Solving Dirac equation in 3D lattice with inverse Hamiltonian method and spectral method

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- Introduction
- Theoretical framework
- Numerical details
- Results and discussion
- Summary and Perspectives

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Introduction

- To get a better convergence description of the nuclei
  - ✓ far from the β-stability line;
  - ✓ with exotic shapes;
  - ✓ with exotic excitation modes;
  - ✓ …

  one should investigate them in coordinate space or coordinate-equivalent space.

- In CDFT framework, the existing methods
  - Runge-Kutta / Shooting method Meng, *NPA* 635, 3 (1998)
  - Dirac Woods-Saxon basis Zhou, Meng, and Ring, *PRC* 68, 034323 (2003); Zhou, Meng, Ring, and Zhao, *PRC* 82, 011301 (2010)

  However, it's difficult to extend these methods to 3D case.

- Imaginary time method (ITM) is a good choice for the calculation in coordinate space. Davies, Flocard, Krieger, and Weiss, *NPA* 342, 111 (1980).

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Introduction

- ITM is a iteratively method for self-consistent mean field problem, and it has been applied to nonrelativistic mean field calculations in 3D coordinate space successfully. Bonche, Flocard, and Heenen, *Comput. Phys. Comm.* 171, 49 (2005); Maruhn, Reinhard, Stevenson, and Umar, *Comput. Phys. Comm.* 185, 2195 (2014).

- However, there are two challenges when one applies ITM to CDFT naively,
  - Variational collapse;
  - Fermion doubling (spurious solutions).

- To avoid these problems, Zhang, Liang and Meng applied the ITM to the Schr o dinger-equivalent form of the Dirac equation, and developed a spherical RMF code based on this method. Zhang, Liang, and Meng, *CPC* 33, 113 (2009); Zhang, Liang, and Meng, *IJMPE* 19, 55 (2010).

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Introduction

- To avoid variational collapse, Hagino and Tanimura creatively proposed inverse Hamiltonian method (IHM); to avoid Fermion doubling problem, Tanimura, Hagino and Liang introduced high-order Wilson terms. Based on these two methods, they performed 3D lattice calculations for CDFT.

  Hagino and Tanimura, *PRC* 82, 057301 (2010); Tanimura, Hagino, and Liang, *PTEP* 2015, 073D01 (2015).

- However, there are some drawbacks when employing high-order Wilson terms,
  - Correction for energies and wave functions.
  - Introducing artificial violation of the rotational symmetry.

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Introduction

In this work:

- To avoid variational collapse, we employ inverse Hamiltonian method.

- To avoid Fermion doubling problem, we perform the spatial derivatives of Dirac equation in momentum space with the help of discrete Fourier transform (spectral method). S. J. Shen, T. Tang, and L. L. Wang, *Spectral methods : algorithms, analysis and applications* (Springer, 2011).

- Combining these two methods, we propose a new method to solve Dirac equation in 3D lattice space.

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Imaginary time method

- If Hamiltonian h is independent on time, the evolution of $|\psi(0)\rangle$ reads

$$|\psi(t)\rangle = \mathrm{e}^{-\mathrm{i}ht}\ |\psi_0\rangle$$

- Basic idea of ITM is $t \to -\mathrm{i}\tau$, and now the evolution of $|\psi(0)\rangle$ becomes

$$|\psi(\tau)\rangle = \mathrm{e}^{-\hat{h}\tau}|\psi_0\rangle = \sum_k \mathrm{e}^{-\varepsilon_k \tau}|\phi_k\rangle\langle\phi_k|\psi_0\rangle$$

where

$$\varepsilon_0 \le \varepsilon_1 \le \varepsilon_2 \le \cdots$$

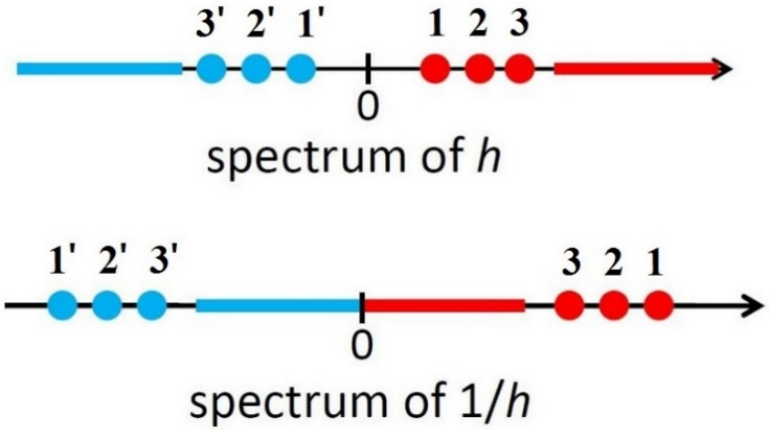
Obviously, with $\tau \to \infty$, $|\psi(\tau)\rangle$ will converge to ground state of Hamiltonian h. Davies, Flocard, Krieger, and Weiss, *NPA* 342, 111 (1980).

- In practice, the imaginary time τ is cut into steps by $\Delta\tau$, and the evolution is carried out iteratively. Then, the evolution operator is expanded to the linear order of $\Delta\tau$.

$$|\psi^{(n+1)}\rangle \propto \left(1 - \Delta\tau\hat{h}\right)|\psi^{(n)}\rangle$$

Inverse Hamiltonian method

- Because of the Dirac sea, a direct extension of ITM to Dirac equation will meet so-called variational collapse problem. Zhang, Liang, and Meng, *CPC* 33, 113 (2009); Zhang, Liang, and Meng, *IJMPE* 19, 55 (2010).
- To avoid similar problem in Ritz variational principle – maximizing $\langle 1/\hat{h} \rangle$ instead of minimizing $\langle \hat{h} \rangle$ Hill and Krauthauser, *PRL* 72, 151(1994)



- Hagino and Tanimura combined this idea with ITM and proposed IHM. The evolution of wave functions reads $|\psi\downarrow(\tau)\rangle = \mathrm{e}^{\uparrow \tau/\hat{h}-W} |\psi\downarrow 0\rangle$, who will converge to the ground state in Fermi sea as $\tau \to \infty$ with a suitable W. Hagino and Tanimura, *PRC* 82, 057301 (2010);

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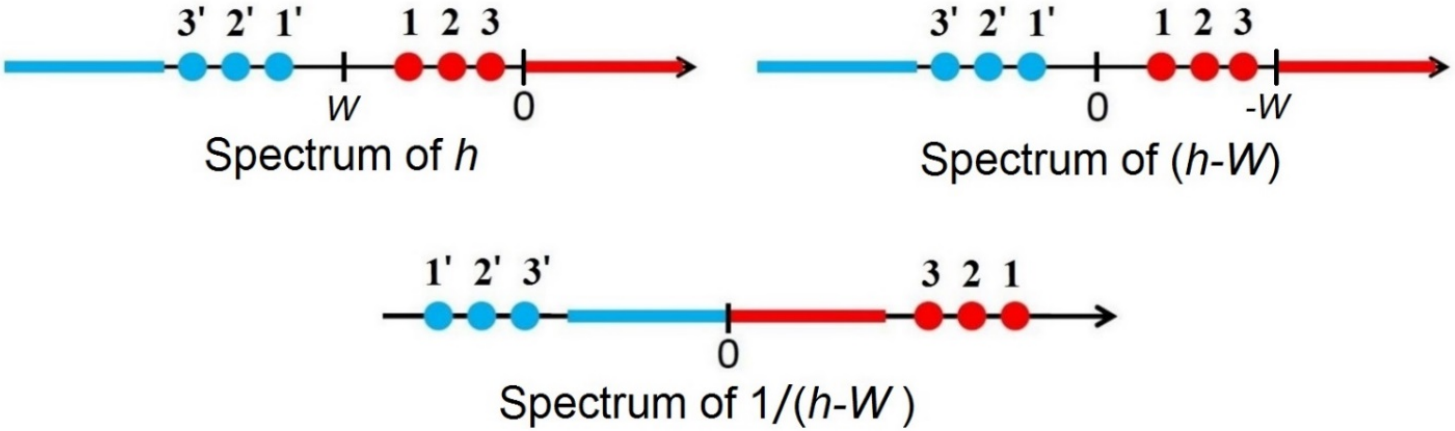

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Fermion doubling problem

- Solving Dirac equation in lattice space one may get spurious states with high momentum but low energy. Wilson1977Quarks and strings on a lattice
- 1D free Dirac equation:

$$(-\mathrm{i}\alpha\partial_x + \beta m)\psi(x) = \varepsilon\psi(x)$$

its solutions have the following form

$$\psi(x) = \tilde{\psi}(k)\exp(\mathrm{i}kx),$$

- Taking finite difference method,

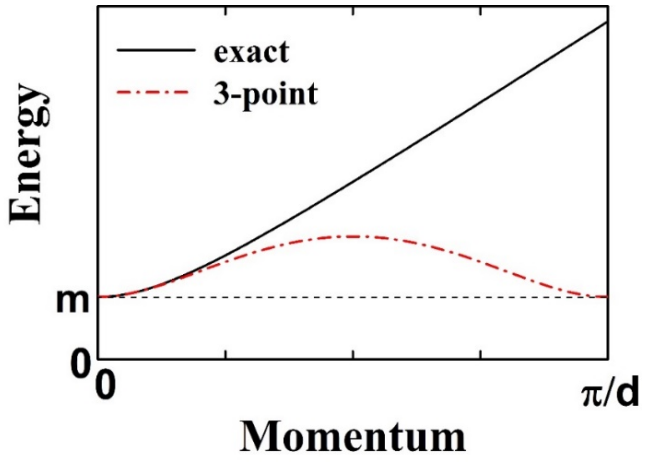
$$\partial_x\psi(x) \to \left[\psi(x_{i+1}) - \psi(x_{i-1})\right]/2d.$$

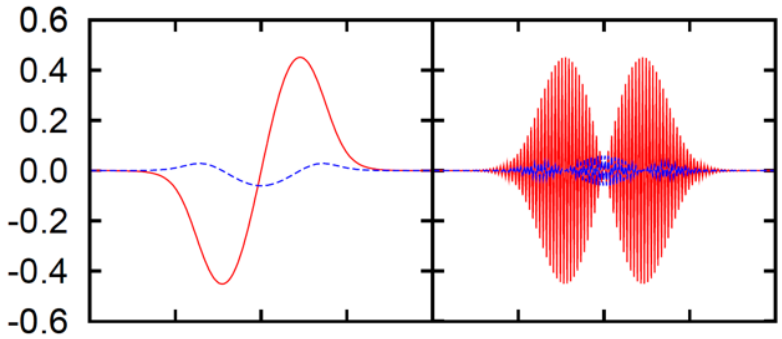
one will get

$$\left[\frac{1}{d}\alpha\sin(kd) + \beta m\right]\tilde{\psi}(k) = \varepsilon\tilde{\psi}(k)$$

- Dispersion relation $\varepsilon^2 = k^2 + m^2$ becomes

$$\varepsilon^2 = \frac{1}{d^2}\sin^2(kd) + m^2$$





Taken from Tanimura, Hagino, and Liang, *PTEP* 2015, 073D01 (2015).

Spectral method

- In momentum space, 1D free Dirac equation

$$(-\mathrm{i}\alpha\partial_x + \beta m)\psi(x) = \varepsilon\psi(x) \rightarrow (\alpha k + \beta m)\tilde{\psi}(k) = \varepsilon\tilde{\psi}(k)$$

It gives exact dispersion relation: $\varepsilon^2 = k^2 + m^2$, i.e. no Fermion doubling.

- In lattice space, spatial derivatives can be performed in momentum space with the help of discrete Fourier transform. In numerical physics, this method is so-called (Fourier) spectral method.
- Assuming $f(x_\nu)$ in momentum space is $f(k_n)$, m-th derivative of $f(x_\nu)$

$$f^{(m)}(x_\nu) = \frac{1}{n_x}\sum_{n=1}^{n_x}\exp(\mathrm{i}k_n x_\nu)(\mathrm{i}k_n)^m \tilde{f}(k_n)$$

$$= \frac{1}{n_x}\sum_{n=1}^{n_x}\exp(\mathrm{i}k_n x_\nu)\tilde{f}^{(m)}(k_n)$$

$$\Rightarrow \quad \tilde{f}^{(m)}(k_n) = (\mathrm{i}k_n)^m \tilde{f}(k_n)$$

$f_\nu^{(m)}(x_\nu)$ can be get from following procedure (FT: Fourier transform),

$$f(x_\nu) \xrightarrow{\mathrm{FT}} \tilde{f}(k_n) \xrightarrow{\tilde{f}^{(m)}(k_n)=(\mathrm{i}k_n)^m \tilde{f}(k_n)} \tilde{f}^{(m)}(k_n) \xrightarrow{\text{inverse FT}} f^{(m)}(x_\nu)$$

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Numerical details

- Potential of Dirac equation

$$V(\boldsymbol{r}) + S(\boldsymbol{r}) = \frac{V_0}{1 + \exp\left[(r - R_0 F(\Omega))/a\right]}$$

$$V(\boldsymbol{r}) - S(\boldsymbol{r}) = \frac{-\lambda V_0}{1 + \exp\left[(r - R_{ls} F(\Omega))/a_{ls}\right]}$$

$$F(\Omega) = [1 + \beta_{20} Y_{20}(\Omega) + \beta_{22}(Y_{22}(\Omega) + Y_{2-2}(\Omega)) + \beta_{30} Y_{30}(\Omega)]$$

with

V_0 [MeV]	R_0 [fm]	a [fm]	λ	R_{ls} [fm]	a_{ls} [fm]
−65.796	4.482	0.615	11.118	4.159	0.648

- The box sizes and step sizes for three direction are identical, denoted as L and d respectively. In calculations, L=23 fm and d=1 fm if not specified.
- Imaginary time step size: $\Delta\tau$=100 MeV.
- The inverse Hamiltonian is calculated by conjugate residual method. *S. Yousef, Iterative methods for sparse linear systems, (Siam, 2003)*

Numerical Details

To get a faster convergence, we suggest two procedures:

- **Changing *W***:

$$W_i = \varepsilon_i - \Delta W_i$$

where $\Delta W\downarrow 1 = 6\ MeV$, and for $i > 1$

$$\Delta W_i = \begin{cases} \varepsilon_i - \varepsilon_{i-1}, & \varepsilon_i - \varepsilon_{i-1} > \Delta W_1 \\ \Delta W_{i-1}, & \varepsilon_i - \varepsilon_{i-1} \leqslant \Delta W_1 \end{cases}$$

- **Diagonalizing Hamiltonian** within the space of the evelution wave functions every 10 iterations, the eigen functions are taken as initial wave functions for the next iteration.

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Iteration times

- Taking spherical potential as an example, we count the required iteration times for the convergence of all bound states.

- The convergence in the following calculations is defined as the energy dispersions

$$\delta = \sqrt{\langle h^2 \rangle - \langle h \rangle^2}$$

for all bound states are smaller than 10^{-4} MeV.

- The required iteration times:
  - (1) Normal choice: **>130,000**
  - (2) Changing W only: **27,184**
  - (3) Diagonalizing Hamiltonian only: **232**
  - (4) Changing W and diagonalizing Hamiltonian: **39**

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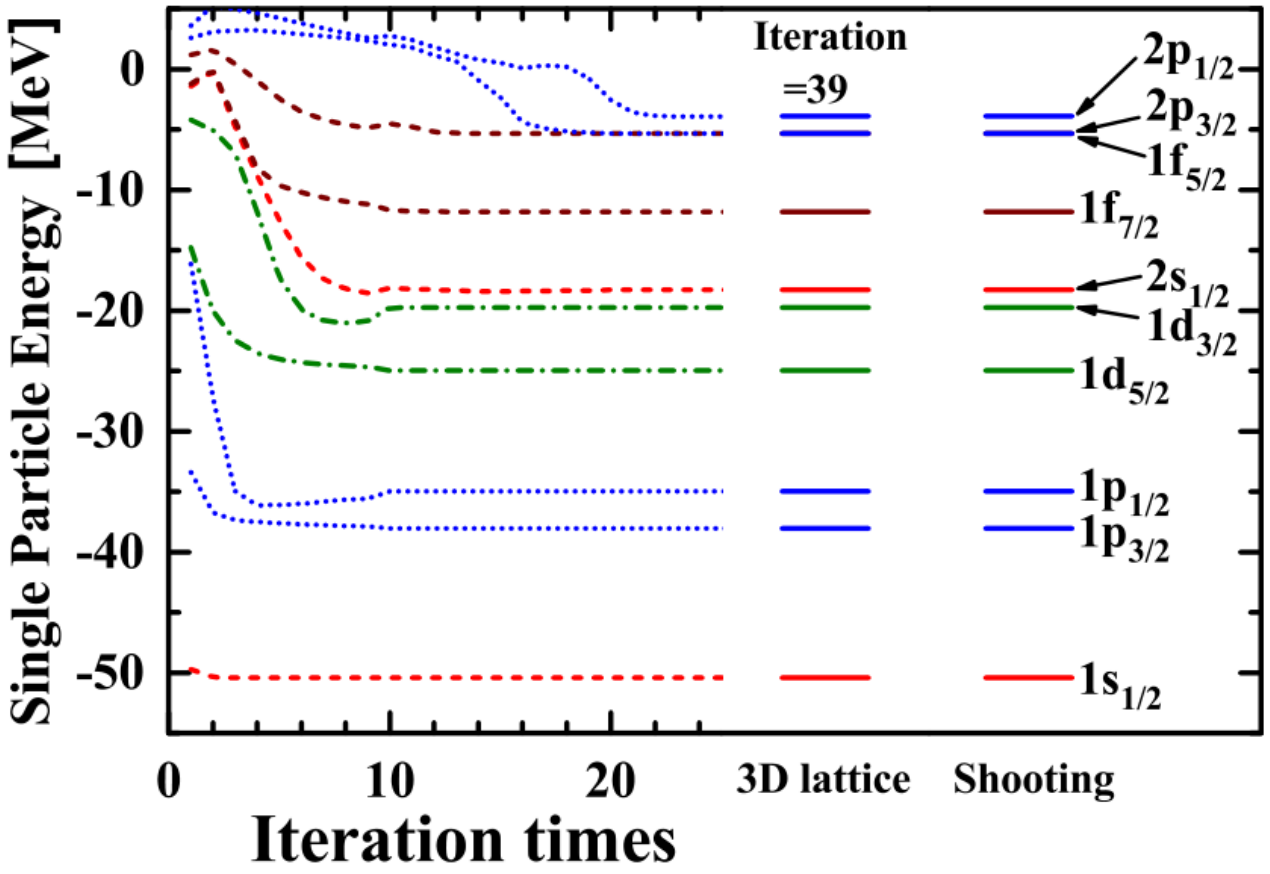
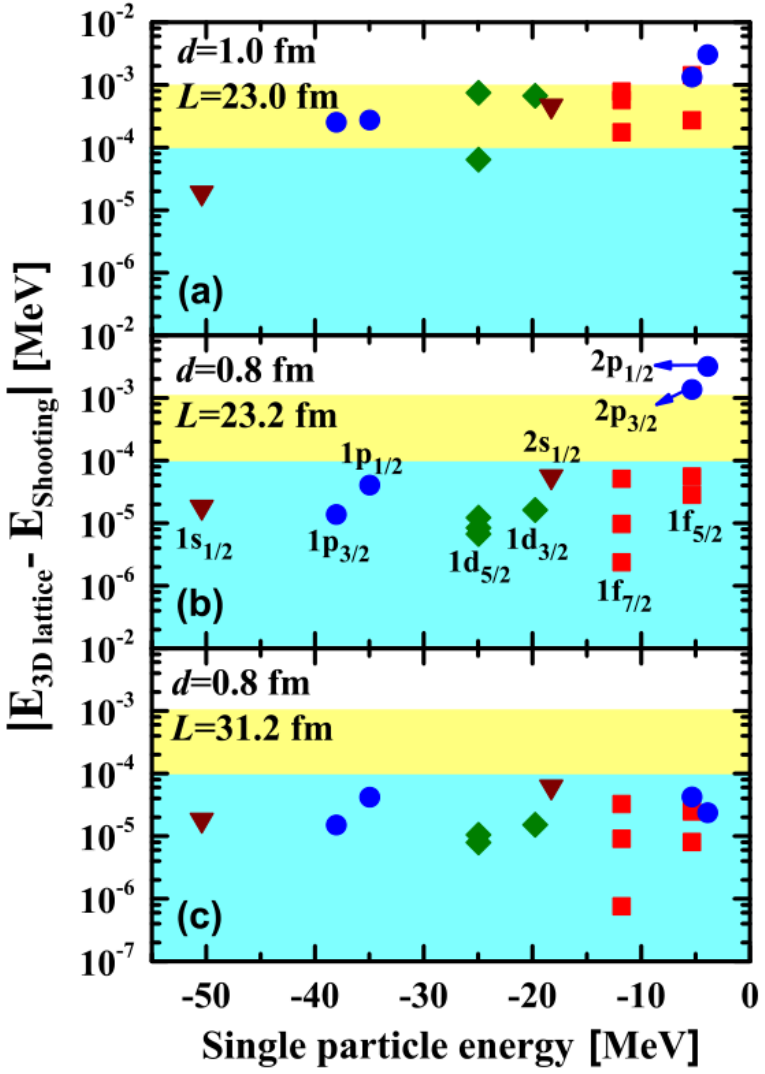
Spherical single particle levels



- For clarity, only one energy level of the degenerate ones is shown.
- After 39-th iteration, all the energy dispersions of bound sates are smaller than 10^{-4} MeV .

Energy accuracy



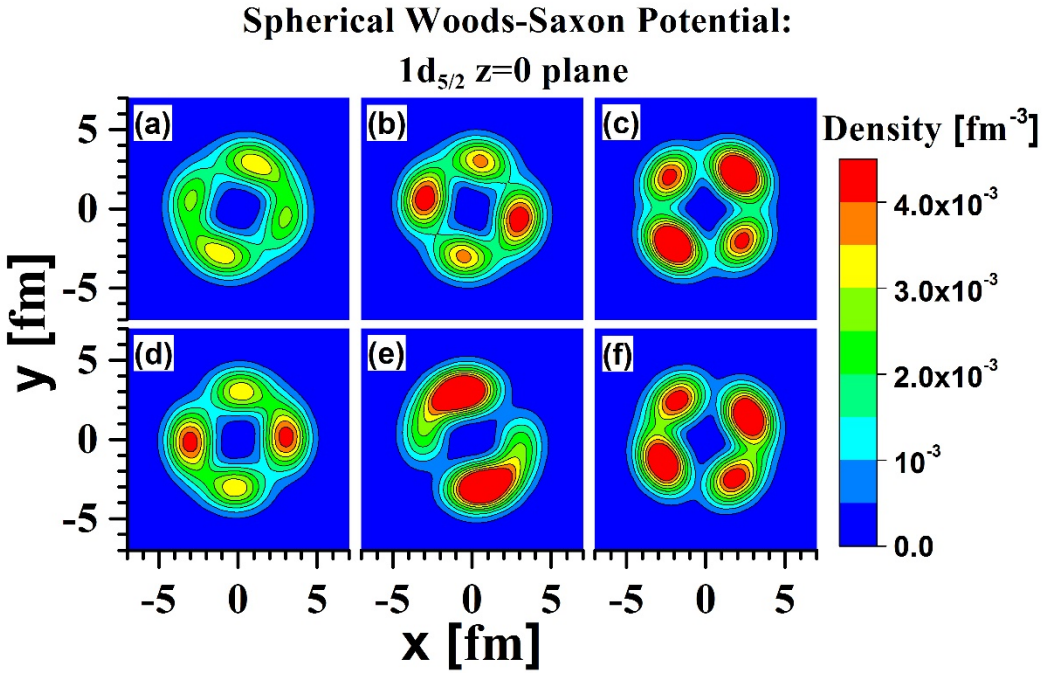
- Fig. (a) and Fig. (b):
  - $L\downarrow a \approx L\downarrow b \approx 23$ fm
  - $d\downarrow a = 1.0$ fm, $d\downarrow b = 0.8$ fm

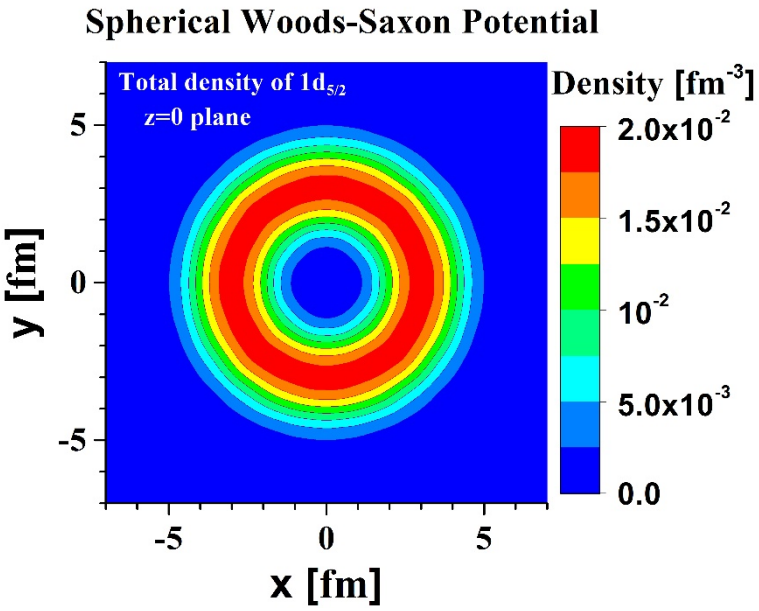
  Except weak bound $2\mathrm{p}\downarrow 3/2$ and $2\mathrm{p}\downarrow 1/2$ orbitals, the deviations are smaller than $10\uparrow -4$ MeV.

- Fig. (b) and Fig. (c):
  - $L\downarrow b$ =23.2 fm, $L\downarrow c$ =31.2 fm
  - $d\downarrow b = d\downarrow c = 0.8$ fm

  the deviations of $2\mathrm{p}\downarrow 3/2$ and $2\mathrm{p}\downarrow 1/2$ orbitals drop obviously, whereas the others are almost unchanged.

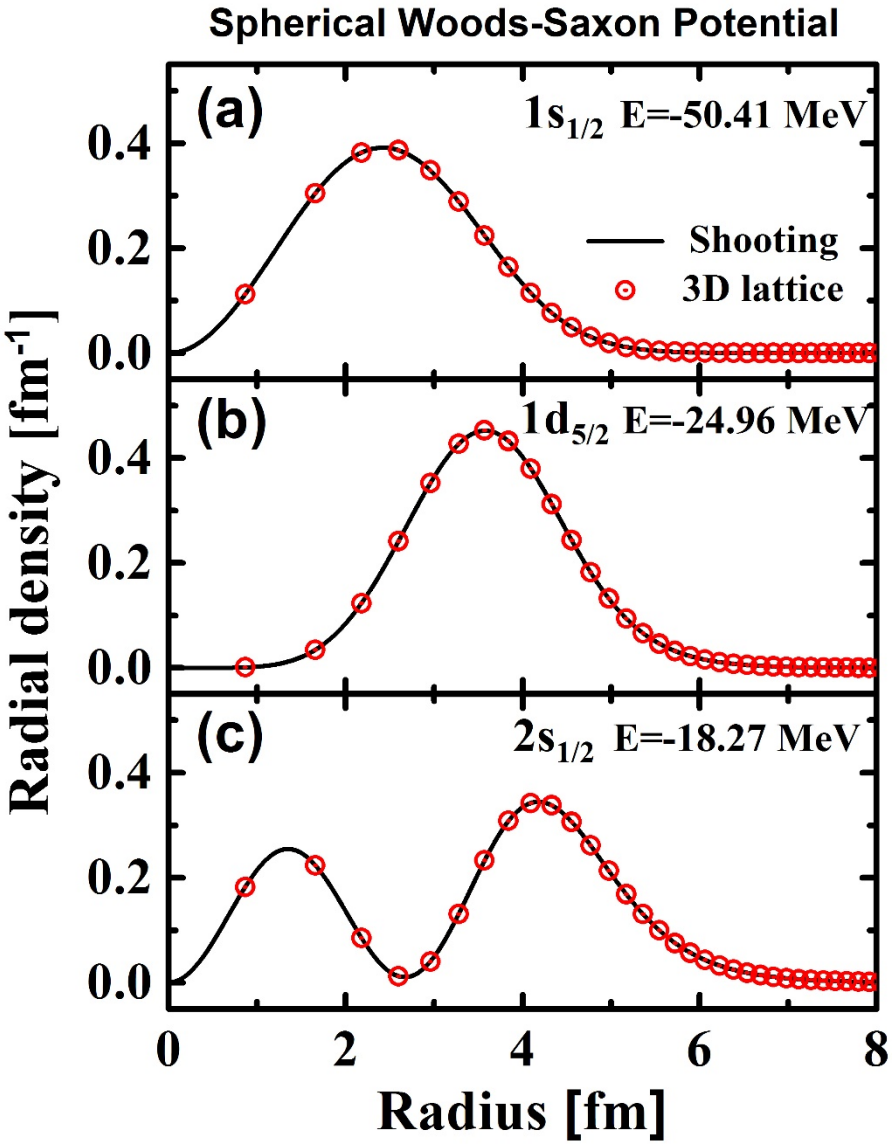
Density distribution





- The distribution of total density of six states of $1d\downarrow 5/2$ orbit is spherical.

Radial density distribution



- In 3D lattice calculations, radial (vector) densities are obtained by following equation

$$\rho^V_{nlj}(r) = \frac{1}{2j+1} 4\pi r^2 \sum_{i\in\{nlj\}} \psi^\dagger_i(\boldsymbol{r})\psi_i(\boldsymbol{r})$$

- The radial densities obtained by shooting method and 3D lattice calculations are almost identical.

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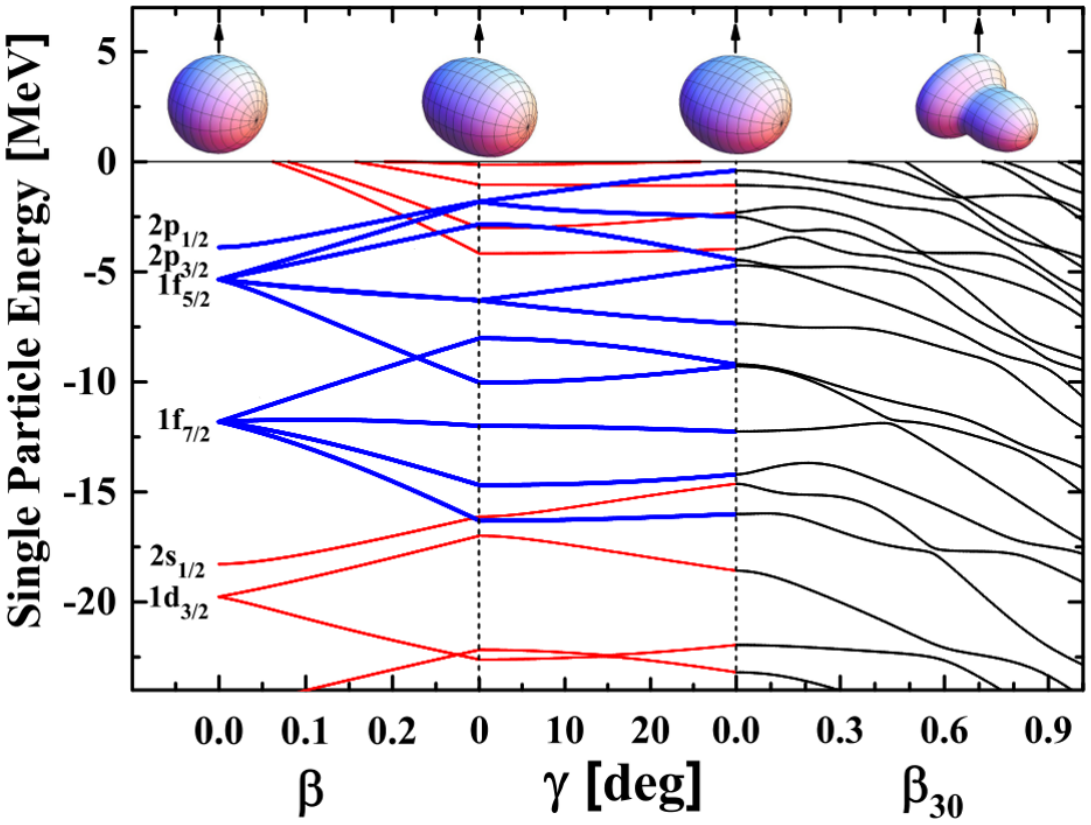
Deformed single particle levels



$$V(\boldsymbol{r}) + S(\boldsymbol{r}) = \frac{V_0}{1 + \exp[(r - R_0 F(\Omega))/a]}$$

$$F(\Omega) = [1 + \beta_{20} Y_{20}(\Omega) + \beta_{22}(Y_{22}(\Omega) + Y_{2-2}(\Omega)) + \beta_{30} Y_{30}(\Omega)]$$

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Summary and perspectives

☐ Summary

- In this work, Dirac equation is solved in 3D lattice by imaginary time method. The variational collapse is avoided by invers Hamiltonian method; Fermion doubling problem is avoided by spectral method, i.e. performing spatial derivatives in momentum space by discrete Fourier transform.

- Then, the new method is used to solve Dirac equations with spherical, quadrapole, octupole potential efficiently.

☐ Perspectives

- This method could be combined with CDFT:
  - 3D CDFT (finished);
  - 3D Cranking CDFT (in progress);
  - 3D Time-dependent CDFT (in progress).

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THANK YOU !

Conjugate Residual Algorithm

- Conjugate Residual Algorithm for linear equation $\boldsymbol{Ax=b}$:

1. Compute $r_0 := b - Ax_0$, $p_0 := r_0$
2. For $j = 0, 1, \ldots,$ until convergence Do:
3. $\quad \alpha_j := (r_j, Ar_j)/(Ap_j, Ap_j)$
4. $\quad x_{j+1} := x_j + \alpha_j p_j$
5. $\quad r_{j+1} := r_j - \alpha_j Ap_j$
6. $\quad \beta_j := (r_{j+1}, Ar_{j+1})/(r_j, Ar_j)$
7. $\quad p_{j+1} := r_{j+1} + \beta_j p_j$
8. $\quad$ Compute $Ap_{j+1} = Ar_{j+1} + \beta_j Ap_j$
9. EndDo

Functional PC-PK1: spherical nuclei

Nucleus: ^{16}O

	3D Lattice (n=24, d= 0.8 fm)	Spherical Code (R=20 fm, dr=0.1fm)	Axial def. Code (Nf=18)
Binding Energy [MeV]	127.285	127.286	127.230
Charge Radius r_c [fm]	2.767	2.768	2.768
$r_n - r_p$ [fm]	−0.023	−0.024	−0.024

Nucleus: ^{208}Pb

	3D Lattice (n=30, d= 1 fm)	Spherical Code (R=20 fm, dr=0.1fm)	Axial def. Code (Nf=18)
Binding Energy [MeV]	1637.941	1637.915	1637.780
Charge Radius r_c [fm]	5.518	5.518	5.517
$r_n - r_p$ [fm]	0.257	0.257	0.257

Functional PC-PK1: deformed nuclei

Nucleus: ^{20}Ne

	3D Lattice (n=24, d=0.8fm)	Axial def. Code (nf=18)
Binding Energy [MeV]	155.552	155.509
Charge Radius r_c [fm]	3.007	3.006
$r_n - r_p$ [fm]	−0.030	−0.029
β	0.541	0.541
β_{40}	0.494	0.491

Functional DD-ME2: spherical nuclei

Nucleus: ^{16}O

	3D Lattice (n=24, d=0.8 fm)	Lalazissis *et al* PRC71, 024312 (2005)	Absolute deviation
Binding Energy [MeV]	127.809	127.801	0.008
Charge Radius r_c [fm]	2.729	2.727	0.002
$r_n - r_p$ [fm]	-0.03	-0.03	0.00

Nucleus: ^{208}Pb

	3D Lattice (n=30, d=1 fm)	Lalazissis *et al* PRC71, 024312 (2005)	Absolute de viation
Binding Energy [MeV]	1638.483	1638.426	0.057
Charge Radius r_c [fm]	5.519	5.518	0.001
$r_n - r_p$ [fm]	0.19	0.19	0.00