the *reduced mass* of the system. Since the Laplacian of the two-body system separates into the sum of Laplacians of the relative and the center-of-mass coordinates and the potential is a function of \vec{r} only, the eigenfunction Ψ [expressed as a function of \vec{r} and \vec{R} , using Eqs. (2.10) and (2.11)] becomes separable into a product of the relative and the center-of-mass wave functions

$$\Psi(\vec{r}, \vec{R}) = \psi(\vec{r}) \Phi(\vec{R}). \quad (2.14)$$

Substituting Eq. (2.12) in Eq. (2.8) and dividing throughout by Ψ , we have

$$\frac{1}{\psi(\vec{r})} \left[-\frac{\hbar^2}{2\mu} \nabla_r^2 + V(\vec{r}) \right] \psi(\vec{r}) = \frac{1}{\Phi(\vec{R})} \left[\frac{\hbar^2}{2M} \nabla_R^2 \right] \Phi(\vec{R}) + E_T. \quad (2.15)$$

We note that the left side is a function of \vec{r} only, while the right side is a function of \vec{R} only. This can be true for arbitrary values of \vec{r} and \vec{R} , only if each side is a constant, independent of \vec{r} and \vec{R} . Calling this separation constant E , we have

$$\left[-\frac{\hbar^2}{2\mu} \nabla_r^2 + V(\vec{r}) \right] \psi(\vec{r}) = E \psi(\vec{r}) \quad (2.16)$$

$$\left[-\frac{\hbar^2}{2M} \nabla_R^2 \right] \Phi(\vec{R}) = E_{CM} \Phi(\vec{R}), \quad (2.17)$$

where $E_{CM} = E_T - E$ is the energy of the center-of-mass motion, E is the energy of the relative motion, and E_T is the total energy. Equation (2.17) shows that the center-of-mass of the system moves like a *free particle* of mass M (sum of the individual masses) and momentum $\vec{P} = \hbar \vec{K}$

$$\Phi(\vec{R}) = C e^{i \vec{K} \cdot \vec{R}}, \quad (2.18)$$

where C is a normalization constant and $E_{CM} = \frac{\hbar^2 K^2}{2M}$. This is expected, since there is no *external force* and the entire system of two particles moves like a free body as a single entity. Since only the relative motion of the two particles under their mutual force is of physical interest, we need to consider only Eq. (2.16). This is the same as the one-body Schrödinger equation (2.1). Thus a two-body system under mutual force only is equivalent to the motion of a single *fictitious particle* of mass μ moving in a *potential field* $V(\vec{r})$. This equation can be solved as discussed in the last section.

2.2.2 Two Identical Particles: Symmetry of Wave Function

As mentioned at the beginning of this section, we have to worry about the symmetry of the wave function, if the particles are identical (hence $m_1 = m_2$). The two-body wave function should be symmetric for two identical bosons (integral spin particles) and antisymmetric for two identical fermions (half-integral spin particles).

We first discuss the symmetry of the space part of the wave function, ignoring the spin degrees of freedom for the time being. The symmetric (upper sign) and antisymmetric (lower sign) wave functions under pair exchange operator P_{12} satisfy

$$P_{12} \Psi(\vec{r}_1, \vec{r}_2) = \Psi(\vec{r}_2, \vec{r}_1) = \pm \Psi(\vec{r}_1, \vec{r}_2). \quad (2.19)$$

Now, Eqs. (2.10) and (2.11) show that under this exchange \vec{r} becomes $-\vec{r}$, while \vec{R} remains unchanged. Hence, the center-of-mass motion remains unaffected while the relative wave function $\psi(\vec{r})$ becomes $\psi(-\vec{r})$. This corresponds to the parity operation, $\vec{r} \rightarrow -\vec{r} = (r, \pi - \theta, \pi + \phi)$, and the spherical harmonics in Eq. (2.6) becomes

$$Y_{lm}(\pi - \theta, \pi + \phi) = (-1)^l Y_{lm}(\theta, \phi). \quad (2.20)$$

Hence, Eq. (2.19) will be satisfied only if l is even for upper sign (symmetric wave function) and odd for lower sign (antisymmetric wave function). In the following, we will see how the full wave function (including spin wave function) should be properly symmetrized.

2.2.3 Inclusion of Spin Degrees of Freedom

Next we consider a two-body system in which spin degrees of freedom come into play. In the most general case, the forces may depend on spin, position, and orbital angular momentum. The total spin S (where $\vec{S} = \vec{s}_1 + \vec{s}_2$, \vec{s}_i being the spin operator of the i th particle, $i = 1, 2$) and its projection M_S , as well as the orbital angular momentum l (where $\vec{l} = \vec{l}_1 + \vec{l}_2$, \vec{l}_i being the orbital angular momentum of the i th particle), and its projection m_l are good quantum numbers, if either the total mutual force is spin independent or if it contains $\vec{s}_1 \cdot \vec{s}_2$ only. However, if there is spin-orbit force ($\vec{l} \cdot \vec{S}$) the good quantum numbers are l, S, J, M_J where J and M_J are the eigenvalues corresponding to the total angular momentum ($\vec{J} = \vec{l} + \vec{S}$) and its projection. For tensor force [given by $3(\vec{\sigma}_1 \cdot \hat{r})(\vec{\sigma}_2 \cdot \hat{r}) - (\vec{\sigma}_1 \cdot \vec{\sigma}_2)$, where $\vec{\sigma}_i$ is the Pauli spin operator for the i th particle], there can be l mixing.

First, we consider two distinct particles for the simple case where l, S, m_l, M_S are good. Typical examples are the simple model of the hydrogen atom, where the interaction between the proton and the electron is spin independent or a simple model of the deuteron nucleus, where the interaction between the proton and the neutron depends on S (ignoring the tensor force). For the simple model of the hydrogen atom, since spin does not appear at all, the spin wave function is either singlet ($S = 0$) or triplet ($S = 1$) and is commonly suppressed. The most important part of nuclear force is spin dependent (contains $\vec{s}_1 \cdot \vec{s}_2$), the force in the triplet state being more strongly attractive than that in the singlet state. In the simple model of deuteron (with proton and neutron treated as distinct particles), the singlet ($S = 0$) and triplet ($S = 1$) states are independently calculated (temporarily suppressing spin variables) with singlet and triplet potentials, respectively.

The total wave function now becomes a product of space and spin wave functions

$$\Psi^{Total}(1, 2) \equiv \Psi^{Total}(\vec{r}_1, \vec{s}_1, \vec{r}_2, \vec{s}_2) = \Psi(\vec{r}_1, \vec{r}_2) \chi(\vec{s}_1, \vec{s}_2), \quad (2.21)$$

where \vec{s}_i is the spin variable, given by the spin and its projection operators, $\{\hat{s}_i, \hat{s}_{iz}\}$, of the i th particle ($i = 1, 2$). If the particles are distinct, there is no requirement of symmetry of the total wave function. If the interaction is spin independent (as in the case of simple hydrogen atom), $\chi(\vec{s}_1, \vec{s}_2)$ can take any of the possible S, M_S values, while $\Psi(\vec{r}_1, \vec{r}_2)$ remains the same. If there is spin-dependent force (as in the simple deuteron model), for each possible $\chi(\vec{s}_1, \vec{s}_2)$, the space wave function $\Psi(\vec{r}_1, \vec{r}_2)$ will be different, depending on the potential, which depends on $\vec{s}_1 \cdot \vec{s}_2$.

Next consider two identical particles. Since the *total wave function* has to be symmetric for identical bosons and antisymmetric for identical fermions, the product $\Psi \chi$ should have the appropriate symmetry. Thus for bosons, both space and spin wave functions must be symmetric or both must be antisymmetric. For fermions, if one is symmetric, the other must be antisymmetric. We already saw that Ψ is symmetric or antisymmetric for even or odd l , respectively. The spin wave function χ is symmetric or antisymmetric for $S = 1$ or $S = 0$, respectively. If l, S, m_l, M_S are good (no mixing of l and S), we simply have to combine appropriate symmetry of Ψ and χ in Eq. (2.21). If there is mixing of l or S , the right side of Eq. (2.21) should be a sum of appropriate combinations of Ψ and χ , corresponding to possible (l, S) values.

Two-Body Spin Wave Function

Denoting the spin state of the i th particle by $|s_i, m_{s_i}\rangle$ (where m_{s_i} is the eigenvalue of \hat{s}_{iz}), the two-body spin wave function becomes

$$\chi(\vec{s}_1, \vec{s}_2) \equiv |s_1, s_2, S, M_S\rangle = \sum_{m_{s_1}, m_{s_2}} \langle s_1, m_{s_1}, s_2, m_{s_2} | S, M_S \rangle |s_1, m_{s_1}\rangle |s_2, m_{s_2}\rangle, \quad (2.22)$$

where $\langle s_1, m_{s_1}, s_2, m_{s_2} | S, M_S \rangle$ is a Clebsch–Gordan (CG) coefficient. The spin wave function is represented by the ket vector. S and M_S are, respectively, the total spin and its projection

$$\begin{aligned} \vec{S} &= \vec{s}_1 + \vec{s}_2, \\ M_S &= m_{s_1} + m_{s_2}. \end{aligned} \quad (2.23)$$

By angular momentum selection rule $|s_1 - s_2| \leq S \leq (s_1 + s_2)$, i.e., S can take the values $|s_1 - s_2|, |s_1 - s_2| + 1, |s_1 - s_2| + 2, \dots, (s_1 + s_2)$. It can easily be seen that the state with the maximum spin $S = s_1 + s_2$ will be symmetric, the state with next lower S will be antisymmetric, the next lower one symmetric, and so on.

2.2.4 Introduction of Isospin Degrees of Freedom for Nucleons

The nucleons, viz., the proton and the neutron, have nearly the same mass and both are spin $\frac{1}{2}$ particles. It is known experimentally that the nuclear parts of their interactions

are the same, at least at low energies. So they can be treated as two states of a single particle called *nucleon*. A fictitious ‘spin,’ in analogy with the common spin, is associated with the nucleon and called *isospin*, such that the proton and the neutron are two states with a different ‘isospin projection’ of the *nucleon*. Since there are only two projection states of the nucleon, its isospin is $t = \frac{1}{2}$. The projections (called t_{i3} instead of t_{i_z} , since \vec{t}_i is not really a vector in three-dimensional coordinate space) of proton and the neutron are $\frac{1}{2}$ and $-\frac{1}{2}$, respectively. Note that this is a purely mathematical construction for convenience and the *isospin* is not a physical quantity. If \vec{t}_i is the isospin of the i th particle, the total isospin of two nucleons is $\vec{T} = \vec{t}_1 + \vec{t}_2$. Then in exact analogy with Eq. (2.22), one can construct isospin state $|t_1, t_2, T, M_T\rangle$ of two nucleons. Clearly, T can take two values, viz. 0 and 1, which are, respectively, antisymmetric and symmetric under P_{12} in the isospin space. With the introduction of this isospin degree of freedom, the total wave function becomes

$$\Psi^{Total}(1, 2) \equiv \Psi^{Total}(\vec{r}_1, \vec{s}_1, \vec{t}_1; \vec{r}_2, \vec{s}_2, \vec{t}_2) = \Psi(\vec{r}_1, \vec{r}_2)\chi(\vec{s}_1, \vec{s}_2)\tau(\vec{t}_1, \vec{t}_2), \quad (2.24)$$

where $\tau(\vec{t}_1, \vec{t}_2)$ is the two-body isospin wave function. The total wave function must be antisymmetric under P_{12} , i.e., out of the space, spin, and isospin wave functions, either all three can be antisymmetric, or only one antisymmetric and the other two symmetric. Thus for two nucleons, $T = 1$ states can be spin-triplet odd l (abbreviated as triplet-odd) or spin-singlet even l (singlet-even). Similarly, $T = 0$ states can be triplet-even or singlet-odd. Note that with the introduction of isospin, the deuteron is a two-body system of identical particles. However, without the isospin, it is a system of two distinct particles. Both the descriptions are valid, although imposition of symmetry actually reduces the number of possibilities and thus simplifies the problem.

2.3 System of Several Particles

The situation becomes already complicated, when three mutually interacting particles are involved, since it will involve two relative vectors, after removal of the CM motion. Clearly, the situation worsens rapidly as the number of interacting particles in the system increases. In the next chapter, we will discuss the three-body system in detail. In this section, we discuss some general features of the A -body system.

The Schrödinger equation for a system of A particles of mass m_i ($i = 1, A$), interacting through pair-wise mutual forces, is

$$\left[-\sum_{i=1}^A \frac{\hbar^2}{2m_i} \nabla_i^2 + \sum_{i < j=2}^A V(\vec{r}_i - \vec{r}_j) \right] \Psi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_A) = E \Psi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_A). \quad (2.25)$$

The restriction $i < j = 2$, A in Eq. (2.25) is needed to avoid double counting of pair-wise interactions. In this case also, we can separate the center-of-mass (CM) motion in terms of the CM vector \vec{R} . In addition, there will be $N = (A - 1)$ relative vectors to describe the space part of the relative motion. For a mutually interacting system without any externally applied field, the CM motion is not important, and only the relative motion has to be studied. This involves $(3A - 3)$ degrees of freedom for the space part alone. Associated algebraic procedure is very involved, as we will see in the following chapters. Imposition of symmetry is also very complicated. For $A \geq 3$, there will be states of mixed symmetry, in addition to states, which are totally symmetric or totally antisymmetric under pair exchanges. Introduction of spin of the particles (and isospin, if it is relevant) will further complicate the form of the total wave function. For a system of identical bosons or fermions, the total wave function with the appropriate symmetry will be obtained as a sum of products of space and spin (and also isospin, where the latter is relevant) wave functions of conjugate symmetry, such that each product has the desired symmetry. Clearly, this is going to be a nontrivial exercise and will be dealt in the following chapters.

2.3.1 Independent Particle Model: Mean-Field Description

However, the situation simplifies immensely, if the total interaction of a system of identical particles (with $m_i = m$, $i = 1, A$) is separable and $\sum_{i < j=2}^A V(\vec{r}_i - \vec{r}_j)$ can be replaced by $\sum_{i=1}^A \bar{V}(\vec{r}_i)$, such that each individual particle is subjected to the *same* potential field $\bar{V}(\vec{r})$. Then Eq. (2.25) is replaced by

$$\left[-\sum_{i=1}^A \frac{\hbar^2}{2m} \nabla_i^2 + \sum_{i=1}^A \bar{V}(\vec{r}_i) \right] \Psi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_A) = E \Psi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_A). \quad (2.26)$$

In this case, the many-body wave function is separable into a product of single-particle (s.p.) wave functions

$$\Psi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_A) = \prod_{i=1}^A \psi_{\alpha_i}(\vec{r}_i), \quad (2.27)$$

with

$$E = \sum_{i=1}^A \epsilon_{\alpha_i}, \quad (2.28)$$

where $\psi_{\alpha_i}(\vec{r}_i)$ satisfies a single particle Schrödinger equation

$$\left[-\frac{\hbar^2}{2m} \nabla_i^2 + \bar{V}(\vec{r}_i) \right] \psi_{\alpha_i}(\vec{r}_i) = \epsilon_{\alpha_i} \psi_{\alpha_i}(\vec{r}_i). \quad (2.29)$$

Here α_i represents an abbreviated form of s.p. quantum numbers (a set of three quantum numbers for the space wave function) associated with a particular s.p. state $|\alpha_i\rangle$ of the Hamiltonian $\hat{h}_i = -\frac{\hbar^2}{2m}\nabla_i^2 + \bar{V}(\vec{r}_i)$. The full Hamiltonian of the system is $\hat{H} = \sum_i \hat{h}_i$. Since \hat{h}_i is the same for all i , the subscript i can be dropped in Eq. (2.29). Thus the many-body problem reduces immediately to the solution of a one-body problem, which is easy to solve and has already been discussed.

It may appear that the satisfaction of the condition $\sum_{i < j=2}^A V(\vec{r}_i - \vec{r}_j) = \sum_{i=1}^A \bar{V}(\vec{r}_i)$ is extremely fortuitous and very unlikely in a real physical situation. Indeed, we may never be so lucky as to have this condition exactly satisfied. However, in a real situation like a nucleus (with many nucleons) or an atom (with many electrons), it may not be very far from truth. In such a case, each one of the particles (nucleons or electrons) moves in the *same* common field produced by all the remaining particles in the system. Hence, to a good approximation, each particle moves in the *same mean field* $\bar{V}(\vec{r})$, produced as a result of interactions and motions of all the remaining particles. This physical scenario may be understood by the following crude analogy. Consider a merry-go-round, in which each individual can go in completely random and fast orbital motion. Then a particular individual will not ‘see’ any other particular individual, but only a cloud (‘field’) around himself, due to fast relative motions of all others. However, every other individual will ‘see’ the *same* cloud. Thus, the sum total of all the individual interactions will effectively be seen as each individual experiencing the same common field. This is the physical basis of the *mean-field theory* (MFT). This leads to the highly successful *shell model* in a nucleus or in an atom. The difference $\sum_{i < j=2}^A V(\vec{r}_i - \vec{r}_j) - \sum_{i=1}^A \bar{V}(\vec{r}_i)$, called *residual interaction*, can be treated as a perturbation. In the MFT, the mean field $\bar{V}(\vec{r})$ can be calculated using suitably chosen trial single-particle wave function $\psi_{\alpha_i}(\vec{r}_i)$. This is then substituted in Eq. (2.29) and a fresh set of $\psi_{\alpha_i}(\vec{r}_i)$ recalculated. This process is repeated until convergence is achieved.

If the particles in the system (a nucleus or an atom in the above example) are identical, we have to symmetrize the wave function appropriately. Since the particles are identical, any permutation of the particle indices leaves the Hamiltonian invariant. Thus the system obeys permutation symmetry and energy eigenvalues are degenerate under permutation operations. We can see this from Eqs. (2.27) and (2.28). Any permutation of the particle indices produces another wave function which is different and orthogonal to the original one, but corresponds to the same energy. Hence, any linear combination of these degenerate eigenfunctions is also a solution belonging to the same energy. The symmetrization postulate demands that the physical wave function be totally symmetric or totally antisymmetric under any pair exchange, for a system of identical bosons or identical fermions, respectively. Hence, totally symmetric or totally antisymmetric linear combinations of Eq. (2.27) should be chosen for a boson system or a fermion system, respectively. Now, any permutation (\hat{P}) can be obtained as a set of n_P successive pair exchanges. Hence, the symmetric wave function is

$$\Psi^{(symmetric)}(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_A) = \frac{1}{\sqrt{A!}} \sum_{\hat{P}} \hat{P} \prod_{i=1}^A \psi_{\alpha_i}(\vec{r}_i), \quad (2.30)$$

and the antisymmetric wave function is

$$\Psi^{(antisymmetric)}(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_A) = \frac{1}{\sqrt{A!}} \sum_{\hat{P}} (-1)^{n_P} \hat{P} \prod_{i=1}^A \psi_{\alpha_i}(\vec{r}_i). \quad (2.31)$$

The factor $\frac{1}{\sqrt{A!}}$ in front is the normalization constant, since each s.p. wave function $\psi_{\alpha_i}(\vec{r}_i)$ [as also $\Psi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_A)$] is normalized and there are $A!$ permutations. As spin (and isospin for nucleons) degrees are relevant for identical particles, the abbreviated quantum number α_i will now include spin (and isospin for nucleons) and their projections. Including the spin degrees of freedom, the variable \vec{r}_i is replaced by the abbreviated notation i (for the i th particle), which stands for $\{\vec{r}_i, \vec{s}_i\}$. With the addition of isospin, i represents $\{\vec{r}_i, \vec{s}_i, \vec{t}_i\}$. With this notation, the antisymmetric wave function, Eq. (2.31), is just the determinantal wave function

$$\Psi^{(antisymmetric)}(1, 2, \dots, A) = \frac{1}{\sqrt{A!}} \begin{vmatrix} \psi_{\alpha_1}(1) & \psi_{\alpha_1}(2) & \dots & \psi_{\alpha_1}(A) \\ \psi_{\alpha_2}(1) & \psi_{\alpha_2}(2) & \dots & \psi_{\alpha_2}(A) \\ \dots & \dots & \dots & \dots \\ \psi_{\alpha_A}(1) & \psi_{\alpha_A}(2) & \dots & \psi_{\alpha_A}(A) \end{vmatrix}. \quad (2.32)$$

This determinant is called the *Slater determinant*. Any pair exchange of two particles corresponds to exchanging two columns of this determinant, which results in the same determinant with a negative sign. Thus, it clearly shows that this wave function is antisymmetric under any pair exchange.

2.3.2 Many-Body Description

The discussion in the previous subsection considers the total wave function as a product wave function. This is an independent particle model of the system and is exact only if the total Hamiltonian is separable in the particle indices. For an exact treatment of a realistic case, Eq. (2.25) must be solved. As we explained earlier, the treatment of the space part becomes very complicated as the number of particles increases. In addition, imposition of the required symmetry of the total wave function becomes quite involved. This is because unlike the simple product wave function where only a particular linear combination of the s.p. wave functions gives the desired symmetry, one has to sum combinations of space wave function of a particular (including mixed) symmetry with spin wave function (and isospin wave function, where it is relevant) of the conjugate symmetry. We will see how this can be done for the trinucleon system in Chap. 5.

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