

A Novel Method for Determining the Mean-Field Directly From the Single Particle Matter Density

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Outline

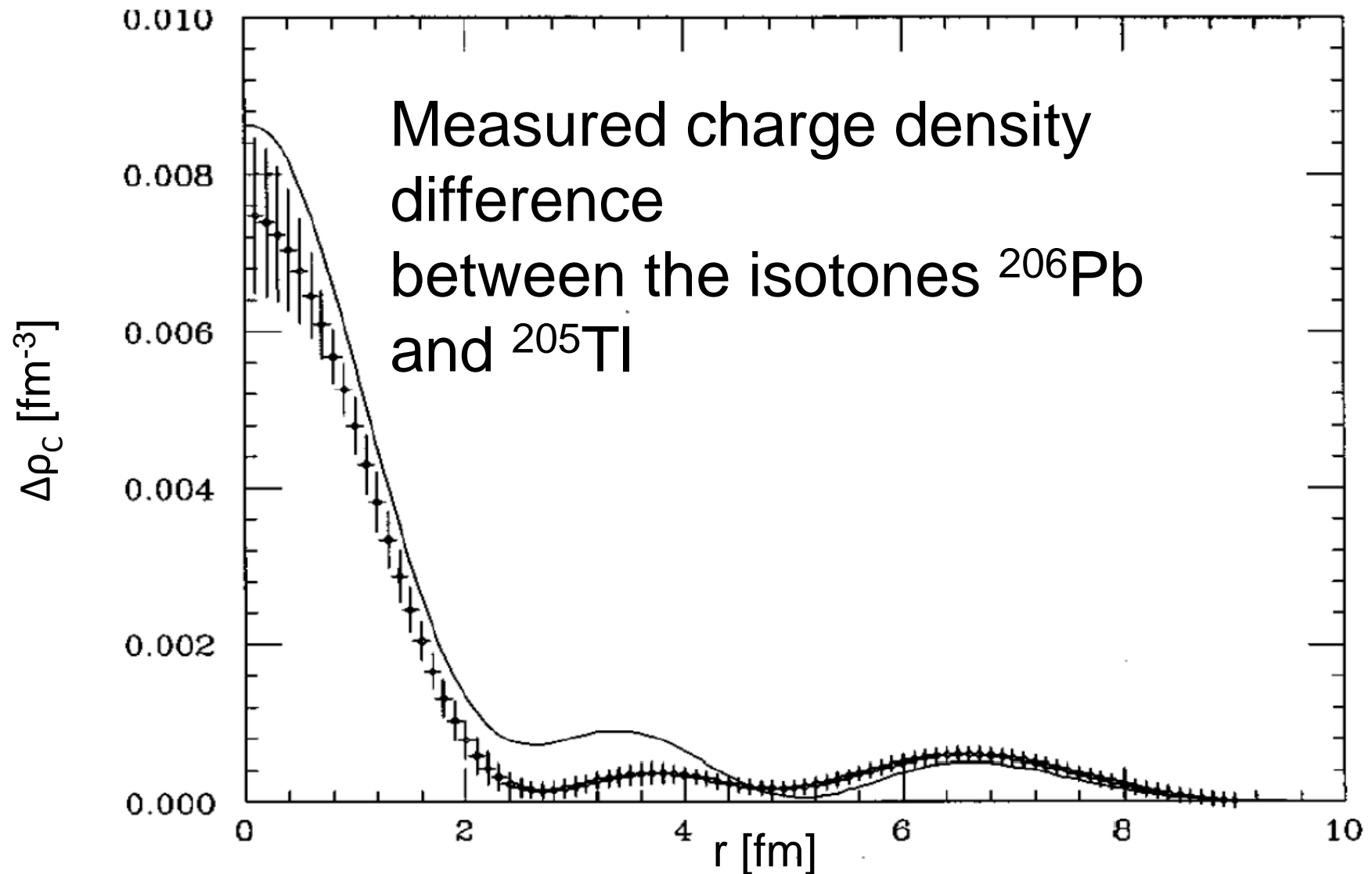
1. Introduction
2. Derivation of method, mean field from matter density
3. Application to $3s_{1/2}$ state in ^{206}Pb
4. Conclusions

Introduction

- The shell model, which is based on the assumption that nucleons in the atomic nucleus move independently in single particle orbits associated with a single particle potential, has been very successful in explaining many features of nuclei.
- In this talk I will present a novel method, using the single particle Schrodinger equation for a wave function $\Psi(\vec{r})$ with eigen-energy E , to determine the central potential $V(\vec{r})$ directly from the measured single particle matter density, $\rho(\vec{r}) = [\Psi(\vec{r})]^2$ and its first and second derivatives, assuming known for all \vec{r} .
- I present the results of an application of the method to the experimental data of the charge distribution of the proton $3s_{1/2}$ orbit given by the charge density difference, $\Delta\rho_c(r)$, between charge density distributions of the isotones $^{206}\text{Pb} - ^{205}\text{Tl}$, determined by analysis of elastic electron scattering measurements.

Introduction

- I point out that the resulting single particle potential, if found, will provide a stringent limit on the effects of short correlations on the expected values of long-range operators, an important test for the shell model.
- The resulting potential can also be used as an additional experimental constraint in determining a modern energy density functional (EDF) for more reliable prediction of properties of nuclei and nuclear matter.
- The charge density difference, $^{206}\text{Pb} - ^{205}\text{Tl}$, $3s_{1/2}$ state
- Extraction of proton matter density from charge distribution
- The matter density difference is then used to determine the mean-field potential $V(\vec{r})$ for the $3s_{1/2}$ state in ^{206}Pb
- Goal: Develop pure $3s_{1/2}$ state to see if short range correlations are negligible



Solid Line: Adjusted mean field calculation assuming a difference in occupation probabilities of 0.7 in the 3s shell and 0.3 in the 2d shell

Formalism

Single-particle Schrodinger Eq $\frac{\hbar^2}{2m} \Delta\Psi + V\Psi = E\Psi$

$$V(\vec{r}) = E + \frac{\hbar^2}{2m} S(\vec{r}), \quad S(\vec{r}) = \frac{\Delta\Psi(\vec{r})}{\Psi(\vec{r})}$$

If we know single-particle W.F. we can determine $V(\vec{r})$

Nonsingular V : $\Delta\Psi(\vec{r}) = 0$ when $\Psi(\vec{r}) = 0$

Experimentally, one measures density: $\rho(\vec{r}) = [\Psi(\vec{r})]^2$

Operating with Δ on $[\Psi(\vec{r})]^b$

b is positive and real

Using the relation $\vec{\nabla} \Psi^b = b \Psi^{b-1} \vec{\nabla} \Psi$

With the definition $S(\vec{r}) = \frac{\Delta \Psi(\vec{r})}{\Psi(\vec{r})}$

We obtain the general relation:

$$S(\vec{r}) = \frac{\Delta [\Psi(\vec{r})]^b}{b [\Psi(\vec{r})]^b} - \frac{b-1}{b^2} \left[\frac{\vec{\nabla} [\Psi(\vec{r})]^b}{[\Psi(\vec{r})]^b} \right]^2$$

For $b > 2$, $\vec{\nabla} [\Psi(\vec{r})]^b = 0$ and $\Delta [\Psi(\vec{r})]^b = 0$ when $[\Psi(\vec{r})]^b = 0$.

For $b = 1$, Single Particle Schrodinger Equation

For $b = 2$, $\rho(\vec{r}) = [\Psi(\vec{r})]^2$.

$$\text{Spherical: } \Psi_{nlj}(\vec{r}) = \frac{R_{nlj}(r)}{r} Y_{lj}$$

$$-\frac{\hbar^2}{2m} \frac{d^2 R_{nlj}}{dr^2} + \left[V(r) + \frac{\hbar^2}{2m} \frac{l(l+1)}{r^2} \right] R_{nlj} = E R_{nlj}$$

$$V(r) = V_{cen}(r) + \vec{s} \cdot \vec{l} V_{s.o.}(r) + \frac{1}{2} (1 - \tau_z) V_{coul}(r)$$

$$V_{cen}(r) = E + \frac{\hbar^2}{2m} S(r) - \frac{\hbar^2}{2m} \frac{l(l+1)}{r^2} - \frac{1}{2} (1 - \tau_z) V_{coul}(r) - c_{ls} V_{s.o.}(r)$$

$\tau_z = 1$ for a neutron and -1 for a proton

$c_{ls} = -l(l+1)$ and l for $j = l - 1/2$ and $j = l + 1/2$, respectively

$$S(r) = \frac{d^2 R_{nlj}(r)}{dr^2} \frac{1}{R_{nlj}(r)}$$

$$\frac{d(R_{nlj}^2)}{dr} = 2R_{nlj} \frac{dR_{nlj}}{dr}$$

$$\frac{d^2(R_{nlj}^2)}{dr^2} = 2\left(\frac{dR_{nlj}}{dr}\right)^2 + 2R_{nlj} \frac{d^2R_{nlj}(r)}{dr^2}$$

And using $S(r) = \frac{d^2R_{nlj}(r)}{dr^2} \frac{1}{R_{nlj}(r)}$

$$S(r) = \frac{1}{2R_{nlj}^2} \left[\frac{d^2(R_{nlj}^2)}{dr^2} - \frac{1}{2} \frac{1}{R_{nlj}^2} \left[\frac{d(R_{nlj}^2)}{dr} \right]^2 \right]$$

When $R_{nlj} = 0$: $\frac{dR_{nlj}}{dr} = 0$

$$\frac{d^2(R_{nlj}^2)}{dr^2} - \frac{1}{2} \frac{1}{R_{nlj}^2} \left[\frac{d(R_{nlj}^2)}{dr} \right]^2 = 0$$

Using the relation:

$$R_{nlj}^2(r) = 4\pi r^2 \rho_{nlj}(r)$$

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

When $\rho_{nlj} = 0$:

$$\frac{d\rho_{nlj}}{dr} = 0$$
$$\frac{d^2 \rho_{nlj}}{dr^2} + \frac{2}{r} \frac{d\rho_{nlj}}{dr} - \frac{1}{2\rho_{nlj}} \left(\frac{d\rho_{nlj}}{dr} \right)^2 = 0$$

Examples of application of method for $3s_{1/2}$:

$$R_{3s/2} \sim \sin(kr + \varphi)$$

We get constant potential:

$$V = E - \frac{\hbar^2 k^2}{2m}$$

Harmonic Oscillator:

$$R_{3s/2}(r) = \left(\frac{15}{2\sqrt{\pi}} \nu^{3/2} \right)^{1/2} r e^{-\frac{1}{2}\nu r^2} \left[1 - \frac{4}{3}\nu r^2 + \frac{4}{15}(\nu r^2)^2 \right]$$

We get expected potential:

$$V(r) = E - \frac{11}{2} \hbar\omega + \frac{1}{2} m\omega^2 r^2$$

For commonly used potential, Woods-Saxon potential:

$$V(r) = V_0/[1 + \exp((r - R_1)/a_0)]$$

$R_{3s/2}(r)$ obtained numerically

Coulomb potential for equivalent uniform charge distribut

$$V^{coul}(r) = Ze^2 \begin{cases} (3 - r^2/R_c^2)/2R_{ch} & r < R_{ch} \\ 1/r & r > R_{ch} \end{cases}$$

$$R_{ch}^2 = (5/3)\langle r^2 \rangle_{ch}$$

Spin-orbit potential:

$$V_{s.o.}(r) = c dV_{cen.}(r)/dr \quad c \sim 0.2$$

Determining point proton distribution from charge dist

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

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

$$a^2 = \frac{1}{12} r_{pfs}^2 \text{ with } r_{pfs} = 0.85 \text{ fm (rms radius of } \rho_{pfs}\text{)}$$

$$\langle r^2 \rangle_{ch} = \int r^2 \rho_{ch}(\vec{r}) d\vec{r} / \int \rho_{ch}(\vec{r}) d\vec{r}$$

$$\langle r^2 \rangle_{ch} = \langle r^2 \rangle_p + \langle r^2 \rangle_{pfs}$$

$$\rho_{ch}(\vec{r}) = \frac{1}{4\pi a} \int_0^\infty r' dr' \rho_p(r') \left[\left(1 + \frac{|r - r'|}{a} \right) e^{-|r - r'|/a} - \left(1 + \frac{(r + r')}{a} \right) e^{-(r + r')/a} \right]$$

Define Fourier transform of density:

$$F(q) = \frac{4\pi}{q} \int_0^{\infty} \sin(qr) \rho(r) r dr$$

$$\rho(r) = \frac{1}{(2\pi)^3} \frac{4\pi}{r} \int_0^{\infty} \sin(qr) F(q) q dq$$

$$F_{pfs}(q) = \left(1 + \frac{1}{12} r_{pfs}^2 q^2 \right)^{-2}$$

$$F_{ch}(q) = F_{pfs}(q) F_p(q)$$

We get the point proton density:

$$\rho_p(r) = \frac{1}{(2\pi)^3} \frac{4\pi}{r} \int_0^{\infty} \sin(qr) F_p(q) q dq$$

$$\Delta\rho_c(r) = \rho_{ch}(r; {}^{206}\text{Pb}) - \rho_{ch}(r; {}^{205}\text{Tl})$$

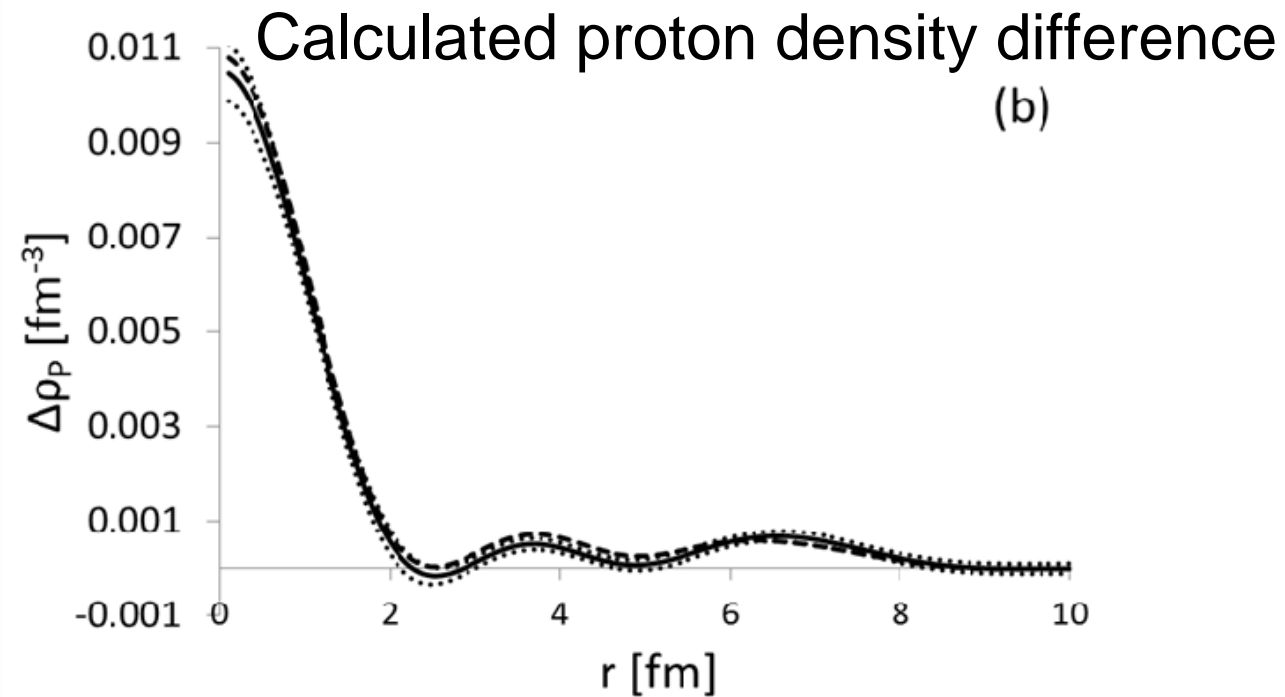
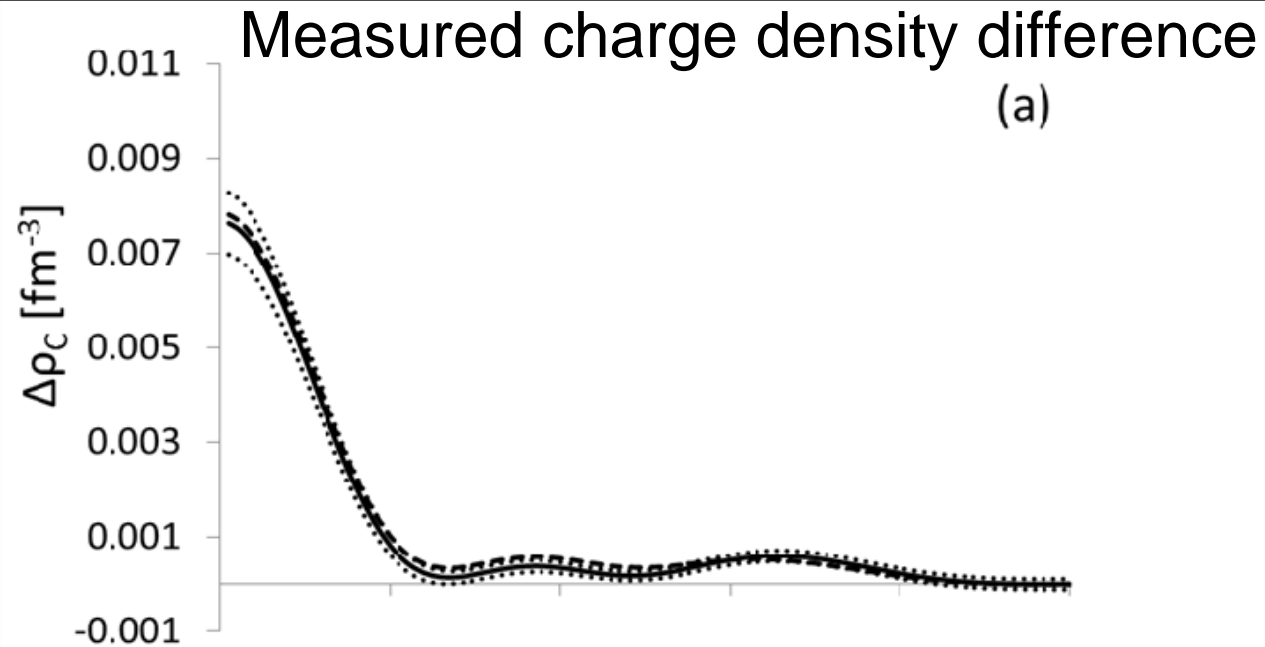
Rearrangement effect :

The charge distribution of ${}^{205}\text{Tl}$ is scaled so that the charge rms radius of the scaled density is equal to that of the 81 core protons in ${}^{206}\text{Pb}$.

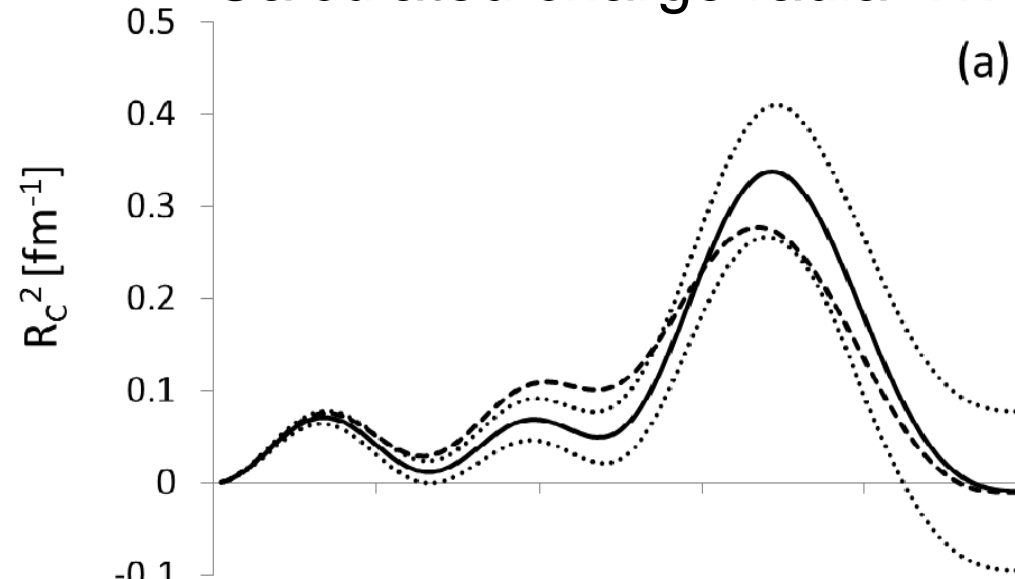
$$\Delta\rho_{Rc}(r) = \rho_{ch}(r; {}^{206}\text{Pb}) - \alpha^3 \rho_{ch}(\alpha r; {}^{205}\text{Tl}),$$

$$\alpha = 5.4792/5.4848 = 0.9990$$

α is obtained by assuming that the charge rms radius of the core 81 protons in ${}^{206}\text{Pb}$ is larger than that of ${}^{205}\text{Tl}$ by 0.005 fm, a value similar to the change in the charge rms radii for isotones in this region

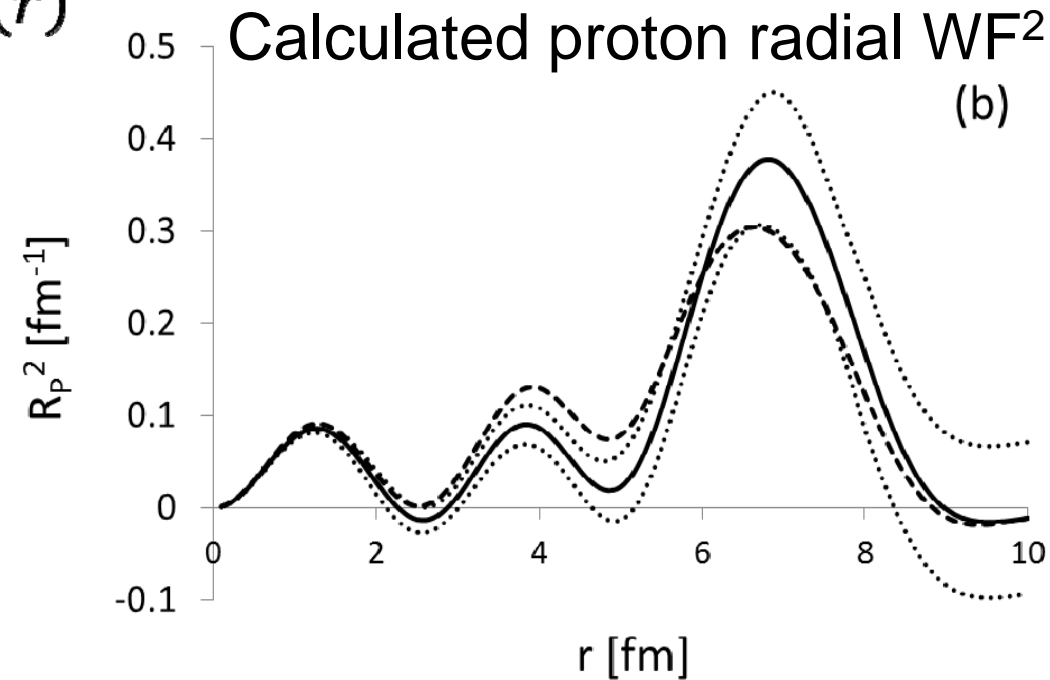


Calculated charge radial WF² difference



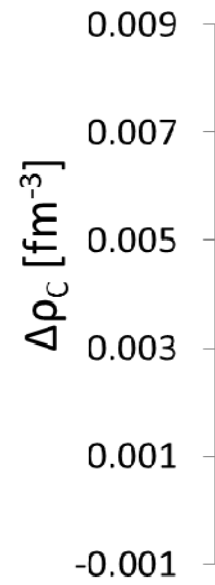
$$R^2(r) = 4\pi r^2 \rho(r)$$

Calculated proton radial WF² difference



Measured charge density difference

(a)



Calculated proton radial WF² difference

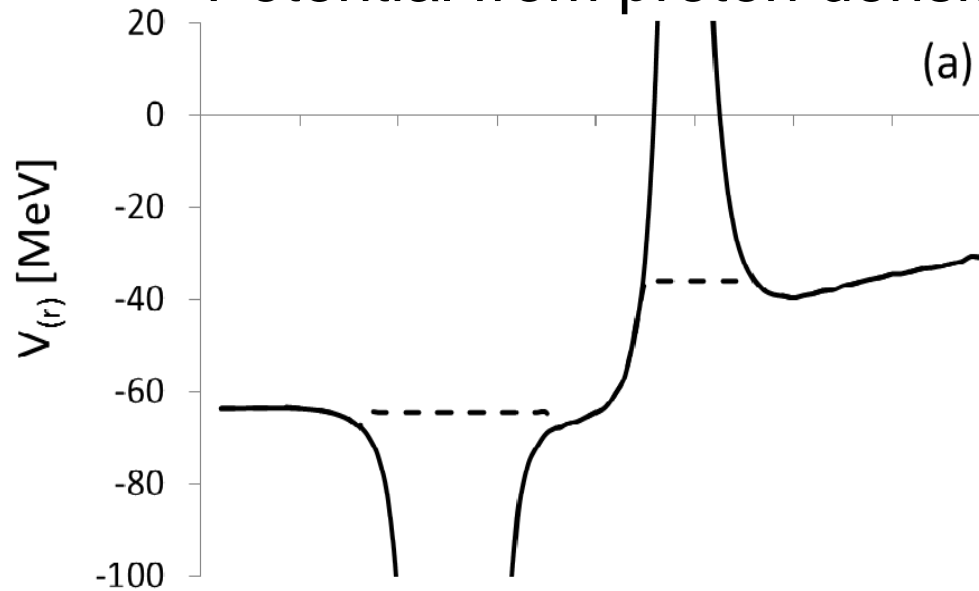
(b)



$$R^2(r) = 4\pi r^2 \rho(r)$$

r [fm]

Potential from proton density difference

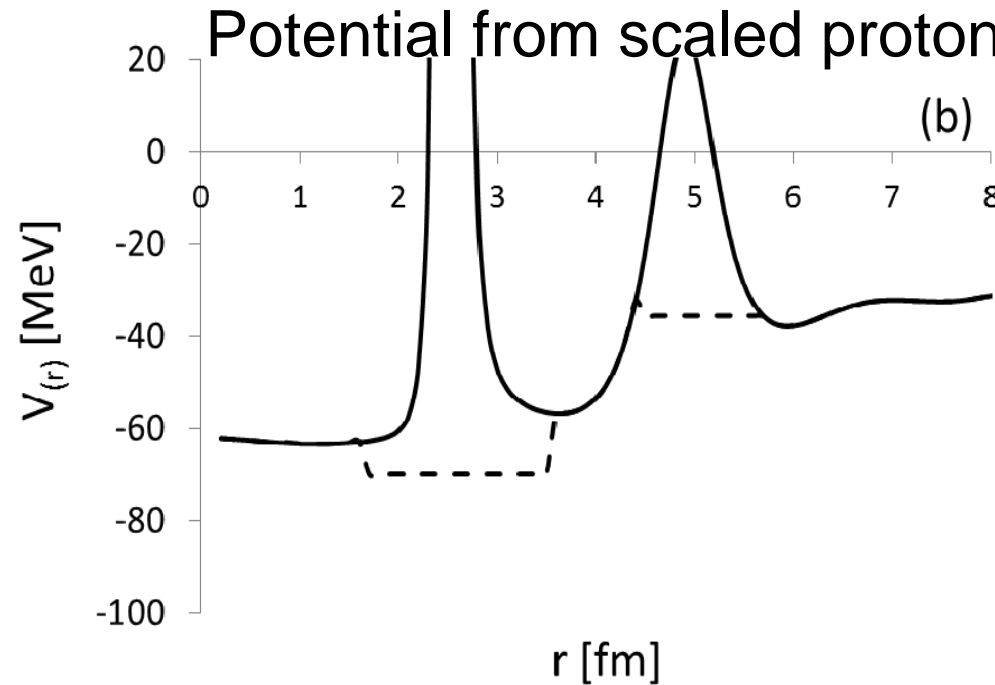


Dashed line potential

$$R \sim \sin(kr + \varphi)$$

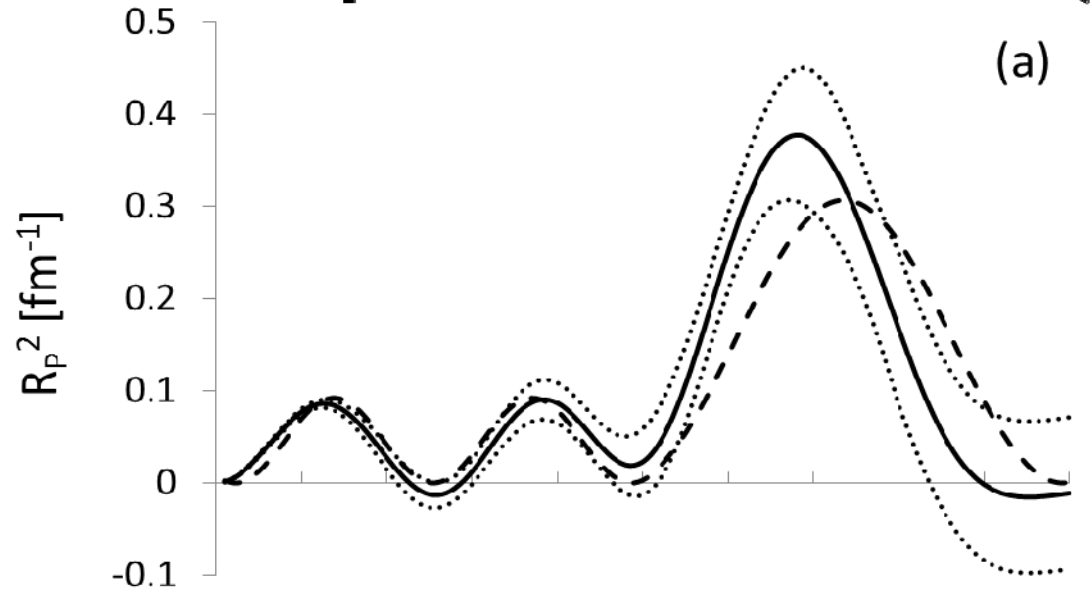
$$V = E - \frac{\hbar^2 k^2}{2m}$$

Potential from scaled proton density difference

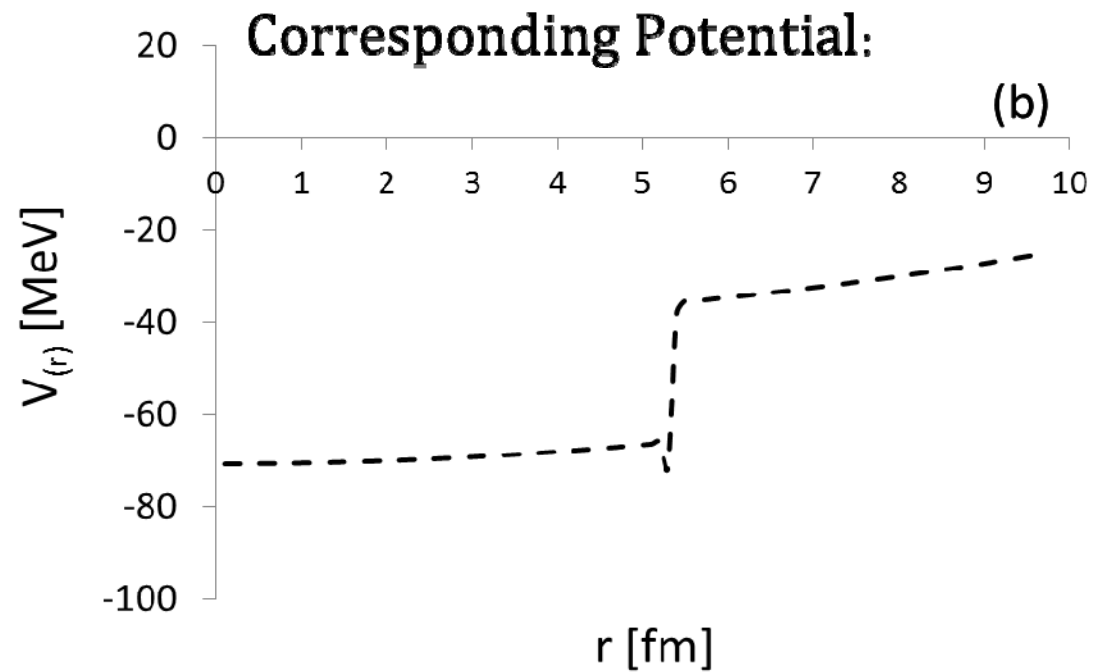


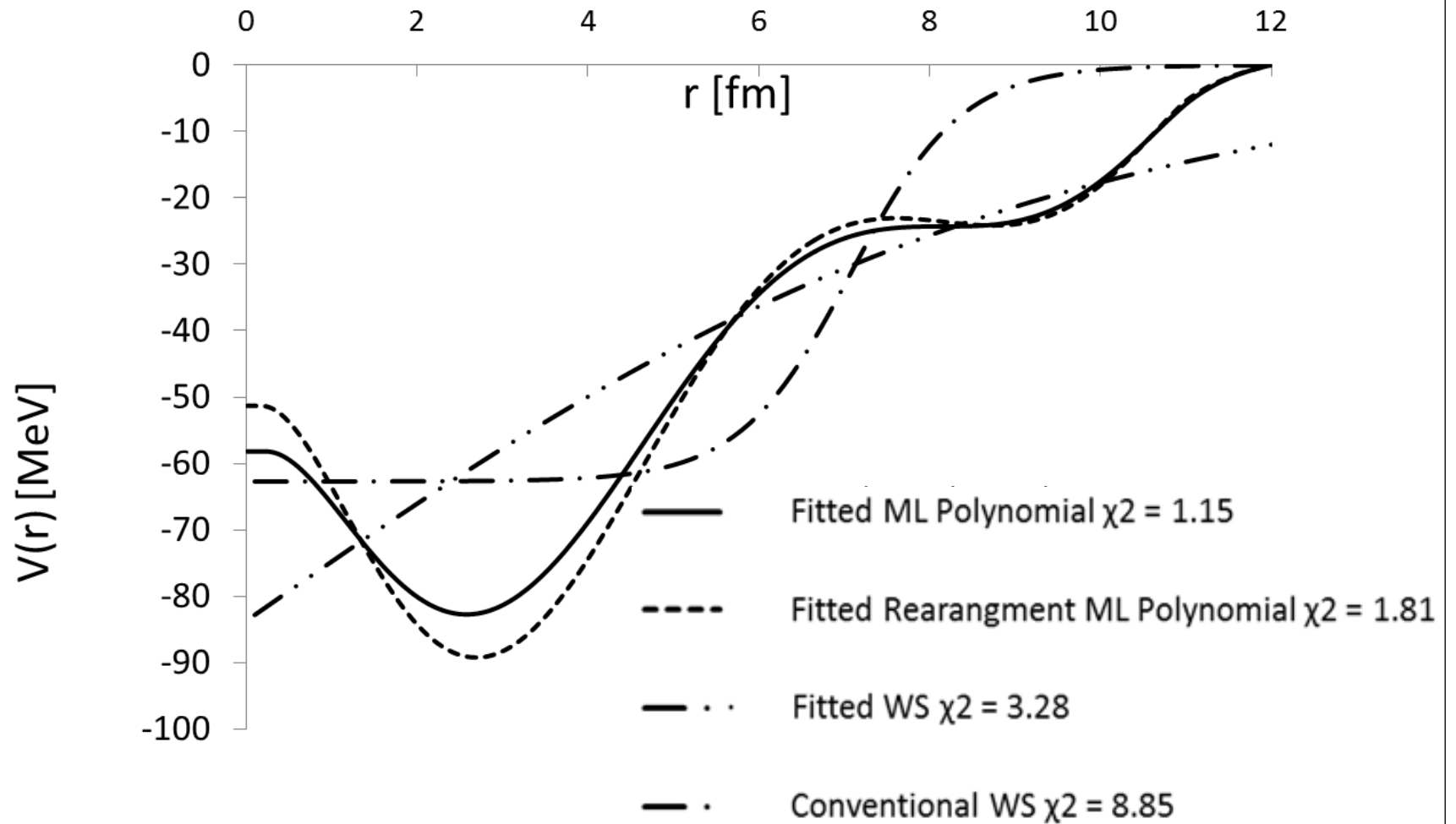
r [fm]

Fit to smooth splice of two sine WFs: $R \sim \sin(kr + \varphi)$



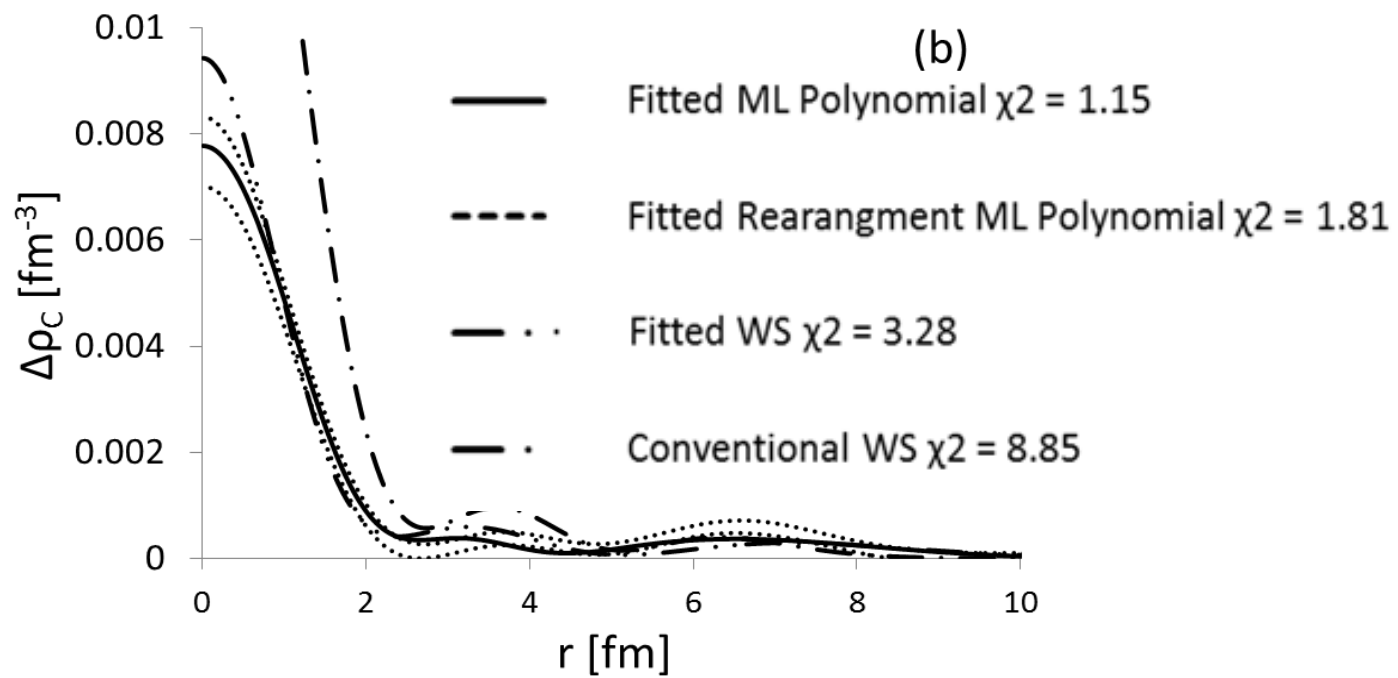
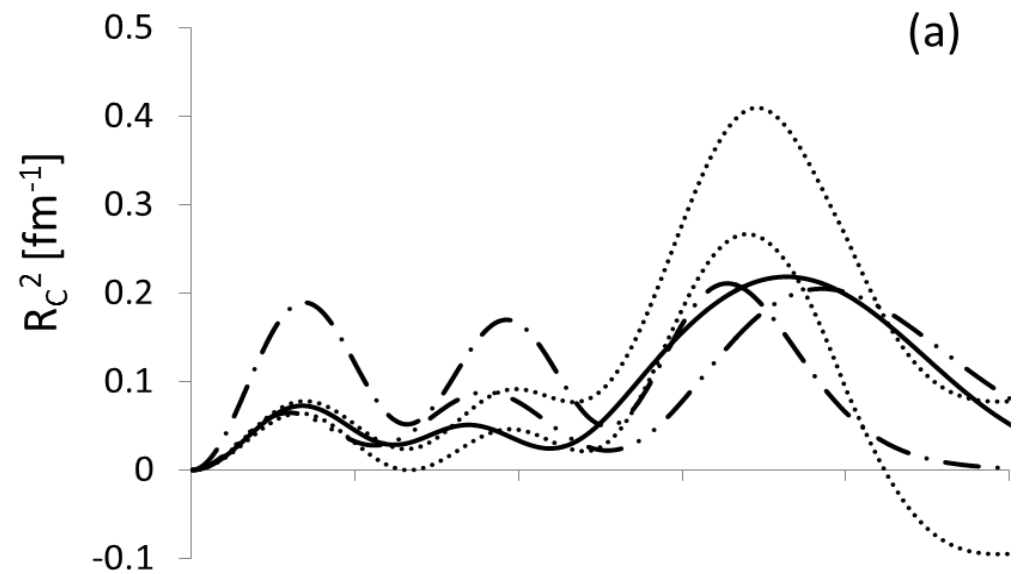
Corresponding Potential:

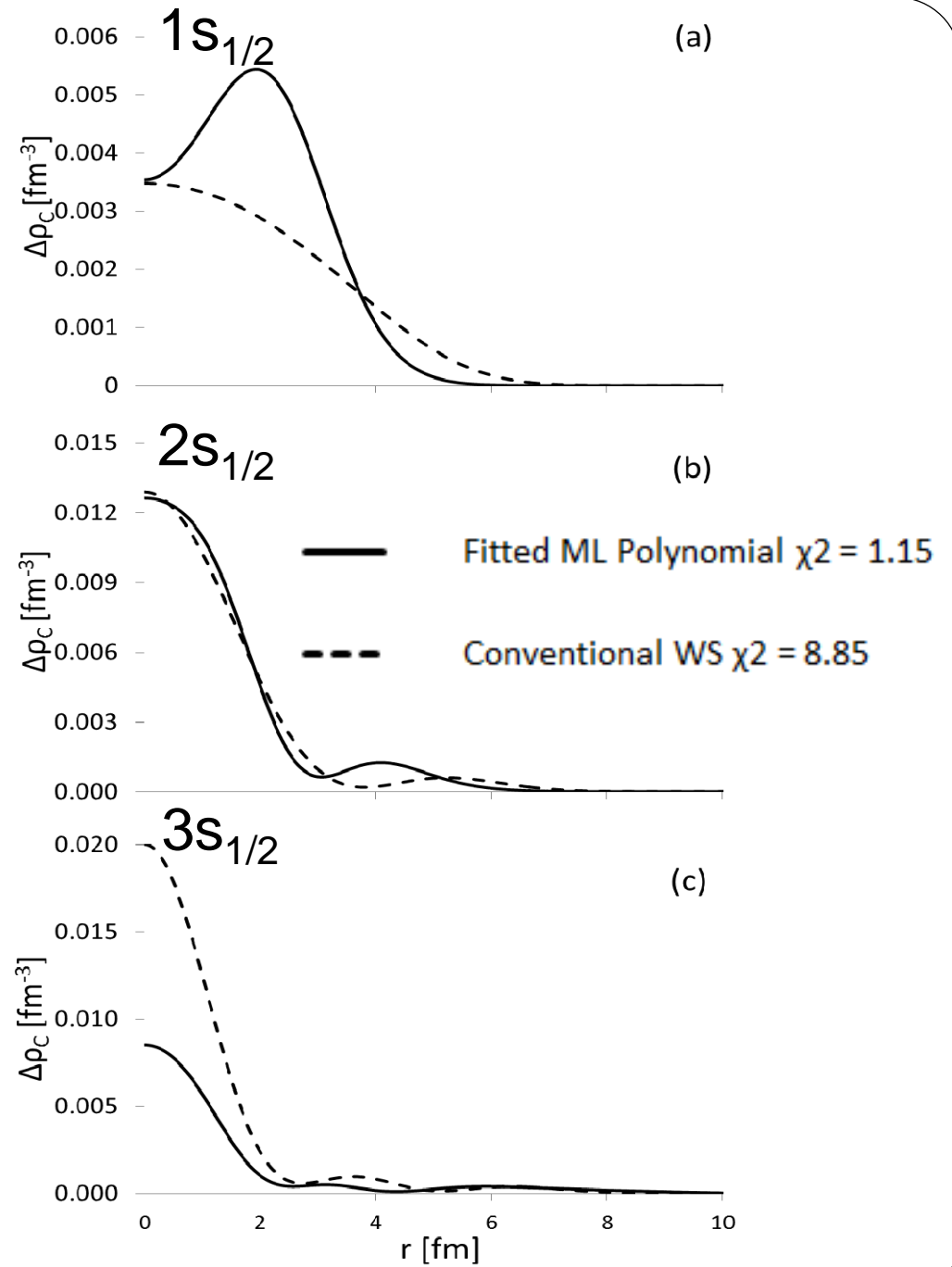
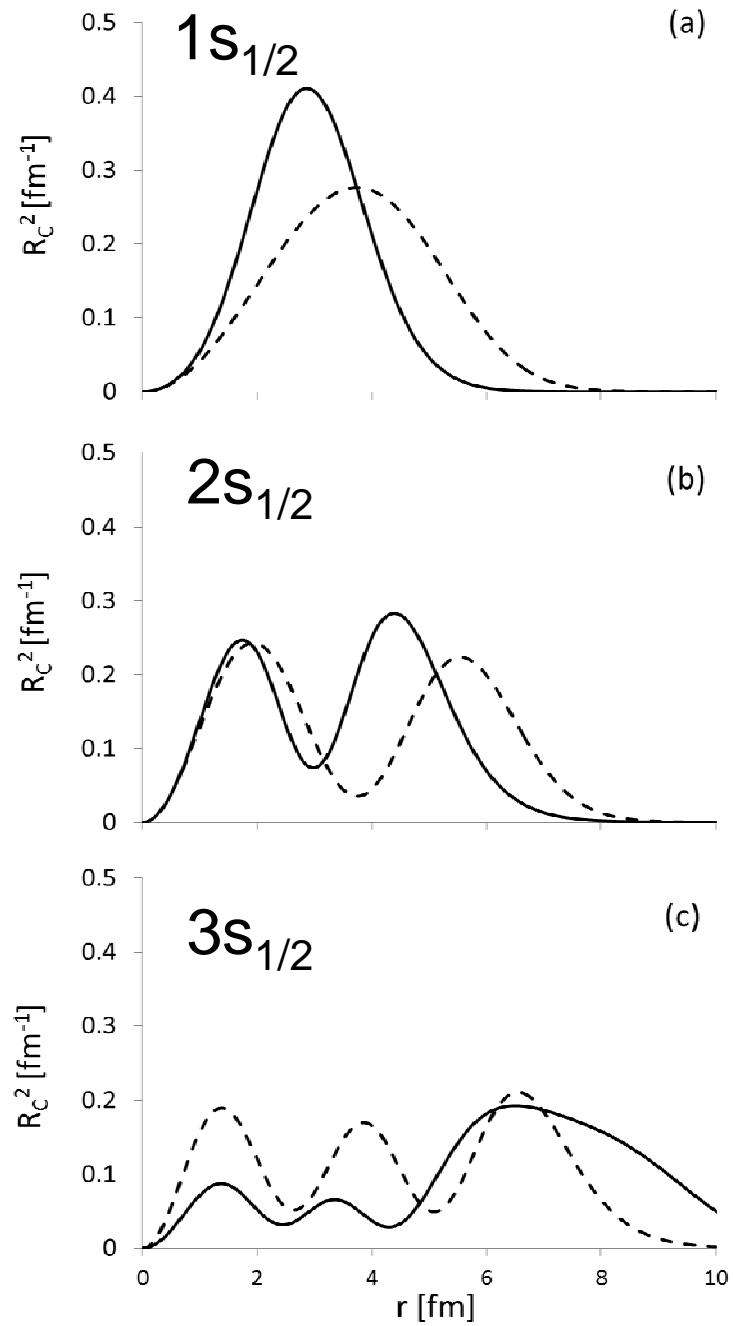




Fitted WS: $V_0 = -167.95$ MeV $R_1 = -0.03$ fm and $a_0 = 4.68$ fm

Conventional WS: $V_0 = -62.712$ MeV $R_1 = 7.087$ fm and $a_0 = 0$





Conclusions

- We have developed a new method of determining the single particle potential directly from the density distributions
- The potential derived from the density distributions of $3s_{1/2}$ state in ^{206}Pb shows large uncertainties around the nodes as the experimental error is larger than the value of the density
- We carried out a least-squares fit of a potential that is fit to the density data which is a much better fit than the conventional Woods-Saxon potential especially near $r = 0$ fm
- Clearly more accurate data is needed to better determine the potential and answer the question how well can the data be reproduced by a

Acknowledgements

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Backup Slides

**A NOVEL METHOD FOR DETERMINING
THE MEAN-FIELD DIRECTLY FROM THE SINGLE
PARTICLE MATTER DENSITY: APPLICATION TO THE
MEASURED CHARGE DENSITY DIFFERENCE BETWEEN
THE ISOTONES $^{206}\text{Pb} - ^{205}\text{Tl}$**

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We present a novel method, using the single particle Schrodinger equation, to determine the central potential directly from the single particle matter density and its first and second derivatives. As an example, we consider the experimental data for the charge density difference between the isotones $^{206}\text{Pb} - ^{205}\text{Tl}$, deduced by analysis of elastic electron scattering measurements and corresponds to the shell model $3s_{1/2}$ proton orbit, and determine the corresponding single particle potential (mean-field). We also present results of 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. The fair agreement with fitted potentials may be an indication that effects of short range correlations on charge distributions due to shell model wave functions are not significant. 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 calculated $3s_{1/2}$ wave function.