Radial Equation of Bound State and Binding Energies of Ξ^- Hypernuclei *

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Abstract The radial equation in its standard form, which can be solved by using the threepoint central difference method from central two points towards outside point by point, is reduced from Schrödinger equation or from the low energy approximation of Dirac equation. In this paper, a method for solving the radial equation of the bound state to get the binding energy and the radial wave function is given, and the binding energies of the ground state (GS) of several Ξ^- hypernuclei are calculated.

Key words radial equation of bound state, central difference method, binding energy of ground state

1 Introduction

In many fields, such as quantum mechanics, atomic and nuclear physics, how to solve the radial equation to get the eigenvalue and the eigenfunction of the bound state is always encountered. Among this kind of equations only a few of them can be solved analytically, and most of them have to be solved with numerical method. In this work we introduce a very useful numerical method with which the radial equation of the bound state can be solved. As an application, the binding energies of the ground states (GS) of several Ξ^- hypernuclei are calculated and analyzed.

2 Formulae and methods

The motion of a particle with spin 1/2 (electron, nucleon, hyperon, and so on) in a central potential field is governed by the Schrödinger equation

$$\left[-\frac{\hbar^2}{2\mu}\nabla^2+V(r)\right]\Psi(\boldsymbol{r},\zeta)=\varepsilon\Psi(\boldsymbol{r},\zeta), \quad (1)$$

or by the Dirac equation

$$[c\boldsymbol{\alpha}\cdot\boldsymbol{p}+\beta(\mu c^2+V_s(r))+V_v(r)+V_c(r)]\Psi(\boldsymbol{r},\zeta)=E\Psi(\boldsymbol{r},\zeta). \quad (2)$$

In the case of a hyperon moving in a hypernucleus, the potential in the Schrödinger equation can be written as

$$V(r)=V_{cen}(r)+V_{so}(r)+V_c(r),$$

where

$$V_{cen}(r)=-\frac{U_{cen}}{\rho_{cen,0}}\rho_{cen}(r)$$

is the central potential,

$$V_{so}(r)=-\frac{\lambda_\pi^2 U_{so}}{\rho_{so,0}\,r}[(j(j+1)-l(l+1)-3/4]\frac{\mathrm{d}\rho_{so}(r)}{\mathrm{d}r}$$

is the spin-orbital coupling potential,

$$V_c(r)(\mathrm{MeV})=\begin{cases}1.440975\,Z_\Xi Z/r & \text{if } r>R_c(\mathrm{fm})\\ \dfrac{0.720488}{R_c}Z_\Xi Z\left(3-\dfrac{r^2}{R_c^2}\right) & \text{if } r\leqslant R_c(\mathrm{fm})\end{cases} \quad (6)$$

is the Coulamb potential, $\rho_i(r)$ takes the Woods-Saxon form

$$\rho_i(r)=\rho_{i,0}\Big/\left[1+\left(\exp\left(\frac{r-R_i}{a_i}\right)\right)\right]$$

$\lambda_\pi^2=(\hbar/m_\pi c)^2\approx 2.0\mathrm{fm}^2$, $R_i=r_i A^{1/3}$, $i=$ cen, so and c, $\varepsilon=-B$, and B denotes the binding energy. Assuming

$$\Psi(\boldsymbol{r},\zeta)=\frac{u_{lj}(r)}{r}\chi_{ljm}(\theta,\varphi,\zeta), \quad (8)$$

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and separating variable r from θ, φ and ζ, we obtain the radial equation

$$u''_{lj}(r) = A_{lj}(r)u_{lj}(r), \tag{9}$$

where

$$A_{lj}(r) = \frac{l(l+1)}{r^2} + \frac{2\mu}{\hbar^2}[B + V(r)]. \tag{10}$$

In the Dirac equation, $\boldsymbol{\alpha}$ and β are Dirac matrices, $E = \mu c^2 + \varepsilon = \mu c^2 - B$ is the total energy,

$$V_s(r) = \frac{-U_s}{1+\exp\left(\frac{r-R_s}{a_s}\right)} \tag{11}$$

is an attractive scalar potential and

$$V_v(r) = \frac{U_v}{1+\exp\left(\frac{r-R_v}{a_v}\right)} \tag{12}$$

is a repulsive potential (time component of the four vector potential), and $V_c(r)$ is the Coulamb potential taken as that in the Schrödinger equation. Dirac spinor $\Psi(\boldsymbol{r}, \zeta)$ can be divided into two Pauli spinors $G(\boldsymbol{r}, \zeta)$ and $F(\boldsymbol{r}, \zeta)$. Assuming

$$V_-(r) = V_s(r) - V_v(r) - V_c(r), \tag{13}$$

$$V_+(r) = V_s(r) + V_v(r) + V_c(r), \tag{14}$$

$$D(r) = E + \mu c^2 + V_-(r), \tag{15}$$

$$G(\boldsymbol{r}) = \frac{\sqrt{D(r)}}{r}u_{lj}(r)\chi_{ljm}(\theta,\varphi,\zeta), \tag{16}$$

and separating variable r from θ, φ and ζ, we can also obtain a radial equation similar to Eq.(9) except

$$A_{lj}(r) = \frac{l(l+1)}{r^2} + \frac{2\mu}{\hbar^2}[B' + V_{cen}(r) + V_{so}(r)], \tag{17}$$

with the central potential

$$V_{cen}(r) = V_+(r) + \frac{B^2}{2\mu c^2} + \frac{\hbar^2}{2\mu}\left[\frac{1}{\hbar^2 c^2}(V_+(r)-B)(V_-(r)-B) - \frac{D'(r)}{rD(r)} - \frac{D''(r)}{2D(r)} + \frac{3}{4}\left(\frac{D'(r)}{D(r)}\right)^2\right], \tag{18}$$

the spin-orbital potential

$$V_{so}(r) = -\frac{\hbar^2}{2\mu}[(j(j+1) - l(l+1) - 3/4]\frac{D'(r)}{rD(r)}, \tag{19}$$

$$B' = B - B^2/2\mu c^2,\ D'(r) = \frac{dD(r)}{dr},$$

$$D''(r) = \frac{d^2D(r)}{dr^2}.$$

There is no first order differential quotient in the radial Eq.(9), thus it can be solved by Gowell central difference method (the corresponding cut-down error is $0(h^6)$). Gowell three-point recurrence formula can be writen as

$$u_{lj}(r_{i+1}) = \frac{\left[2 + \frac{5}{6}h^2A_{lj}(r_i)\right]u_{lj}(r_i) - \left[1 - \frac{h^2}{12}A_{lj}(r_{i-1})\right]u_{lj}(r_{i-1})}{1 - \frac{h^2}{12}A_{lj}(r_{i+1})}, \tag{20}$$

with $r_i = ih$, $h = 0.1$fm, $i = 0, 1, 2, \cdots$, and starting conditions

$$u_{lj}(0) = 0,\ u_{lj}(h) = h^{l+1},$$

$$A_{lj}(0)u_{lj}(0) = \lim_{r\to 0}\frac{l(l+1)}{r^2}r^{l+1} = 2\delta_{l1}. \tag{21}$$

The detailed Gowell formula is derived in the appendix. The radial Eq.(9) and the Gowell three-point recurrence Eq.(20) can be used in both the scattering and the bound state problem. In scattering problem, for a given incidental energy ε (E for Dirac equation), the radial wave function can be derived by using Eqs.(20,21) from central two points towards outside point by point to the nucleus boundary. And the complex phase shift or the S matrix element can be derived from the connection condition on the nucleus boundary between above calculated inner wave function and the outer Coulamb wave function. Then the total, elastic and absorption cross section as well as the elastic scattering angular distribution can be calculated from the S matrix element. This is the typical approach in optical model calculation, such as in Ref.[1].

In bound state problem, for a given binding energy B (B' for Dirac equation), in terms of Eq.(20), the radial wave function can also be calculated point by point from the starting conditions (21). It should be pointed out that the calculated radial wave function is not normalized, it should be normalized with certain condition that would be different for different real problems. The method for solving Eq.(20) is outlined as follows: If B_0 is a trial value near the eigenvalue of the binding energy B, the asymptotic form of the numerical solution of $u_{lj}^{B_0}(r)$ at large r is given by the linear combination of a regular ($g(B_0)\exp(-k_0r)$) and an irregular ($f(B_0)\exp(k_0r)$) solutions with $k_0^2 = 2\mu B_0/\hbar^2$. Then the radial wave function at large r can be expressed as

$$u_{lj}^{B_0}(r) = f(B_0)\exp(k_0r), \tag{22}$$

because $\exp(-k_0 r)\to 0$. For another trial value B_1, we have

$$u_{lj}^{B_1}(r) = f(B_1)\exp(k_1 r) \quad (23)$$

with $k_1^2 = 2\mu B_1/\hbar^2$. If $f(B)$ is an analytic function (slowly varying with respect to r), $f(B_1)$ can be expanded as

$$f(B_1) = f(B_0) + f'(B_0)(B_1 - B_0) + \cdots . \quad (24)$$

If $|B_1 - B_0|$ is sufficiently small, we can only keep first two terms. Then the derivative $f'(B_0)$ is given by

$$f'(B_0) = \frac{f(B_1) - f(B_0)}{B_1 - B_0} = \frac{u_{lj}^{B_1}(r)\exp(-k_1 r) - u_{lj}^{B_0}(r)\exp(-k_0 r)}{B_1 - B_0} . \quad (25)$$

If B is just the eigenvalue of the binding energy, $f(B)$ should be zero, that is

$$f(B) = f(B_0) + f'(B_0)(B - B_0) = 0, \quad (26)$$

consequently,

$$B = B_0 - f(B_0)/f'(B_0). \quad (27)$$

In the numerical calculation the recurrence method is used to calculate the eigenvalue B. Let

$$B_1 \to B_0,\ u_{lj}^{B_1}(r) \to u_{lj}^{B_0}(r),\ B \to B_1, \quad (28)$$

then calculate new $u_{lj}^{B_1}(r)$ by Eqs.(20,21) and new B value by Eqs.(25,27),⋯, until the new and old B values approach to each other within a given accuracy.

3 Binding energy of Ξ⁻ hypernuclei

In calculating the GS binding energy of the Ξ⁻ hypernucleus, phenomenological optical potentials in Eqs. (4)—(7), (11)—(15), (18)—(19) are used. The potential parameters are optimized by minimizing the χ^2 value

$$\chi^2 = \frac{1}{N}\sum_{k=1}^{N}\frac{(B_k^{ex} - B_k^{th})^2}{\sigma_k^2}, \quad (29)$$

where B_k^{ex} and B_k^{th} are the experimental and theoretical GS binding energies of k-th Ξ⁻ hypernucleus, respectively, σ_k is the error of B_k^{ex}, N is the total number of Ξ⁻ hypernuclei used in the least-square fit. There are only three adjustable potential parameters a_{cen}, r_{cen} and U_{cen} for the Schrödinger equation, and four adjustable parameters $a_s = a_v$, $r_s = r_v$, U_s and U_v for the Dirac equation, $r_c = 1.15$ fm is fixed for both cases.

The resultant potential parameters are $a_{cen} = 0.31333$ fm, $r_{cen} = 0.93333$ fm and $U_{cen} = 26.66098$ MeV with $\chi^2 = 0.21611$ for the Schrödinger equation, and $a_s = a_v = 0.29221$ fm, $r_s = r_v = 0.955016$ fm, $U_s = 218.3073$ MeV and $U_v = 191.3731$ MeV ($U_+ = U_s - U_v = 26.9342$ MeV, $U_- = U_s + U_v = 409.6804$ MeV) with $\chi^2 = 0.23336$ for the Dirac equation. The experimental and theoretical GS binding energies for five known Ξ⁻ hypernuclei are given in table 1. The experimental values are taken from Ref.[2].

Table 1. GS binding energies of five Ξ⁻ hypernuclei (in MeV).

Ξ⁻ hypernuclei	$B_{\Xi^-}^{ex}$	$B_{\Xi^-}^{th}$	
		Schrödinger equation	Dirac equation
$^{8}_{\Xi^-}$He	5.9 ± 1.2	6.0134	5.9554
$^{11}_{\Xi^-}$B	9.2 ± 2.2	10.7410	10.6011
$^{15}_{\Xi^-}$C	16.0 ± 4.7	13.7277	13.5447
$^{17}_{\Xi^-}$O	16.0 ± 5.5	15.8672	15.6528
$^{28}_{\Xi^-}$Al	23.2 ± 6.8	21.5568	21.2869

It is seen from table 1 that the calculated values of $B_{\Xi^-}^{th}$ by using the Schrödinger equation and the Dirac equation are very close to each other. Also the theoretical B_{Ξ^-} are usually quite close to the experimental values, except those of $^{15}_{\Xi^-}$C. We guess that the experimental B_{Ξ^-} value of $^{15}_{\Xi^-}$C may be questionable. The obtained Ξ⁻ potential well depth $U_{cen} = 26.66$ MeV and $U_+ = 26.93$ MeV are reasonable in comparison with previous empirical values of 20 MeV[3] and 28 MeV[4], respectively, deduced by fitting the binding energies of Ξ⁻ hypernuclei in the emulsion experiment. This Ξ⁻ potential well depth is about 1/2 of that for a nucleon in the center of nucleus.

Appendix A

Deduction of Gowell recurrence formula

The Taylor expansions of $u_{lj}(r_{i+1})$ and $u_{lj}(r_{i-1})$ at the point r_i are, respectively, (for simplicity, we omit the subscripts lj in following formulae)

$$u(r_{i+1}) = u(r_i) + hu'(r_i) + \frac{h^2}{2}u''(r_i) + \frac{h^3}{6}u'''(r_i) + \frac{h^4}{24}u^{(4)}(r_i) + \frac{h^5}{120}u^{(5)}(r_i) + \frac{h^6}{720}u^{(6)}(r_i) + \cdots, \tag{A1}$$

and

$$u(r_{i-1}) = u(r_i) - hu'(r_i) + \frac{h^2}{2}u''(r_i) - \frac{h^3}{6}u'''(r_i) + \frac{h^4}{24}u^{(4)}(r_i) - \frac{h^5}{120}u^{(5)}(r_i) + \frac{h^6}{720}u^{(6)}(r_i) + \cdots, \tag{A2}$$

consequently,

$$u(r_{i+1}) - 2u(r_i) + u(r_{i-1}) = h^2u''(r_i) + \frac{h^4}{12}u^{(4)}(r_i) + \frac{h^6}{360}u^{(6)}(r_i) + \cdots. \tag{A3}$$

When h is sufficiently small, we have

$$u(r_{i+1}) - 2u(r_i) + u(r_{i-1}) \approx h^2u''(r_i) \tag{A4}$$

with the cut-down error $0(h^4)$, or

$$u(r_{i+1}) - 2u(r_i) + u(r_{i-1}) \approx h^2u''(r_i) + \frac{h^4}{12}u^{(4)}(r_i) \tag{A5}$$

with the cut-down error $0(h^6)$. Differentiating Eq.(A4) twice we obtain

$$h^2u^{(4)}(r_i) \approx u''(r_{i+1}) - 2u''(r_i) + u''(r_{i-1}). \tag{A6}$$

Substituting Eq.(A6) into Eq.(A5), we get

$$u(r_{i+1}) - 2u(r_i) + u(r_{i-1}) \approx \frac{5}{6}h^2u''(r_i) + \frac{h^2}{12}(u''(r_{i+1}) + u''(r_{i-1})). \tag{A7}$$

From Eq.(9) we know that $u''(r) = A(r)u(r)$. Substituting it into Eq.(A7), we obtain that

$$\left(1 - \frac{h^2}{12}A(r_{i+1})\right)u(r_{i+1}) \approx \left(2 + \frac{5}{6}h^2A(r_i)\right)u(r_i) - \left(1 - \frac{h^2}{12}A(r_{i-1})\right)u(r_{i-1}). \tag{A8}$$

Adding the omitted subscripts lj in Eq.(A8) we obtain the Gowell three-point recurrence formula.

$$u_{lj}(r_{i+1}) = \frac{\left[2 + \frac{5}{6}h^2A_{lj}(r_i)\right]u_{lj}(r_i) - \left[1 - \frac{h^2}{12}A_{lj}(r_{i-1})\right]u_{lj}(r_{i-1})}{1 - \frac{h^2}{12}A_{lj}(r_{i+1})}. \tag{A9}$$

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束缚态径向方程和 Ξ^- 超核的结合能*

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摘要 无论从薛定谔方程或是 Dirac 方程的低能近似出发都可导出同一标准形式的径向方程,这种径向方程可用三点中央差分格式从中心两点出发向外递推求解. 给出了一种求解束缚态的能量本征值及其径向波函数的方法并计算分析了几个 Ξ^- 超核的基态结合能.

关键词 束缚态径向方程 中央差分格式 基态结合能

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