Introduction My adventure Summary and Perspectives

Second EMMI-EFES Workshop on Neutron-Rich Exotic Nuclei RIKEN, June 16 \sim 18, 2010

Gradient method to solve the Hartree-Fock-Bogoliubov equation in the coordinate space

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June 18, 2010



Peking University Jie Meng



Niigata University Masayuki Matsuo





2 My adventure

- ITS method to solve the Dirac equation
- ITS method to solve the Hartree-Fock-Bogoliubov equation
- Gradient method to solve the HFB equation



Outline



2 My adventure

- ITS method to solve the Dirac equation
- ITS method to solve the Hartree-Fock-Bogoliubov equation
- Gradient method to solve the HFB equation



Introduction

Exotic phenomena in nuclear physics



Tanihata PRL 55(1985)2676, Hansen ARNPS 45(1995)591, Jensen RMP 76(2004)215,...

Features:

_ _ _ _ _ _ _

- ✓ Weakly bound
- \checkmark Coupling to the continuum
- \checkmark Large spacial density distribution

To describe the exotic nuclei

one expects to present the appropriate asymptotic behavior for the w.f. of nucleons in the coordinate space.

Introduction

Current status of investigation

Candidate theory for the description of exotic nuclei

Hartree-Fock-Bogoliubov (HFB) theory: Bogoliubov quasiparticle \Rightarrow unified description of both the mean field & paring correlation

- Non-relativistic: Skyrme Dobaczewski NPA(1984)
- Relativistic: covariant density functional theory

Vretenar PR(2005), Meng PPNP(2006), Long PRC(2010)

★ Technique to solve the HFB equation in coordinate space

- ✓ Shooting method
- ✓ Runge-Kutta scheme for coupled channels: Price PRC (1987)
- ✓ Woods-Saxon basis: *Zhou PRC(2003), ISPUN07(2008)*
- ✓ Green function method: *Oba PRC(2009)*

√ ...

Introduction

Current status of investigation

★ Candidate theory for the description of exotic nuclei

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★ Technique to solve the HFB equation in coordinate space

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- ✓ Green function method: *Oba PRC(2009)*
- ✓ …
- ? Gradient step method: Reinhard NPA(1982)
 - Gradient method: *Mang ZPA(1976)*
 - Imaginary time step (ITS) method: Davies NPA(1980), Gall ZPA(1994)

Gradient evolution to solve the Hartree-Fock-Bogoliubov equation

★ Gradient step method

Starts from an initial state and search for the local minimum on the energy surface

- Imaginary time step (ITS) method
- Gradient method

Gradient evolution to solve the Hartree-Fock-Bogoliubov equation

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 \checkmark Bound from the bottom

Introduction My adventure Summary and Perspectives

Gradient evolution to solve the Hartree-Fock-Bogoliubov equation

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Introduction My adventure Summary and Perspectives

Gradient evolution to solve the Hartree-Fock-Bogoliubov equation

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✓ Bound from the bottom

My adventure

- ITS method to solve the Dirac equation
- ITS method to solve the HFB equation
- **③** Gradient method to solve the HFB equation



? Not bound from the bottom

directly in the coordinate space!

Outline



2 My adventure

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Introduction ITS metho My adventure ITS metho Summary and Perspectives Gradient r

ITS method to solve the Dirac equation ITS method to solve the Hartree-Fock-Bogoliubov equation Gradient method to solve the HFB equation

ITS method to solve the Dirac equation

★ Imaginary time step (ITS) method Davies NPA(1980)

• Evolution of the w. f.

$$\left. \Phi_{j}^{(n+1)}
ight
angle \ = \ \left(1 - \eta \hat{h}
ight) \left| \phi_{j}^{(n)}
ight
angle$$

• Dirac equation

$$\begin{pmatrix} V+S & -\frac{d}{dr}+\frac{\kappa_a}{r} \\ +\frac{d}{dr}+\frac{\kappa_a}{r} & V-S-2M \end{pmatrix} \begin{pmatrix} F_a(r) \\ G_a(r) \end{pmatrix} = \varepsilon_a \begin{pmatrix} F_a(r) \\ G_a(r) \end{pmatrix},$$

• Schrödinger-like equation

$$\begin{cases} G_a = \frac{1}{2M_+} \left(\frac{dF_a}{dr} + \frac{\kappa_a}{r} F_a \right), \text{ where } M_+ = M + \frac{S - V + \varepsilon_a}{2}, \\ \hat{h}_F F_a = \varepsilon_a F_a \end{cases}$$

$$\hat{h}_{F} = -\frac{1}{2M_{+}}\frac{d^{2}}{dr^{2}} + \frac{1}{2M_{+}^{2}}\frac{dM_{+}}{dr}\frac{d}{dr} + \left[(V+S) + \frac{1}{2M_{+}^{2}}\frac{dM_{+}}{dr}\frac{\kappa_{a}}{r} + \frac{1}{2M_{+}}\frac{\kappa_{a}(\kappa_{a}+1)}{r^{2}} \right]$$

Introduction IT My adventure IT Summary and Perspectives Gr

ITS method to solve the Dirac equation ITS method to solve the Hartree-Fock-Bogoliubov equation Gradient method to solve the HFB equation

ITS method to solve the Dirac equation

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Introduction IT My adventure IT Summary and Perspectives G

ITS method to solve the Dirac equation ITS method to solve the Hartree-Fock-Bogoliubov equation Gradient method to solve the HFB equation

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Y. Zhang, et al., IJMPE 19(2010)55

Introduction IT My adventure IT Summary and Perspectives G

ITS method to solve the Dirac equation ITS method to solve the Hartree-Fock-Bogoliubov equation Gradient method to solve the HFB equation

ITS method to solve the Hartree-Fock-Bogoliubov equation

Hartree-Fock-Bogoliubov equation

$$\begin{pmatrix} h-\lambda & \Delta \\ -\Delta^* & -h^*+\lambda \end{pmatrix} \begin{pmatrix} U_k \\ V_k \end{pmatrix} = \begin{pmatrix} U_k \\ V_k \end{pmatrix} E_k$$
(1)

TS evolution for HFB equation

$$\begin{pmatrix} U'\\V' \end{pmatrix} = \left\{ 1 - \eta \begin{pmatrix} h - \lambda & \Delta\\ -\Delta^* & -h^* + \lambda \end{pmatrix} \right\} \begin{pmatrix} U\\V \end{pmatrix},$$
(2)

Introduction ITS My adventure ITS Summary and Perspectives Grav

ITS method to solve the Dirac equation ITS method to solve the Hartree-Fock-Bogoliubov equation Gradient method to solve the HFB equation

ITS method to solve the Hartree-Fock-Bogoliubov equation

★ Hartree-Fock-Bogoliubov equation

$$\sum_{\sigma'} \int d^3 r' \begin{pmatrix} h(\mathbf{r},\sigma;\mathbf{r}',\sigma') - \lambda & \Delta(\mathbf{r},\sigma;\mathbf{r}',\sigma') \\ \Delta(\mathbf{r},\sigma;\mathbf{r}',\sigma') & -h(\mathbf{r},\sigma;\mathbf{r}',\sigma') + \lambda \end{pmatrix} \begin{pmatrix} \psi_U^k(\mathbf{r}',\sigma') \\ \psi_V^k(\mathbf{r}',\sigma') \end{pmatrix} = \begin{pmatrix} \psi_U^k(\mathbf{r},\sigma) \\ \psi_V^k(\mathbf{r},\sigma) \end{pmatrix} E_k$$

ITS evolution for HFB equation

$$\begin{pmatrix} \psi_{U}^{k'}(\mathbf{r},\sigma) \\ \psi_{V}^{k'}(\mathbf{r},\sigma) \end{pmatrix} = \begin{pmatrix} \psi_{U}^{k}(\mathbf{r},\sigma) \\ \psi_{V}^{k}(\mathbf{r},\sigma) \end{pmatrix} - \eta \sum_{\sigma'} \left\{ \int d^{3}r' \begin{pmatrix} h(\mathbf{r},\sigma;\mathbf{r}',\sigma') - \lambda & \Delta(\mathbf{r},\sigma;\mathbf{r}',\sigma') \\ \Delta(\mathbf{r},\sigma;\mathbf{r}',\sigma') & -h(\mathbf{r},\sigma;\mathbf{r}',\sigma') + \lambda \end{pmatrix} \begin{pmatrix} \psi_{U}^{k}(\mathbf{r}',\sigma') \\ \psi_{V}^{k}(\mathbf{r}',\sigma') \end{pmatrix} \right\}$$

Simple test

• single-particle hamiltonian,

$$\hat{h}(\mathbf{r},\sigma;\mathbf{r}',\sigma') = \left[\frac{\hat{p}^2}{2M} + V\right] \delta(\mathbf{r}-\mathbf{r}')\delta_{\sigma\sigma'}$$

• the pairing potential,

$$\Delta(\mathbf{r}\sigma,\mathbf{r}'\sigma') = \sum_{ljm} Y_{ljm}(\hat{\mathbf{r}}\sigma) \frac{\Delta_{lj}(r,r')}{rr'} Y^*_{ljm}(\hat{\mathbf{r}}'\sigma')$$

• single-quasiparticle wave function

$$\psi_{U(V)}^{i}(\mathbf{r}\sigma) = \frac{\varphi_{U(V)}^{i}(\mathbf{r})}{\mathbf{r}}Y_{ljm}(\hat{\mathbf{r}}\sigma), \quad i = (nljm)$$

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Introduction ITS method to solve the Dirac equation My adventure ITS method to solve the Hartree-Fock-Bogoliubov equation Gradient method to solve the HFB equation

ITS method to solve the Hartree-Fock-Bogoliubov equation

Details for evolution

• V(r): Harmonic oscillator potential for ¹²C neutron

$$V(r) = \frac{1}{2}m\omega^2 r^2 = \frac{1}{2}\frac{mc^2}{\hbar^2 c^2}(\hbar\omega)^2 r^2, \text{ where } \hbar\omega = \frac{41}{A^{1/3}} \text{ MeV},$$
 (1)

• Pairing potential:

$$\Delta(r,r') = -V_{p} \ e^{-\frac{(r-R_{0})^{2}}{a^{2}}} \ \delta(r-r'), \qquad (2$$

- $-V_p = 0$ MeV
- $R_0 = r_0 A^{1/3}$, with $r_0 = 1.04$ fm
- -a = 0.65 fm
- Fermi level is fixed: $\lambda = -10$ MeV
- Step parameter: $\eta = \Delta t / \hbar$, $\Delta t = 10^{-26}$ s
- Box: R = 20 fm, dr = 0.1 fm
- Initial wave functions: $\psi_V \rightarrow$ spherical Bessel function, $\psi_U \rightarrow 0$

ITS method to solve the Hartree-Fock-Bogoliubov equation



Figure: ITS evolution of the energy for the first $s_{1/2}$ quasi-particle state



Figure: ITS evolution result of the wave function for the first $s_{1/2}$ quasi-particle state

Gradient method to solve the Hartree-Fock-Bogoliubov equation

Gradient method

The energy functional expressed in quasi-particle representation

$$E(Z) = \frac{\langle \Phi' | H | \Phi' \rangle}{\langle \Phi' | \Phi' \rangle} = H^0 + \left(\begin{array}{cc} H^{20*} & H^{20} \end{array} \right) \left(\begin{array}{c} Z \\ Z^* \end{array} \right) + \frac{1}{2} \left(\begin{array}{cc} Z^* & Z \end{array} \right) \left(\begin{array}{c} A & B \\ B^* & A^* \end{array} \right) \left(\begin{array}{c} Z \\ Z^* \end{array} \right),$$

the first order derivative of E(Z) is

$$\left. \frac{\partial E(Z)}{\partial Z^*_{\mu\nu}} \right|_{Z=0} = H^{20}_{\mu\nu} \tag{3}$$

Therefore, the energy difference between $|\Phi\rangle$ and $|\Phi'\rangle$ can be expanded as *Mang NPA(1976)*

$$\Delta E = \sum_{\mu\nu} H^{20}_{\mu\nu} Z_{\mu\nu} + O(Z^2_{\mu\nu})$$
(4)

If $Z_{\mu\nu}$ is chosen to be the direction of the steepest energy descent as,

$$Z_{\mu\nu} = -\eta \left. \frac{\partial E}{\partial Z^*_{\mu\nu}} \right|_{Z=0} = -\eta H^{20}_{\mu\nu}, \text{ where } \eta > 0$$
(5)

the energy difference can be written as

$$\Delta E = -\eta (H^{20})^2. \tag{6}$$

The total energy will decrease during this evolution until it finds the state with the lowest energy.

Gradient method to solve the Hartree-Fock-Bogoliubov equation

★ Gradient evolution for HFB equation

$$\begin{cases} U' = U + V^* Z^*, \\ V' = V + U^* Z^* \end{cases}$$
(7)

where

$$Z = -\eta (H^{20} - \lambda N^{20}).$$
(8)

with

$$H^{20} = U^{\dagger} h V^{*} - V^{\dagger} h^{*} U^{*} + U^{\dagger} \Delta U^{*} - V^{\dagger} \Delta^{*} V^{*}, \quad N^{20} = U^{\dagger} V^{*} - V^{\dagger} U^{*}$$
(9)

Since one should have the relation between U and V as

$$\boldsymbol{U}^{\dagger}\boldsymbol{U} + \boldsymbol{V}^{\dagger}\boldsymbol{V} = 1, \quad \boldsymbol{U}\boldsymbol{U}^{\dagger} + \boldsymbol{V}^{*}\boldsymbol{V}^{T} = 1, \tag{10}$$

$$U^{T}V + V^{T}U = 0, \quad UV^{\dagger} + V^{*}U^{T} = 0.$$
 (11)

and the HFB equation they should satisfy, one could get the evolution for U and V can be expressed as

$$\begin{pmatrix} U'\\V' \end{pmatrix} = \left\{ 1 - \eta \begin{pmatrix} -h + \lambda + E & -\Delta\\\Delta^* & h^* - \lambda + E \end{pmatrix} \right\} \begin{pmatrix} U\\V \end{pmatrix}$$
(12)

Introduction ITS me My adventure ITS me Summary and Perspectives Gradien

ITS method to solve the Dirac equation ITS method to solve the Hartree-Fock-Bogoliubov equation Gradient method to solve the HFB equation

Gradient method to solve the Hartree-Fock-Bogoliubov equation

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$$\begin{pmatrix} \psi_{U}^{k}(\mathbf{r}',\sigma') \\ \psi_{V}^{k}(\mathbf{r}',\sigma') \end{pmatrix} \right\}$$

IntroductionITS method to solve the Dirac equationMy adventureITS method to solve the Hartree-Fock-Bogoliubov equationSummary and PerspectivesGradient method to solve the HFB equation

Gradient method to solve the Hartree-Fock-Bogoliubov equation

★ Comparison between the Gradient and ITS evolution

$$\begin{pmatrix} h-\lambda & \Delta \\ -\Delta^* & -h^*+\lambda \end{pmatrix} \begin{pmatrix} U \\ V \end{pmatrix} = \begin{pmatrix} U \\ V \end{pmatrix} E,$$
(12)

Gradient evolution

$$\begin{pmatrix} U'\\V' \end{pmatrix} = \left\{ 1 - \eta \begin{pmatrix} -h + \lambda + E & -\Delta\\\Delta^* & h^* - \lambda + E \end{pmatrix} \right\} \begin{pmatrix} U\\V \\ (13) \end{pmatrix}$$

ITS evolution

$$\begin{pmatrix} U'\\V' \end{pmatrix} = \left\{ 1 - \eta \begin{pmatrix} h - \lambda & \Delta\\ -\Delta^* & -h^* + \lambda \end{pmatrix} \right\} \begin{pmatrix} U\\V \end{pmatrix},$$
(14)

Gradient method to solve the Hartree-Fock-Bogoliubov equation

★ Details for evolution

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(15)

• Pairing potential:

$$\Delta(r,r') = -V_p \ e^{-\frac{(r-R_0)^2}{a^2}} \ \delta(r-r'), \tag{16}$$

- $-V_p = 0$ MeV
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IntroductionITS method to solve the Dirac equationMy adventureITS method to solve the Hartree-Fock-Bogoliubov equationSummary and PerspectivesGradient method to solve the HFB equation

Gradient evolution to solve the Hartree-Fock-Bogoliubov equation

Gradient evolution for $\Delta = 0$



Figure: Gradient evolution of the energy for the first $s_{1/2}$ quasi-particle state



Figure: Gradient evolution result of the wave function for the first $s_{1/2}$ quasi-particle state

Gradient evolution to solve the Hartree-Fock-Bogoliubov equation

★ Gradient evolution for $\Delta \neq 0$ ($V_p = 10$ MeV)



Figure: Gradient evolution of the energy for the first $s_{1/2}$ quasi-particle state



Figure: Gradient evolution result of the wave function for the first $s_{1/2}$ quasi-particle state

Gradient method to solve the Hartree-Fock-Bogoliubov equation

★ Gradient evolution with constraint of N

The Gradient method is extremely useful in cases where we must fulfill a subsidiary condition – for instance, the particle number condition $\langle \hat{N} \rangle = N$. Starting from $|\Phi_0\rangle$ with arbitrary particle number N_0 , we do not proceed in the direction of the gradient H^{20} alone, but we admix the gradient of the particle number N^{20}

$$Z = -\eta (H^{20} - \lambda N^{20}). \tag{17}$$

The parameter λ is determined in such a way that $\Phi(Z_1)$ has the right particle number N up to linear order in Z. This gives

$$N - N_0 = \sum_{k < k'} Z_{kk'}^* N_{kk'}^{20} + c.c. = Z \cdot N^{20} = -\eta (H^{20} - \lambda N^{20}) \cdot N^{20}.$$
 (18)

Therefore, one could have

$$\lambda = \frac{H^{20} \cdot N^{20}}{N^{20} \cdot N^{20}} + \frac{N - N_0}{\eta N^{20} \cdot N^{20}},$$
(19)

where $Z \cdot N$ is the scalar product of the vectors (Z, Z^*) and (N, N^*) .

8

Gradient evolution to solve the Hartree-Fock-Bogoliubov equation

Gradient evolution for $\Delta \neq 0$ ($V_p = 10$ MeV)



 $\sum_{i=1}^{6} Gradient evolution without constraint of <N>$

Figure: Gradient evolution of the energy for the first $s_{1/2}$ quasi-particle state

Figure: Gradient evolution of the particle number expectation

Introduction ITS method to solve the Dirac equation My adventure ITS method to solve the Hartree-Fock-Bogo Gradient method to solve the HFB equation

Gradient evolution to solve the Hartree-Fock-Bogoliubov equation





Figure: Gradient evolution of the energy and the Fermi level for the first $s_{1/2}$ quasi-particle state



Figure: Gradient evolution result of the wave functions for the first $s_{1/2}$ quasi-particle state at convergence.

Introduction ITS method to solve the Dirac equation ITS method to solve the Hartree-Fock-Bogoliubov equation My adventure Summary and Perspectives Gradient method to solve the HFB equation

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Gradient evolution to solve the Hartree-Fock-Bogoliubov equation

Gradient evolution for $\Delta \neq 0$ ($V_p = 10$ MeV)



Fermi level λ (MeV) λ_{con} = 32919.416 MeV 32400 32000 0 200 400 600 800 1000 iterations

Figure: Gradient evolution of the energy for the first $s_{1/2}$ quasi-particle state

Figure: Gradient evolution of the Fermi level for the first $s_{1/2}$ quasi-particle state

Outline



2 My adventure

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Summary and Perspectives

- Recipe in coordinate space for the description of exotic nuclei
 - \longrightarrow Gradient step method
- Dirac equation
 - \longrightarrow Disaster for the direct ITS evolution for Dirac equation
 - \longrightarrow ITS method for the Schrödinger-like equation
- HFB equation
 - \longrightarrow ITS method failed
 - \longrightarrow Gradient method should be promising, but still some problems left...
- To be continued...

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