Short-range correlations and the proton $3s_{1/2}$ wave function in 206Pb

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Outline

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   Experimental data: $3s_{1/2}$ charge density in ^{206}Pb

2. Determining the corresponding Single-Particle potential directly from Matter Density: Derivation of method, application to $3s_{1/2}$ state in ^{206}Pb.

3. Calculation of short-range correlation effect on single particle density; the $3s_{1/2}$ state in ^{206}Pb

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Introduction

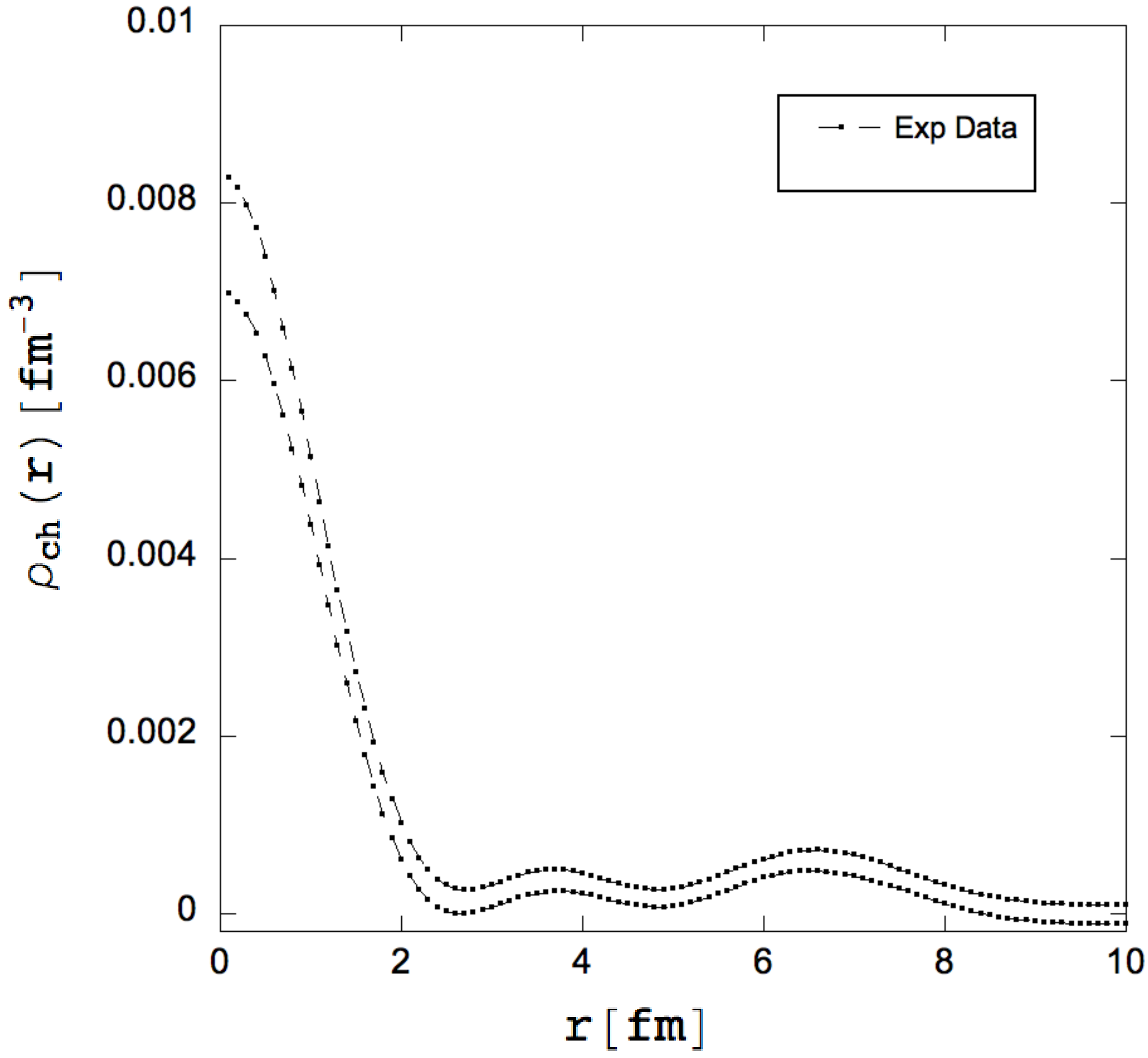
- In this talk I will consider the well-known experimental data of the charge distribution of the proton $3s_{1/2}$ orbit given by the charge density difference, $\Delta\rho_c(r)$, between charge density distributions of the isotones $^{206}Pb - ^{205}Tl$, determined by analysis of elastic electron scattering.
- 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.
- I will present a novel method, using the single particle Schrodinger equation with eigen-energy E, to determine the central potential $V(\vec{r})$ directly from the measured single particle matter density, $\rho(\vec{r})$ and its first and second derivatives, assuming known for all $\vec{r}$. Using the method we obtained the potential for the proton $3s_{1/2}$.

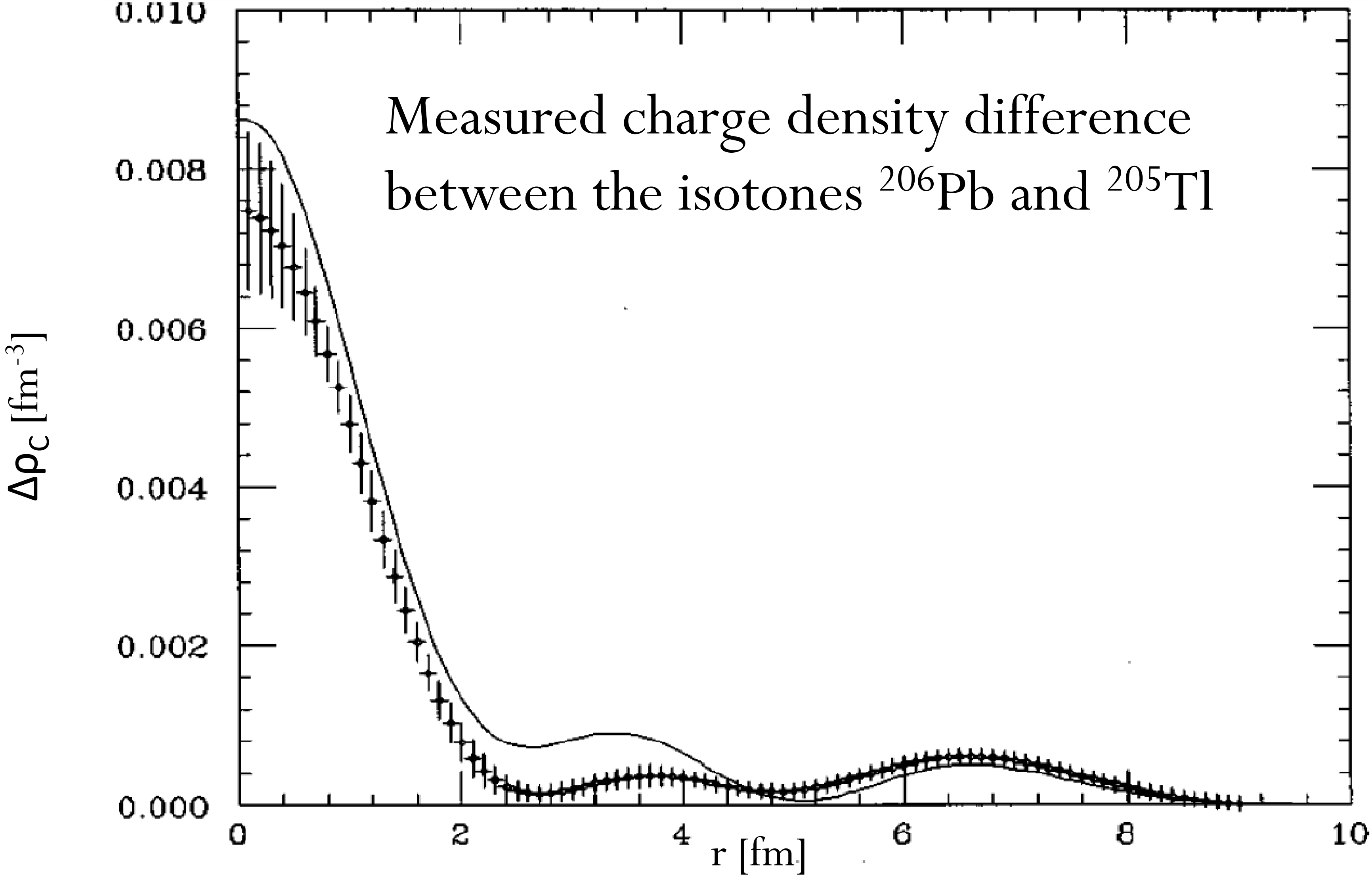
Introduction

- 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.
- We have carried out calculations of the effects of short-range correlations on the charge density difference $^{206}Pb - ^{205}Tl$, $3s_{1/2}$ state, using the Jastrow correlation method. We derive and use a simple approximation for determining the effect of short range correlations on the charge density distribution.
- Goal: Find out how short range correlations affect the charge density distribution and whether it is necessary to help explain the experimental data on the charge density of $3s_{1/2}$ orbit

3s$_{1/2}$

Experimental Data: $\rho_{Ch}(^{206}Pb) - \rho_{Ch}(^{205}Tl)$





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

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Charge distributions of ^{208}Pb, ^{206}Pb, and ^{205}Tl and the mean-field approximation

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Charge distributions of ^{208}Pb, ^{206}Pb, and ^{205}Tl have been calculated within the Hartree-Fock and Hartree-Fock + BCS approximations with the Skyrme interaction. Using the force SkM* designed without any reference to this particular problem, we find good agreement with elastic electron scattering data. The role of pairing correlations beyond the mean field is studied by applying the Lipkin-Nogami method of variation after approximate projection on the good number of particles. We argue in this paper that, in our opinion, there is no *significant* discrepancy between the experimental data and the Hartree-Fock calculations using reasonable effective interactions. In particular, we do not see any compelling need for a large depletion of the occupation number of the proton $3s_{1/2}$ orbital.

Single Particle Potential: Formalism

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

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

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: $\rho(\vec{r}) = [\Psi(\vec{r})]^2$

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

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

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

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

τ_z=1 for a neutron and -1 for a proton

$c_{ls} = -(l+1)$ 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 $R_{nlj} = 0$:

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

We consider the 3s1/2 proton orbit. No S.O. and l=0

Therefore, 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 $\rho_{nlj} = 0$:

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

NOTE Experiment determines charge distribution;
Theory determines point distribution

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

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

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

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

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

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

Define Fourier transform of density:

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

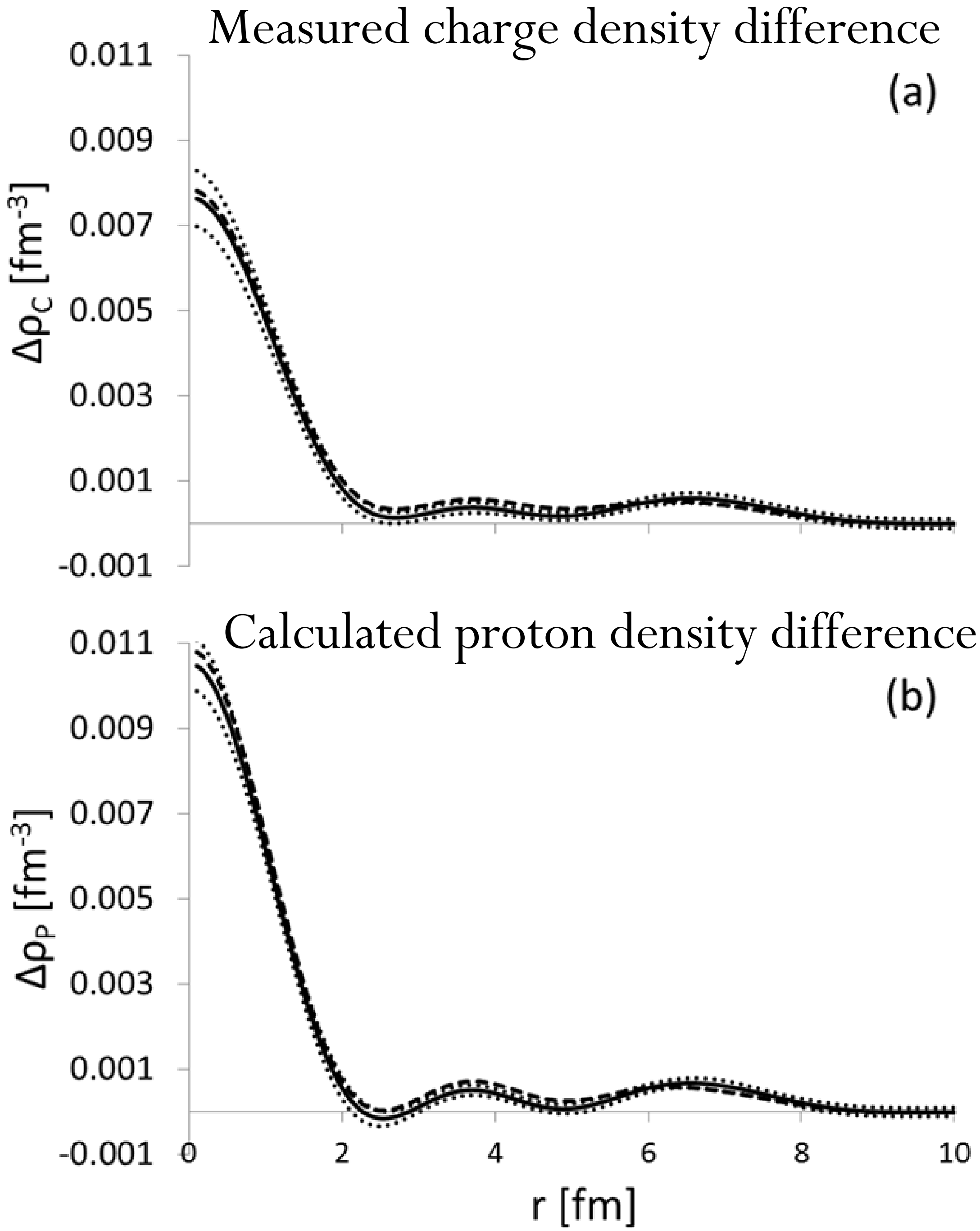
$$\rho(r) = \frac{1}{(2\pi)^3} \frac{4\pi}{r} \int_0^\infty \sin(qr)\, F(q) q dq$$

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

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

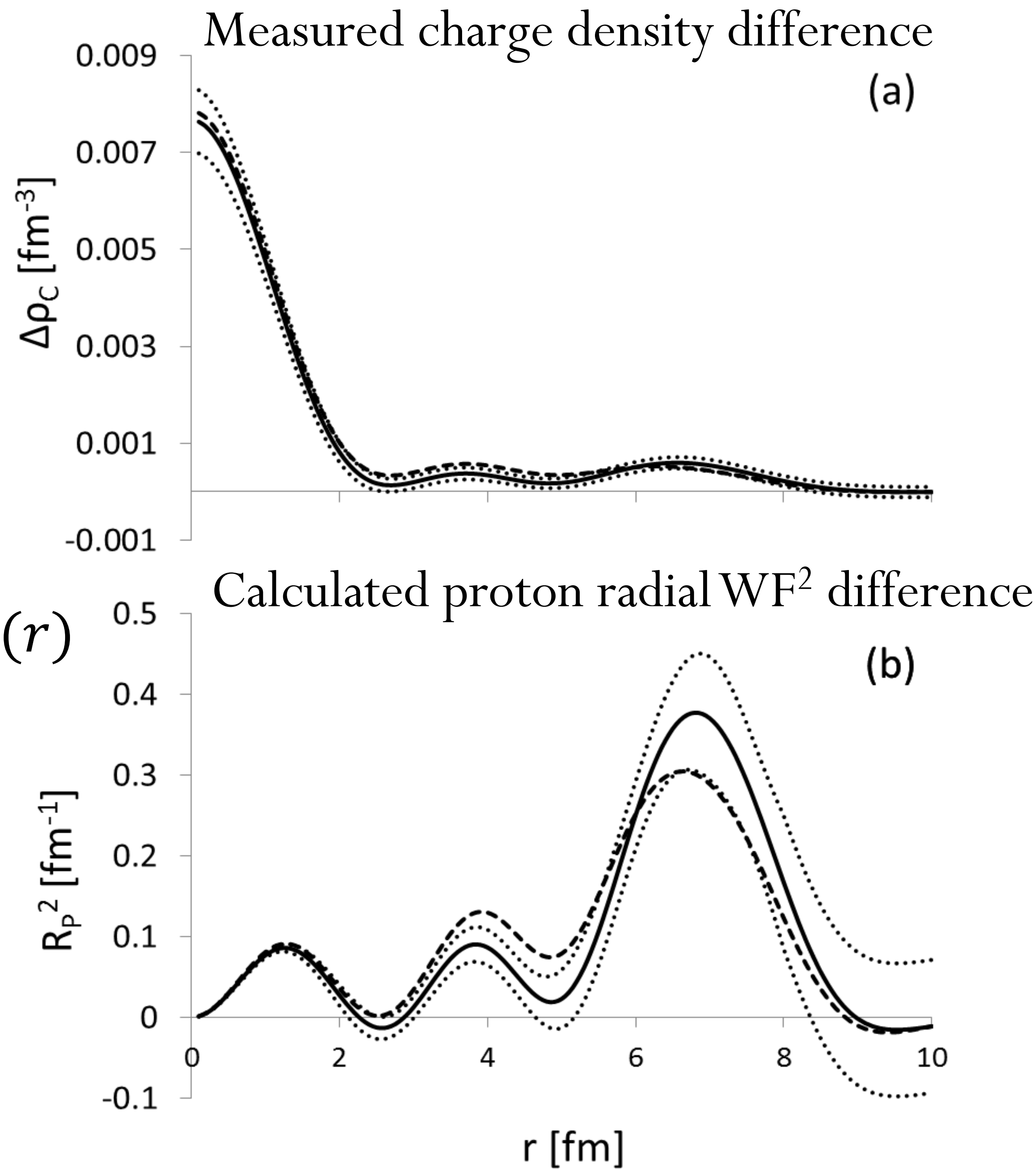
We get the point proton density:

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



Measured charge density difference
(a)
0.011
0.009
0.007
0.005
0.003
0.001
-0.001
$\Delta\rho_C$ [fm^{-3}]
Calculated proton density difference
(b)
$\Delta\rho_P$ [fm^{-3}]
0
2
4
6
8
10
r [fm]

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

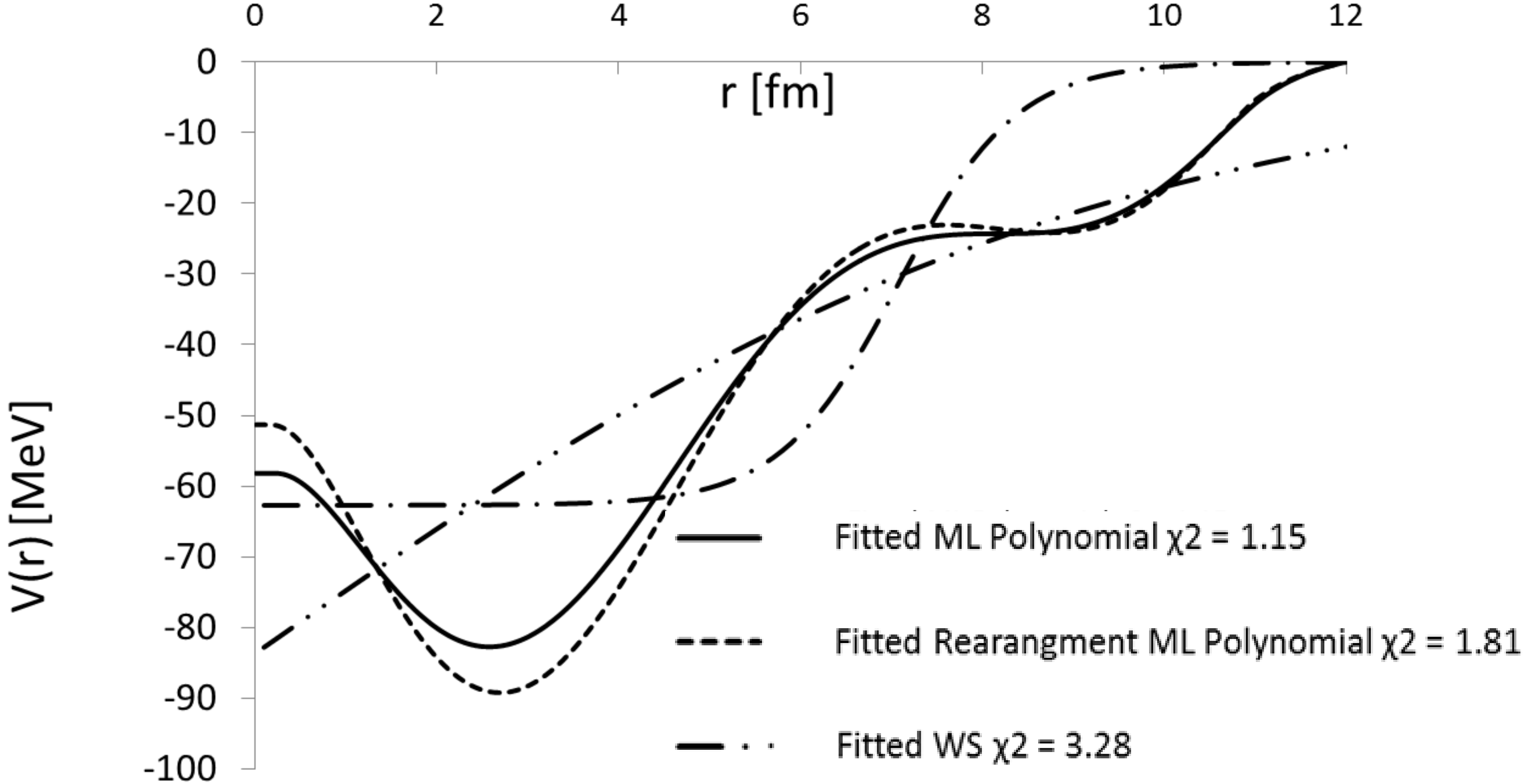


Due to large uncertainty in the experimental data for

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

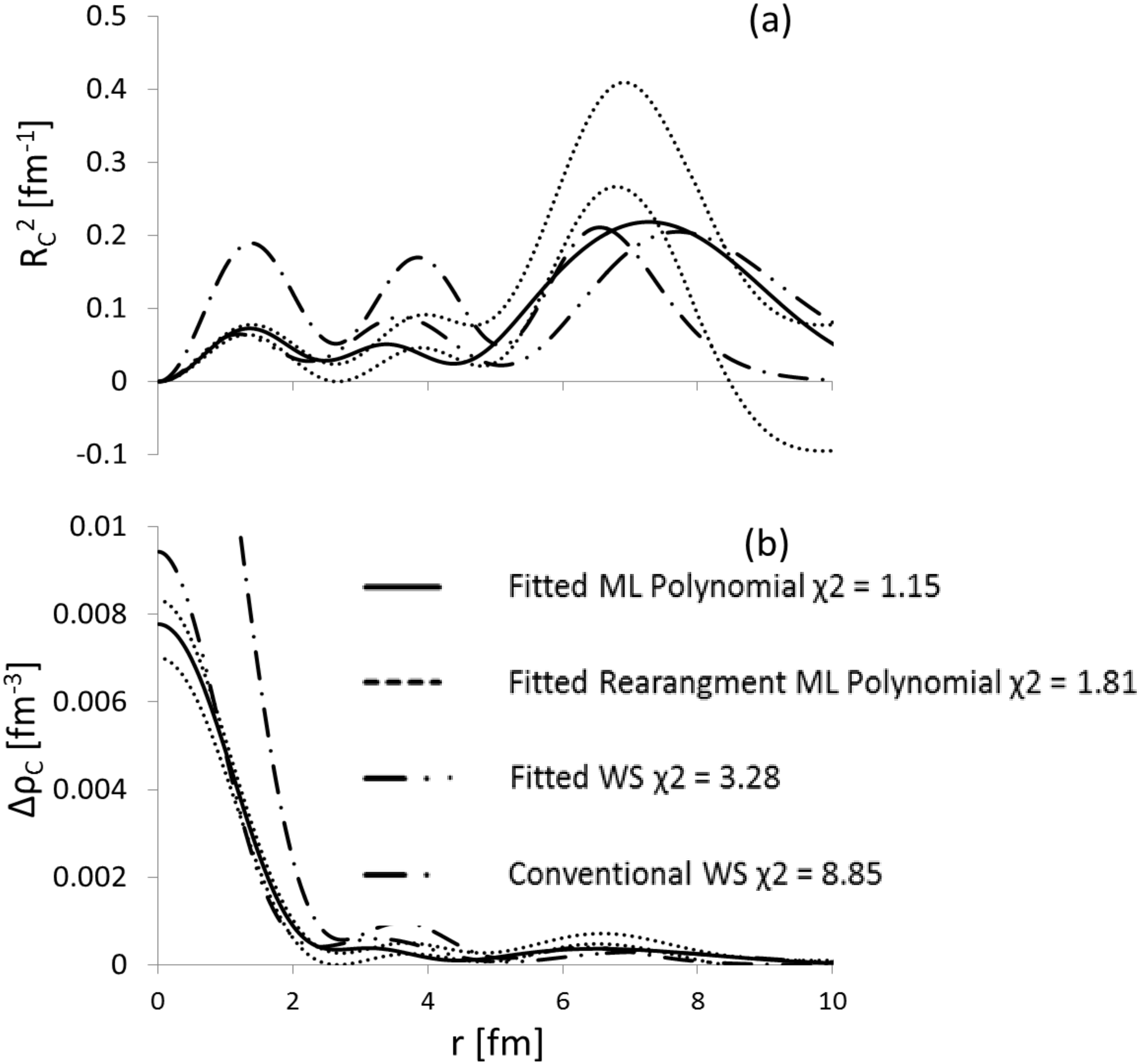
particularly, around the nodes of the 3s1/2 proton wavefunction, we are not able to extract the corresponding potential with reasonable accuracy.

We have therefore determined potentials by fits to the experimental data.



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 = 0.65 fm



(a)
0.5
0.4
0.3
0.2
0.1
0
-0.1
R_C^2 [fm^{-1}]
(b)
0.01
0.008
0.006
0.004
0.002
0
Δρ$_C$ [fm^{-3}]
Fitted ML Polynomial χ2 = 1.15
Fitted Rearangment ML Polynomial χ2 = 1.81
Fitted WS χ2 = 3.28
Conventional WS χ2 = 8.85
0
2
4
6
8
10
r [fm]

Calculation of Short Range correlation effect on 3s1/2 density

- We use the Jastrow many-body correlated wave function with a repulsive two-body correlation factor f_{12} and harmonic oscillator single particle wave functions
- We derive a simple and accurate (within a few percents) approximation for the effect of the two-body correlation factor f_{12} on matter density and calculate the effect of short range correlations on charge density distributions of 206Pb and 205Tl

The Shell Model and the Jastrow Correlated many-body wave functions

$$\Psi^{SM}(\vec{r}_1 \cdots \vec{r}_A) = \frac{1}{\sqrt{A!}} \det\left(\psi_1(\vec{r}_1) \cdots \psi_A(\vec{r}_A)\right)$$

$$\Psi^{corr}(\vec{r}_1 \cdots \vec{r}_A) = \mathrm{N}\left[\prod_{1 \le i < j}^{A} f_{ij}(|\vec{r}_1 - \vec{r}_2|)\right] \Psi^{SM}(\vec{r}_1 \cdots \vec{r}_A)$$

Two-body correlation factor:

$$f_{ij}(|\vec{r}_{ij}|) = 1 - exp\left(-\alpha|\vec{r}_{ij}|^2\right) \qquad \vec{r}_{ij} = \vec{r}_i - \vec{r}_j$$

$$\int_0^\infty d\vec{r}_1 \cdots d\vec{r}_A |\Psi_{12}^{corr}(\vec{r}_1 \cdots \vec{r}_A)|^2 = 1$$

Shell Model single particle density

$$\hat{\rho} = \sum_{i=1}^{A} \delta(\vec{r} - \vec{r}_i)$$

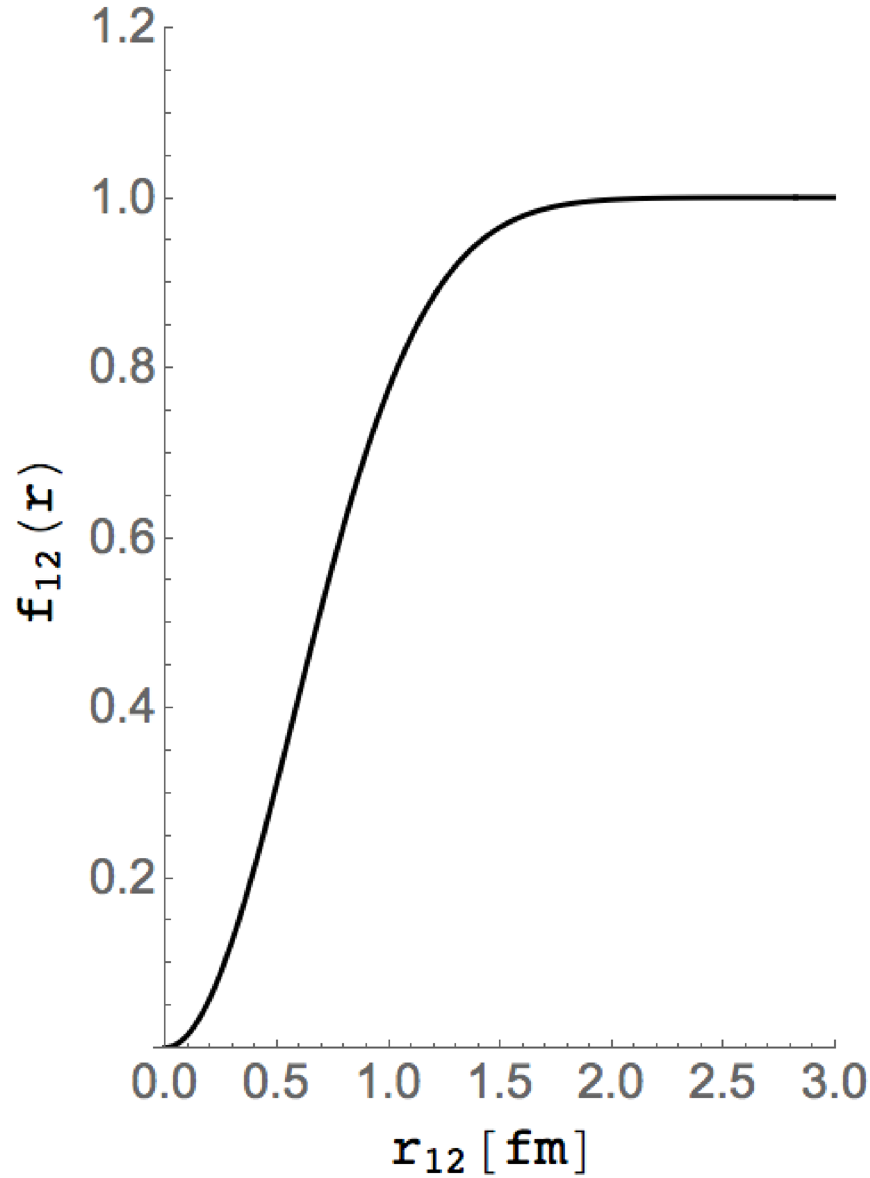
$$\begin{aligned}\rho^{SM}(\vec{r}) &= \langle \psi_{SM} | \hat{\rho} | \psi_{SM} \rangle \\ &= \int |\psi_1(\vec{r}_1)|^2 \cdots |\psi_A(\vec{r}_A)|^2 \sum \delta(\vec{r} - \vec{r}_i)\, d\vec{r}_1 \cdots d\vec{r}_A \\ &= \sum_{i=1}^{A} |\psi_i(\vec{r}_i)|^2\end{aligned}$$

$$\rho_1^{SM}(\vec{r}) = |\psi_1(\vec{r})|^2$$

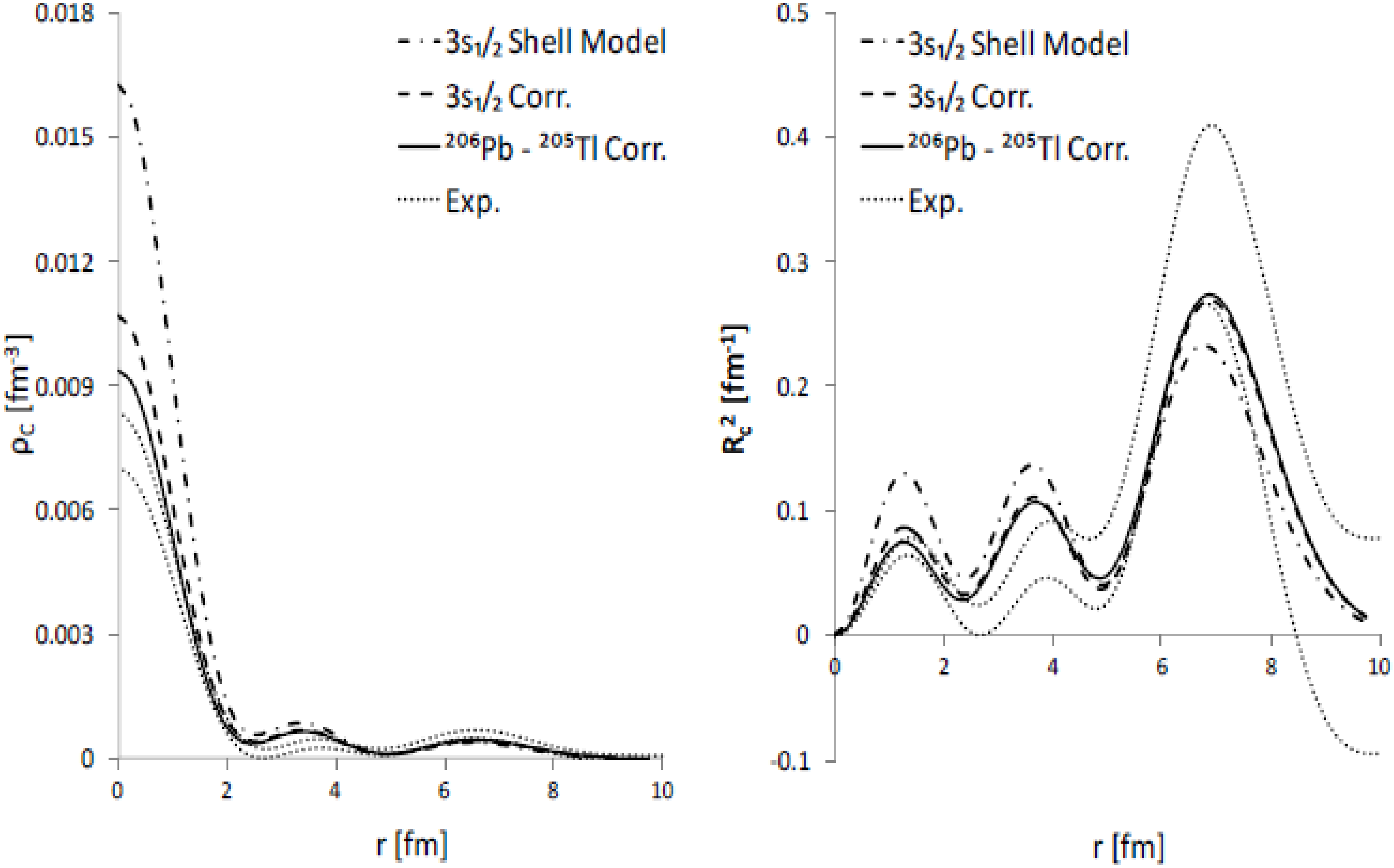
Correlated single particle density

$$\rho^{corr}(\vec{r}) = \langle \psi_{corr} | \hat{\rho} | \psi_{corr} \rangle$$
$$= N^2 \int \left[\prod_{1 \le i < j}^{A} f(\vec{r}_{ij}) \right]^2 |\psi_1(\vec{r}_1)|^2 \cdots |\psi_A(\vec{r}_A)|^2 \sum \delta(\vec{r} - \vec{r}_i)\, d\vec{r}_1 \cdots d\vec{r}_A$$

Two-body Correlation function

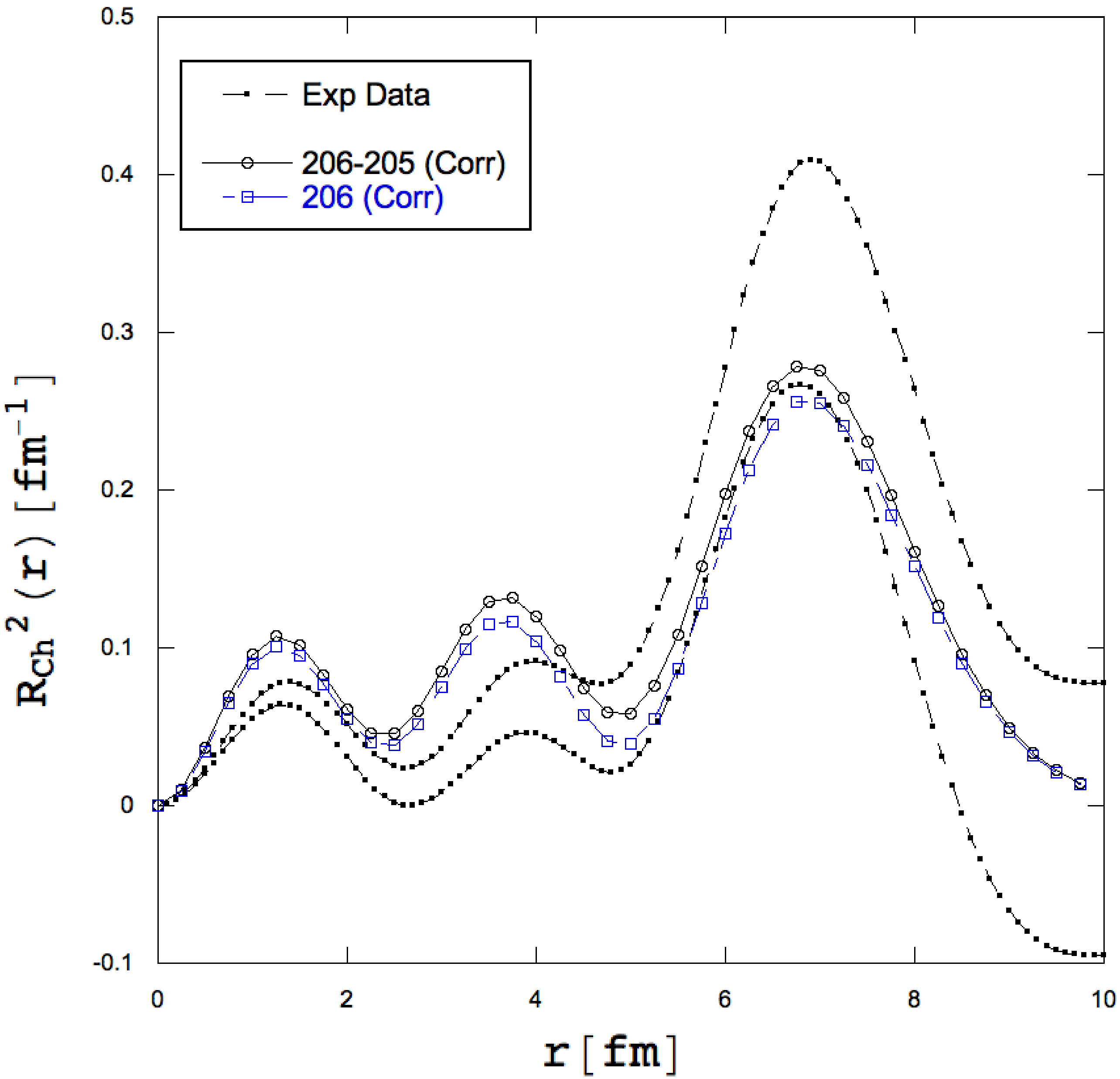


^{206}Pb - ^{205}Tl



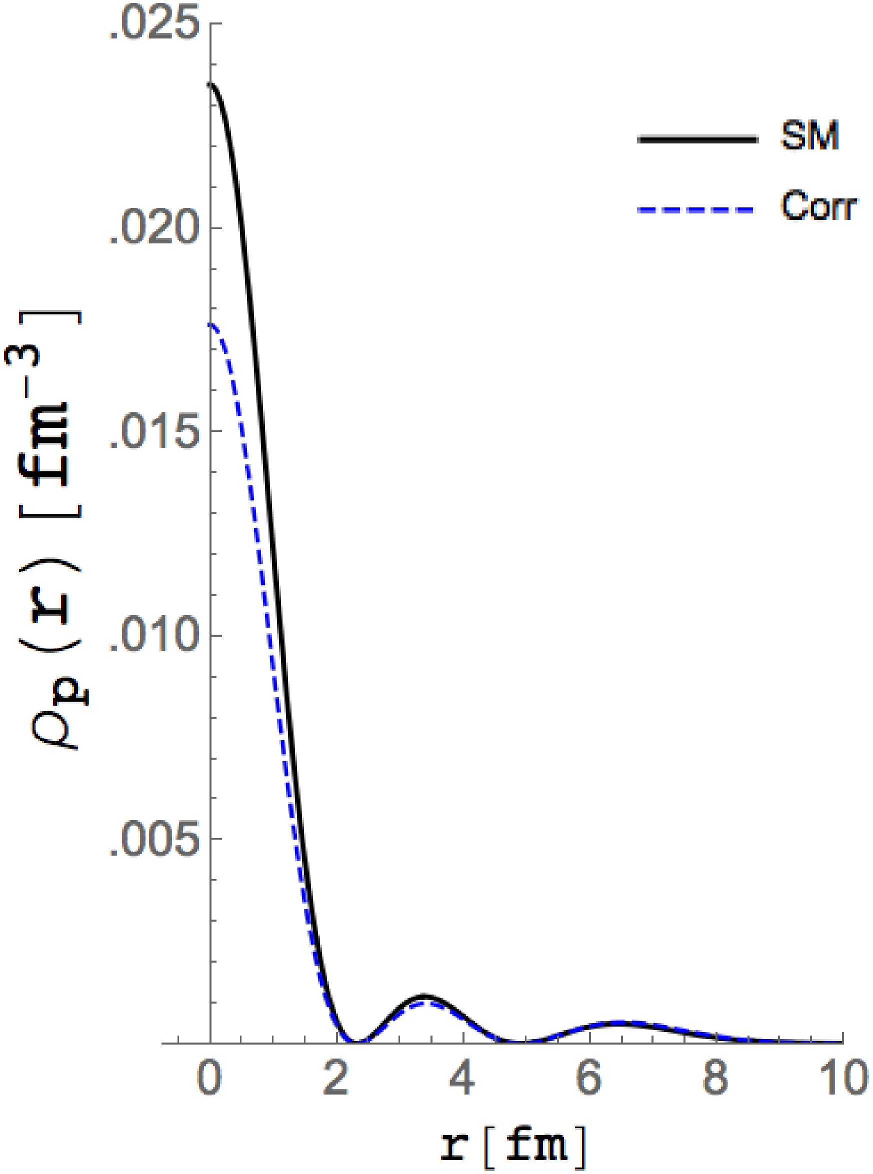
0.018
0.015
0.012
0.009
0.006
0.003
0
ρc [fm-3]
r [fm]
3s1/2 Shell Model
3s1/2 Corr.
206Pb - 205Tl Corr.
Exp.
0.5
0.4
0.3
0.2
0.1
-0.1
Rc2 [fm-1]
0
2
4
6
8
10

$3s_{1/2}$

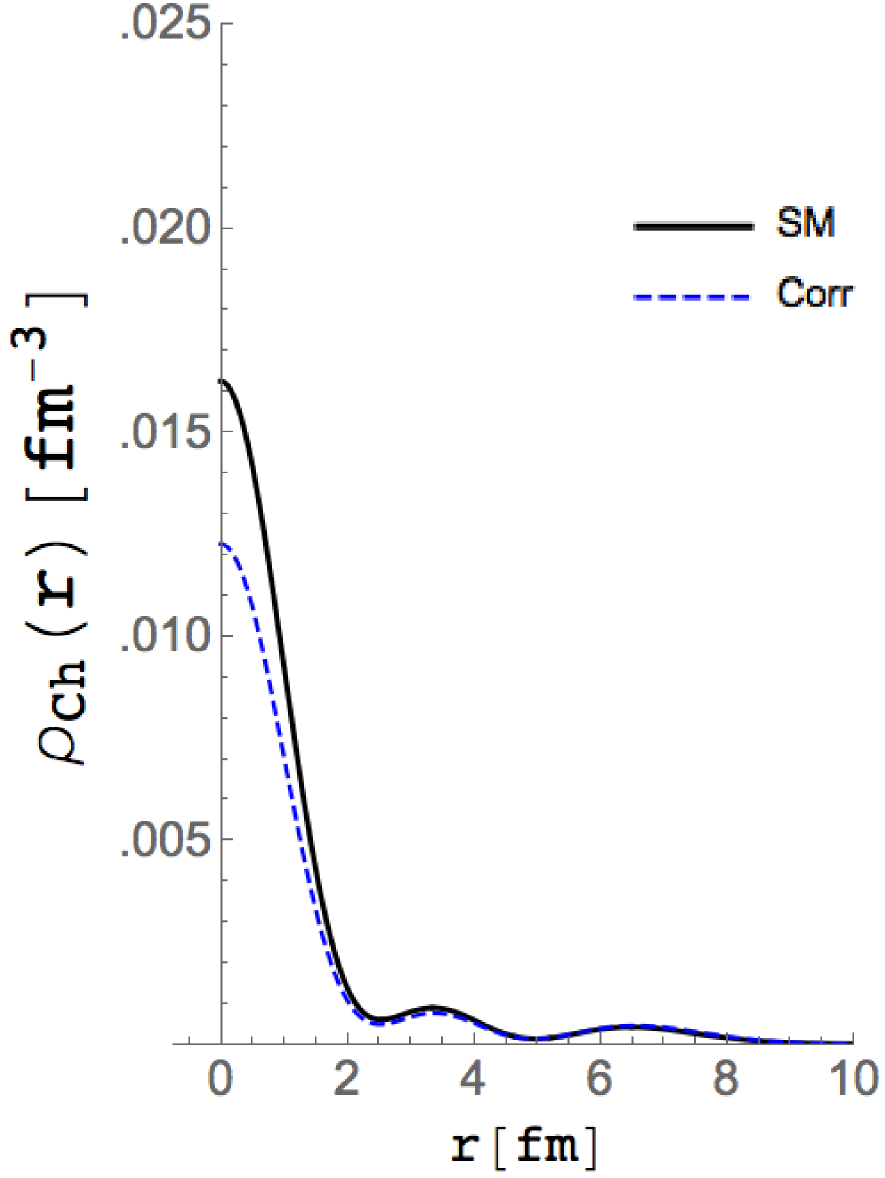


Exp Data
206-205 (Corr)
206 (Corr)
0.5
0.4
0.3
0.2
0.1
0
-0.1
0
2
4
6
8
10
$R_{Ch}^{2}(r)$ [fm^{-1}]
r [fm]

$3s_{1/2}$ Proton Point Density



3s$_{1/2}$ Proton Charge Density



Conclusions

- We have developed and used a new method of determining the single particle potential directly from the density distribution and applied it to the experimentally determined density distributions of the proton $3s_{1/2}$ state in ^{206}Pb and obtaining an acceptable form for the potential.
- We carried out a least-squares fit of a potential providing a 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 calculated $3s_{1/2}$ single particle wave function

Conclusions-Cont.

- We have calculated the effect of short-range correlations on charge densities of 206Pb and 205Tl, using the Jastrow correlated many-body wave function with a repulsive two-body short range correlation function.
- We demonstrated that, although correlated $3s_{1/2}$ charge density at r=0 is reduced 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.
- Further investigations are needed using a more realistic two-body correlation function and determining the effect of short range correlations and the corresponding single particle potential.

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