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Effect of short-range correlations on the single proton $3s_{1/2}$ wave function in ^{206}Pb

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Abstract. We consider the experimental data for difference, $\Delta\rho_c(r)$, between the charge density distributions of the isotones ^{206}Pb – ^{205}Tl, deduced by analysis of elastic electron scattering measurements and corresponds to the shell model $3s_{1/2}$ proton orbit. We investigate the effects of two-body short-range correlations. This is done by: (a) Determining the corresponding single particle potential (mean-field), employing a novel method, directly from the single particle proton density and its first and second derivatives. We also carried out least-square fits to parametrized single particle potentials; (b) Determining the short-range correlations effect by employing the Jastrow correlated many-body wave function to derive a correlation factor for the single particle density distribution. The $3s_{1/2}$ wave functions of the determined potentials reproduce fairly well the experimental data within the quoted errors. The calculated charge density difference, $\Delta\rho_c(r)$, obtained with the inclusion of the short-range correlation effect does not reproduce the experimental data.

1. Introduction

The shell model has been very successful in explaining many features of nuclei [1,2]. The relation between the shell model wave functions and the real nuclear ones is rather complicated. Important information about it may be deduced from the measured charge density difference, $\Delta\rho_c(r)$, between charge density distributions of the isotones ^{206}Pb – ^{205}Tl [3]. The experimental data of $\Delta\rho_c(r)$ show a clear maximum at the center of ^{206}Pb with two additional maxima. This seems to be the shape obtained from a $3s_{1/2}$ single proton wave-function, in agreement with the simple shell model. It was pointed out in the literature that commonly used central potentials, such as the Woods-Saxon potential, lead to a $3s_{1/2}$ charge density in disagreement with experimental data. In particular, the central density obtained from the Woods-Saxon potential is too large by about 30%. This difference between data and the Woods-Saxon results was considered earlier in the literature resulting with the statement that it is accounted for by the effect of two-body short range correlations (SRC) on the shell model wave functions [3,4]. However, it was also stated in Ref, [5] that "there is no *significant* discrepancy between the experimental data and the Hartree-Fock calculations using reasonable effective interactions." In this work we take a closer look at this problem and ask: (i) Is there a single particle potential V(r) whose $3s_{1/2}$ wave function reproduces the experimental data? To answer this question we have developed a novel method, using the single particle Schrodinger equation for a wave function $\psi(\vec{r})$ with eigenenergy E, to determine the central potential $V(\vec{r})$ directly from the measured single particle proton density of

$3s_{1/2}$ wave function and its first and second derivatives, assuming known for all $\vec{r}$. We apply the method to the experimental data of the charge distribution of the proton $3s_{1/2}$ orbit given by the charge density difference, $\Delta\rho_c(r)$ [3]. We have also carried out fits to parametrized single particle potentials. (ii) Is the effect of short-range correlations (SRC) on the nuclear density explains the experimental data? To assess the effect of SRC we have used the Jastrow many-body correlated wave function, with a two-body correlation factor, and derived a simple and a good approximate method for calculating the effect of SRC on the single particle density distribution.

We point out that the resulting single particle potential, if found, will provide a stringent limit on the effects of short correlation on the expected values of long-range operators, an important test for the shell model. The potential can also be used as an additional experimental constraint in determining a modern energy density functional (EDF) for providing more reliable predictions of properties of nuclei and nuclear matter [6,7]. In the next section we provide a short presentation of the novel methods used in the calculations and in section 3 we present some results with the conclusion given in section 4. Some results were presented in Refs. [8,9,10].

2. Formalism

2.1 Deducing the potential from the single-particle density

From the single particle Schrodinger equation,

$$-\frac{\hbar^2}{2m}\Delta\psi + V\psi = E\psi \ , \tag{1}$$

where $V(\vec{r})$ is a real local and non-singular potential, follows that for a given single particle wave function $\psi(\vec{r})$, known for all $\vec{r}$, and given eigenvalue *E,* the corresponding single particle potential *V* is uniquely determined by

$$V(\vec{r}) = E + \frac{\hbar^2}{2m}S(\vec{r}), \qquad S(\vec{r}) = \frac{\Delta\psi(\vec{r})}{\psi(\vec{r})}. \tag{2}$$

For a non-singular *V*, $\Delta\psi(\vec{r}) = 0$, when $\psi(\vec{r}) = 0$. The general relation for $[\psi(\vec{r})]^b$, where b is a positive integer, is given in Refs. [9,10]. Here we limit our consideration to the spherically symmetric case where,

$$\psi_{nlj}(\vec{r}) = \frac{R_{nlj}(r)}{r}Y_{lj} \ . \tag{3}$$

Here, $R_{nlj}(r)$ is the radial wave function for the orbit with principal number *n*, orbital angular momentum *l* and total angular momentum *j* and Y_{lj} is the eigenfunction of the angular momenta *l* and *j*. In the following we limit the discussion to the proton $3s_{1/2}$ orbit, in which the angular momentum *l* = 0 and therefore no centrifugal and spin-orbit potentials appear in $V(\vec{r})$. Substituting (3) in (1) we obtain the Schrodinger equation for the radial wave function $R_{nlj}(r)$. Using the Schrodinger Equation for $R_{nlj}(r)$ we find that,

$$V_{cen}(r) = E + \frac{\hbar^2}{2m}S(r) - \frac{1}{2}(1-\tau_z)V_{coul}(r), \qquad S(r) = \frac{1}{R_{nlj}(r)}\frac{d^2R_{nlj}}{dr^2} \ . \tag{4}$$

where $V_{cen}(r)$ and $\frac{1}{2}(1-\tau_z)V_{coul}(r)$, are the central and coulomb potentials, respectively. Here, τ_z=1 for a neutron and -1 for a proton.

Using the relation

$$R^2_{nlj}(r) = r^2\rho_{nlj}(r) \ , \tag{5}$$

where $\rho_{nlj}(r)$ is obtained by integrating the single particle density distribution over the angles and spin variables, it is possible to extract the wave function $R_{nlj}(r)$ from the experimental data for the charge density of the $3s_{1/2}$ proton orbit and deduce the corresponding single particle potential using Eq. (4). This leads to having some numerical complications. Therefore, we develop below a method to determine the potential directly from $\rho_{nlj}(r)$ and its first and second derivatives. Using Eq. (4) for the relation between $S(r)$ and $R_{nlj}(r)$, we obtain the simple relation between $S(r)$ and R^2_{nlj},

$$S(r) = \frac{1}{2R^2_{nlj}}\left[\frac{d^2(R^2_{nlj})}{dr^2} - \frac{1}{2}\frac{1}{R^2_{nlj}}\left[\frac{d(R^2_{nlj})}{dr}\right]^2\right]. \tag{6}$$

When $R^2_{nlj} = 0$, $dR^2_{nlj}/dr = 0$. From Eq. (4), for non-singular potential, the term on the right hand side (r.h.s) of Eq. (6) in the large square brackets also vanishes. From Eqs. (5) and (6) we obtain the relation,

$$S(r) = \frac{1}{2\rho_{nlj}}\left[\frac{d^2\rho_{nlj}}{dr^2} + \frac{2}{r}\frac{d\rho_{nlj}}{dr} - \frac{1}{2\rho_{nlj}}\left(\frac{d\rho_{nlj}}{dr}\right)^2\right]. \quad (7)$$

When $\rho_{nlj} = 0$, $d\rho_{nlj}/dr = 0$. From Eq. (4), for non-singular potential, the term in the square brackets of (7) vanishes and $\frac{d^2\rho_{nlj}}{dr^2}$ also vanish.

We add that a commonly used central nuclear potential is the Woods Saxon (WS) potential,

$$V(r) = V_0/[1 + exp((r - R_1)/\mathrm{a}_0)]\,, \quad (8)$$

where, V_0, R_1 and a_0 are the depth, half radius and diffuseness parameters, respectively. For the Coulomb potential we adopt the form obtained from a uniform charge distribution of radius R_{ch},

$$V_{coul}(r) = Ze^2\begin{cases}(3 - r^2/R^2_{ch})/2R_{ch} & r \le R_{ch}\\ 1/r & r > R_{ch}\end{cases}, \quad (9)$$

where R_{ch} is deduced from the experimental value of the charge root mean square radius.We emphasize that in elastic electron-nucleus scattering measurements the charge density distribution, $\rho_{ch}(\vec{r})$ is deduced but in theoretical models the point proton density distribution, $\rho_p(\vec{r})$ is calculated. They are related by

$$\rho_{ch}(\vec{r}) = \int \rho_p(\vec{r'})\,\rho_{pfs}(\vec{r} - \vec{r'})d^3\vec{r'}\,, \quad (10)$$

where $\rho_{pfs}(\vec{r})$ is the charge density distribution of the proton. The experimental elastic electron scattering data on a free proton can be well reproduced by the expression

$$\rho_{pfs}(r) = \frac{1}{8\pi a^3}e^{-r/a}\,, \quad (11)$$

where $a^2 = \frac{1}{12}r^2_{pfs}$ with $r_{pfs} = 0.85$ fm being the corresponding charge root mean square (rms) radius [11]. The Fourier transform of the charge density $\rho_{ch}(\vec{r})$, determined by the convolution relation of Eq. (10) is given by

$$F_{ch}(q) = F_{pfs}(q)F_p(q)\,, \quad (12)$$

where $F_{ch}(q)$, $F_{pfs}(q)$ and $F_p(q)$, are the Fourier transfoms of $\rho_{ch}(r)$, $\rho_{pfs}(r)$ and $\rho_p(r)$, respectively. Eq. (12) can be used to determine the form factor $F_p(q)$. Then $\rho_p(r)$ can be obtained from $F_p(q)$ by the inverse Fourier transform and compared with theoretical predictions.

2.2 Effect of short-range correlations on the single particle density

Recently [12], we have derived and employed a simple and a good approximate method for determining the effect of short-range correlations (SRC) on the single particle densities of nucleons in nuclei. The method is obtained assuming: (i) the Jastrow ground state many body wave-function in the independent pair approximation [13,14], and (ii) the relation between the exchange terms and the direct terms of the two-body matrix element of the correlation function is similar to that of the contact interaction $V_0\delta(\vec{r}_i - \vec{r}_j)$. The Jastrow ground state wave-function has the form,

$$\Psi(\vec{r}_1, \cdots \vec{r}_A) = N_{Corr}\prod_{1\le i<j}^{A} f(|\vec{r}_i - \vec{r}_j|)\,\Phi(\vec{r}_1, \cdots \vec{r}_A), \quad (13)$$

where A is the number of nucleons, N_{Corr} is the normalization constant, $\Phi(\vec{r}_1, \cdots \vec{r}_A)$ is the independent particle model (IPM) wave-function for the ground state, given by the Slater determinant,

$$\Phi(\vec{r}_1, \cdots \vec{r}_A) = \frac{1}{\sqrt{A!}}det|\phi_i(\vec{r}_j)|\,, \quad (14)$$

of the single particle wave-functions ϕ_i with $\vec{r}_j$ stands for the set of $\vec{r}$, σ and τ, of space, spin and isospin coordinates, respectively. Note that for open shell nucleus, $\Phi(\vec{r}_1, \cdots \vec{r}_A)$ in (13) is a linear combination of slater determinants. The function $f_{ij} = f(|\vec{r}_i - \vec{r}_j|)$ in (13) is the SRC function taken in the form

$$f_{ij} = f(|\vec{r}_i - \vec{r}_j|) = 1 - e^{-\alpha|\vec{r}_i - \vec{r}_j|^2} = 1 - h_{ij}, \quad (15)$$

where the parameter α is deduced from the experimental data on the charge form factor. The effect of SRC on the proton single particle density distribution is determined by evaluating the matrix element of the density operator using the expansion

$$\prod_{1\le i<j}^{A} f_{ij}^2 = \prod_{1\le i<j}^{A}(1-g_{ij}) = 1 - \sum_{1\le i<j}^{A} g_{ij} + \frac{1}{2}\sum_{\substack{i<j,k<l \\ (ij)\neq(kl)}}^{A} g_{ij}g_{kl} - \cdots, \quad (16)$$

where, $g = 2h - h^2$. We adopt in our calculations the approximation of Ref. [14] with the ratio $d/r_0 \sim 0.5$, where d being the "healing distance" and r_0^3 is the average volume per particle. In the calculations we use the shell model harmonic oscillator wave functions.

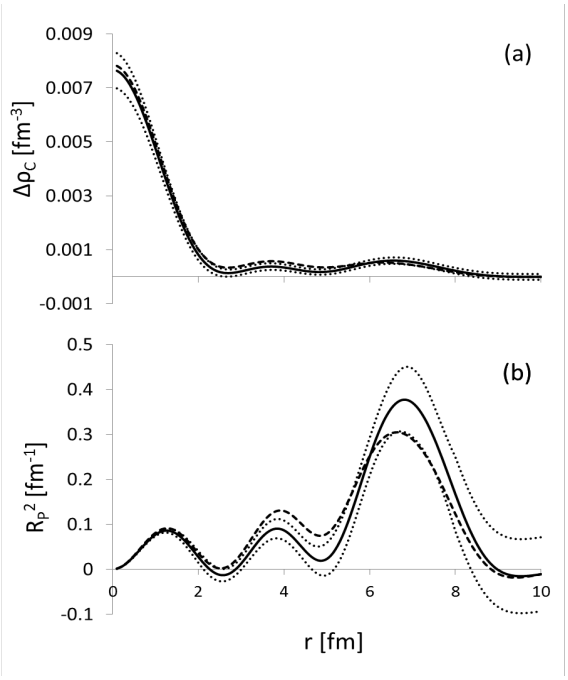

Fig.1. (a) Experimental data for the charge density difference ^{206}Pb – ^{205}Tl. The solid, dashed and dotted lines show the data, data with effect of rearrangement effect and the experimental errors, respectively. (b) Same as (a) for the $R_p^2(r)$ obtained from the experimental data.

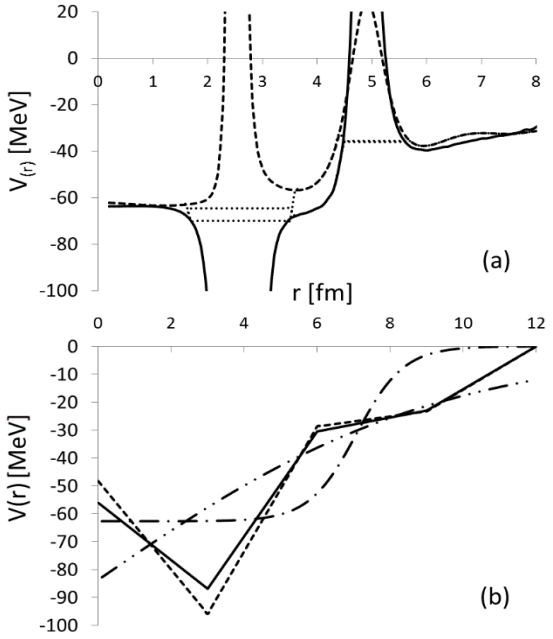

Fig.2. (a) The solid and dashed lines are the potentials deduced from Eq. (6) using Figure 1b. (b) The solid and dashed lines are the fitted broken potentials using Figure 1b. The dashed-dotted line is a fit to Woods-Saxon potential. The dashed-dotted-dotted line is the standard Woods Saxon.

3. Results

We present in Figure 1a (solid line) the experimental data [3] for the charge density difference,

$$\Delta\rho_c(r) = \rho_c(r;\ ^{206}\mathrm{Pb}) - \rho_c(r;\ ^{205}\mathrm{Tl}), \quad (17)$$

between the isotones ^{206}Pb – ^{205}Tl. The dotted lines indicate the experimental uncertainty. The two nodes associated with the proton $3s_{1/2}$ orbit are clearly seen in the figure. To assess the possible rearrangement effect (from ^{205}Tl to ^{206}Pb) on the charge rms radius of the 81 protons core in ^{206}Pb, we adopt the scaling approximation,

$$\Delta\rho_{Rc}(r) = \rho_c(r;\ ^{206}\mathrm{Pb}) - \alpha^3\rho_c(\alpha r;\ ^{205}\mathrm{Tl}), \quad (18)$$

assuming an increase by 0.005 fm, similar to the change between nuclei in this region [15]. We obtain the scaling parameter α = 5.4792/(5.4792 + 0.005) = 0.9990, the ratio between the charge rms radius of ^{205}Tl to that of the 81 core protons in ^{206}Pb. The results for $\Delta\rho_{Rc}(r)$ is shown in Figure1a (dashed line).

We determined the values of $R_p^2(r) = 4\pi r^2 \Delta\rho_p(r)$ and $R_{Rp}^2(r) = 4\pi r^2 \Delta\rho_{Rp}(r)$, deduced from the results of Figure 1a using Eqs. (10) and (12), shown as solid and dashed lines in Figure 1b, respectively The magnitude of the difference between $R_p^2(r)$ and $R_{Rp}^2(r)$ is similar to that of the experimental uncertainty. The corresponding potentials, for $R_p^2(r)$ and $R_{Rp}^2(r)$ of Figure 1b, obtained by employing Eqs. (4) - (6), are shown in Figure 2a by the solid and dashed lines, respectively. The dotted lines (constant potentials) are extracted from fits of the corresponding wave-function to Ψ= Csin(kr+ϕ), in the vicinity of the minima. The Coulomb potential of Eq. (9), with $R_{ch} = 7.1$ fm, was adopted in the calculations. Note the large uncertainties in the extracted potential in the vicinity of the nodes (at 2.6 and 4.9 fm). We have therefore considered several nuclear central potentials with parameters obtained by fits to the corresponding experimental data. In Figure 2b we show the resulting potentials fitted to $R_p^2(r)$ of Figure 1b. The solid line is a fit to broken lines potential to the solid line of Figure 1b, resulting with a good agreement with data and χ^2/N = 1.15. A similar fit to the dashed line of Figure 1b leads to the dashed line of Figure 2b with χ^2/N = 1.81. The dashed-double dotted line is a fit of the solid line of Figure 1b to a parametrized Woods-Saxon potential (9), resulting with χ^2/N = 3.28. The dashed-dotted line is the conventional Woods-Saxon potential (9), resulting with χ^2/N = 8.85 when comparing to the experimental data.

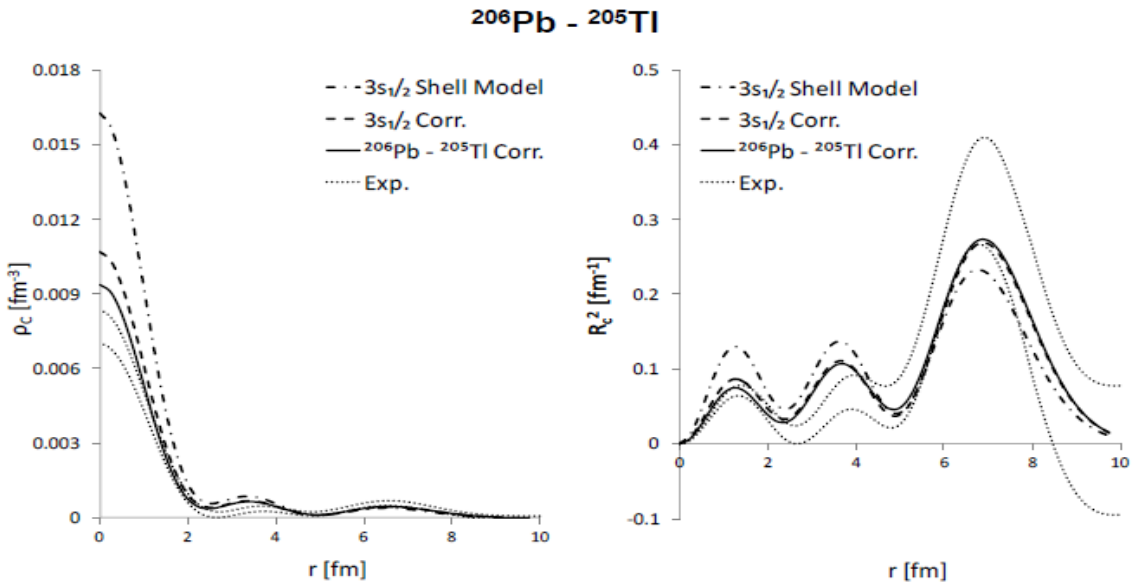

Fig. 3. Comparison between experiment and theory for the charge density of the proton $3s_{1/2}$ orbit using the Jastrow correlated wave function.

Fig. 4. Same as Figure 3 for $R_c^2(r)$.

Using the Jastrow wave function, Eq. (13), we determined the effect of SRC on the charge density distributions of ^{206}Pb and ^{205}Tl. In the calculations we adopted the shell model harmonic oscillator wave function with the size parameter $\nu = 1/5.9$ fm^{-2} and the parameter $\alpha = 1.96$ fm^{-2}. In Figs. 3 and 4 we show the results for the $3s_{1/2}$ proton charge density and the square of the radial wave-function, respectively, and compare with experimental data. The dotted lines show the experimental results for the difference between ^{206}Pb and ^{205}Tl charge distributions and the solid line is the corresponding calculated results. The dashed and dashed dotted lines are for the harmonic oscillator $3s_{1/2}$ proton orbit in ^{206}Pb with and without the effect of correlations, respectively. It is seen from Figures 3 and 4 that although the effect of SRC is to reduce the $3s_{1/2}$ single proton charge density at r = 0 by about 30%, the

calculated density disagrees with the experimental data by more than a factor of 2, particularly in the region of r = 2 – 4 fm.

4. Conclusions

We have considered the experimental data for the charge density difference between the isotones ^{206}Pb – ^{205}Tl, deduced by the analysis of elastic electron scattering measurements and corresponds to the shell model $3s_{1/2}$ proton orbit. We have investigated the effects of two-body short-range correlations. This was done by: (a) Determining the corresponding single particle potential (mean-field), employing a novel method, directly from the single particle proton density distribution and its first and second derivatives. We also carried out least-square fits to parametrized single particle potentials. The $3s_{1/2}$ wave functions of the determined potentials reproduce fairly well the experimental data within the quoted errors.; (b) Determining the effect of short-range effect correlations by employing the Jastrow correlated many-body wave function to derive a correlation factor for the density distributions of single particle orbits. The calculated $3s_{1/2}$ density obtained with the inclusion of the effect of short-range correlations does not reproduce the experimental data. Our conclusion does not contradict the existence of SRC effects in the real nuclear wave function, as demonstrated by the high momentum tail in the experimental data for the charge form factor. Our results indicate that the shell-model wave function may yield charge density distributions which are in agreement with experimental data. More accurate experimental data, with uncertainty smaller by a factor of two or more, may answer the question how well can the data be reproduced by a $3s_{1/2}$ single particle wave function obtain from mean-field calculations. It will also help to determine more exactly the deviation between data and our SRC calculations. Of course, more accurate calculations of the effect of SRC are needed.

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