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

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## Outline

(1) Introduction
(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
(3) Summary and Perspectives


## Outline

## (1) Introduction

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

3 Summary and Perspectives

## Introduction

## * Exotic phenomena in nuclear physics






Tanihata PRL 55(1985)2676,
Hansen ARNPS 45(1995)591,
Jensen RMP 76(2004)215,...
Features:
$\checkmark$ Weakly bound
$\checkmark$ Coupling to the continuum
$\checkmark$ Large spacial density distribution $\checkmark$......

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

## Introduction

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


## Introduction

* 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)
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$\checkmark$ 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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## My adventure

(1) ITS method to solve the Dirac equation
(2) 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

(1) Introduction
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- ITS method to solve the Dirac equation
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## ITS method to solve the Dirac equation

## $\star$ Imaginary time step (ITS) method Davies NPA(1980)

- Evolution of the w. f.

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

- Dirac equation

$$
\left(\begin{array}{cc}
V+S & -\frac{d}{d r}+\frac{\kappa_{a}}{r} \\
+\frac{d}{d r}+\frac{\kappa_{a}}{r} & V-S-2 M
\end{array}\right)\binom{F_{a}(r)}{G_{a}(r)}=\varepsilon_{a}\binom{F_{a}(r)}{G_{a}(r)},
$$

- Schrödinger-like equation

$$
\begin{aligned}
&\left\{\begin{aligned}
G_{a} & =\frac{1}{2 M_{+}}\left(\frac{d F_{a}}{d r}+\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{aligned}\right. \\
& \hat{h}_{F}=-\frac{1}{2 M_{+}} \frac{d^{2}}{d r^{2}}+\frac{1}{2 M_{+}^{2}} \frac{d M_{+}}{d r} \frac{d}{d r} \\
&+\left[(V+S)+\frac{1}{2 M_{+}^{2}} \frac{d M_{+}}{d r} \frac{\kappa_{a}}{r}+\frac{1}{2 M_{+}} \frac{\kappa_{a}\left(\kappa_{a}+1\right)}{r^{2}}\right] .
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## ITS method to solve the Dirac equation

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& \\
& +\left[(V+S)+\frac{1}{2 M_{+}^{2}} \frac{d M_{+}}{d r} \frac{\kappa_{a}}{r}+\frac{1}{2 M_{+}} \frac{\kappa_{a}\left(\kappa_{a}+1\right)}{r^{2}}\right] .
\end{aligned}
$$



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& \\
& +\left[(V+S)+\frac{1}{2 M_{+}^{2}} \frac{d M_{+}}{d r} \frac{\kappa_{a}}{r}+\frac{1}{2 M_{+}} \frac{\kappa_{a}\left(\kappa_{a}+1\right)}{r^{2}}\right]
\end{aligned}
$$


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

## ITS method to solve the Hartree-Fock-Bogoliubov equation

$\star$ Hartree-Fock-Bogoliubov equation

$$
\left(\begin{array}{cc}
h-\lambda & \Delta  \tag{1}\\
-\Delta^{*} & -h^{*}+\lambda
\end{array}\right)\binom{U_{k}}{V_{k}}=\binom{U_{k}}{V_{k}} E_{k}
$$

$\star$ ITS evolution for HFB equation

$$
\binom{U^{\prime}}{V^{\prime}}=\left\{1-\eta\left(\begin{array}{cc}
h-\lambda & \Delta  \tag{2}\\
-\Delta^{*} & -h^{*}+\lambda
\end{array}\right)\right\}\binom{U}{V}
$$

## ITS method to solve the Hartree-Fock-Bogoliubov equation

$\star$ Hartree-Fock-Bogoliubov equation

$$
\sum_{\sigma^{\prime}} \int d^{3} r^{\prime}\left(\begin{array}{cc}
h\left(\mathbf{r}, \sigma ; \mathbf{r}^{\prime}, \sigma^{\prime}\right)-\lambda & \Delta\left(\mathbf{r}, \sigma ; \mathbf{r}^{\prime}, \sigma^{\prime}\right) \\
\Delta\left(\mathbf{r}, \sigma ; \mathbf{r}^{\prime}, \sigma^{\prime}\right) & -h\left(\mathbf{r}, \sigma ; \mathbf{r}^{\prime}, \sigma^{\prime}\right)+\lambda
\end{array}\right)\binom{\psi_{U}^{k}\left(\mathbf{r}^{\prime}, \sigma^{\prime}\right)}{\psi_{V}^{k}\left(\mathbf{r}^{\prime}, \sigma^{\prime}\right)}=\binom{\psi_{U}^{k}(\mathbf{r}, \sigma)}{\psi_{V}^{k}(\mathbf{r}, \sigma)} E_{k}
$$

* ITS evolution for HFB equation

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

$\star$ Simple test

- single-particle hamiltonian,

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

- the pairing potential,

$$
\Delta\left(\mathbf{r} \sigma, \mathbf{r}^{\prime} \sigma^{\prime}\right)=\sum_{l j m} Y_{l j m}(\hat{\mathbf{r}} \sigma) \frac{\Delta_{l j}\left(r, r^{\prime}\right)}{r r^{\prime}} Y_{l j m}^{*}\left(\hat{\mathbf{r}}^{\prime} \sigma^{\prime}\right)
$$

- single-quasiparticle wave function

$$
\psi_{U(V)}^{i}(\mathbf{r} \sigma)=\frac{\varphi_{U(V)}^{i}(r)}{r} Y_{l j m}(\hat{\mathbf{r}} \sigma), \quad i=(n l j m)
$$

## ITS method to solve the Hartree-Fock-Bogoliubov equation

## Details for evolution

- $V(r)$ : Harmonic oscillator potential for ${ }^{12} \mathrm{C}$ neutron

$$
\begin{equation*}
V(r)=\frac{1}{2} m \omega^{2} r^{2}=\frac{1}{2} \frac{m c^{2}}{\hbar^{2} c^{2}}(\hbar \omega)^{2} r^{2}, \quad \text { where } \quad \hbar \omega=\frac{41}{A^{1 / 3}} \mathrm{MeV} \tag{1}
\end{equation*}
$$

- Pairing potential:

$$
\begin{equation*}
\Delta\left(r, r^{\prime}\right)=-V_{p} e^{-\frac{\left(r-R_{0}\right)^{2}}{a^{2}}} \delta\left(r-r^{\prime}\right) \tag{2}
\end{equation*}
$$

$-V_{p}=0 \mathrm{MeV}$
$-R_{0}=r_{0} A^{1 / 3}$, with $r_{0}=1.04 \mathrm{fm}$
$-a=0.65 \mathrm{fm}$

- Fermi level is fixed: $\lambda=-10 \mathrm{MeV}$
- Step parameter: $\eta=\Delta t / \hbar, \Delta t=10^{-26} \mathrm{~s}$
- Box: $R=20 \mathrm{fm}, d r=0.1 \mathrm{fm}$
- Initial wave functions: $\psi_{V} \rightarrow$ spherical Bessel function, $\psi_{U} \rightarrow 0$


## ITS method to solve the Hartree-Fock-Bogoliubov equation

## ITS evolution for $\Delta=0$



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

## $\star$ Gradient method

The energy functional expressed in quasi-particle representation

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

the first order derivative of $E(Z)$ is

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

Therefore, the energy difference between $|\Phi\rangle$ and $\left|\Phi^{\prime}\right\rangle$ can be expanded as Mang NPA(1976)

$$
\begin{equation*}
\Delta E=\sum_{\mu \nu} H_{\mu \nu}^{20} Z_{\mu \nu}+O\left(Z_{\mu \nu}^{2}\right) \tag{4}
\end{equation*}
$$

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

$$
\begin{equation*}
Z_{\mu \nu}=-\left.\eta \frac{\partial E}{\partial Z_{\mu \nu}^{*}}\right|_{Z=0}=-\eta H_{\mu \nu}^{20}, \text { where } \eta>0 \tag{5}
\end{equation*}
$$

the energy difference can be written as

$$
\begin{equation*}
\Delta E=-\eta\left(H^{20}\right)^{2} \tag{6}
\end{equation*}
$$

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

## $\star$ Gradient evolution for HFB equation

$$
\left\{\begin{array}{l}
U^{\prime}=U+V^{*} Z^{*}  \tag{7}\\
V^{\prime}=V+U^{*} Z^{*}
\end{array}\right.
$$

where

$$
\begin{equation*}
Z=-\eta\left(H^{20}-\lambda N^{20}\right) \tag{8}
\end{equation*}
$$

with

$$
\begin{equation*}
H^{20}=U^{\dagger} h V^{*}-V^{\dagger} h^{*} U^{*}+U^{\dagger} \Delta U^{*}-V^{\dagger} \Delta^{*} V^{*}, \quad N^{20}=U^{\dagger} V^{*}-V^{\dagger} U^{*} \tag{9}
\end{equation*}
$$

Since one should have the relation between $U$ and $V$ as

$$
\begin{align*}
U^{\dagger} U+V^{\dagger} V & =1, \tag{10}
\end{align*} \quad U U^{\dagger}+V^{*} V^{T}=1, ~ 子 V^{\top} U=0, \quad U V^{\dagger} U^{T}=0 .
$$

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

$$
\binom{U^{\prime}}{V^{\prime}}=\left\{1-\eta\left(\begin{array}{cc}
-h+\lambda+E & -\Delta  \tag{12}\\
\Delta^{*} & h^{*}-\lambda+E
\end{array}\right)\right\}\binom{U}{V}
$$

## Gradient method to solve the Hartree-Fock-Bogoliubov equation

## $\star$ Gradient evolution for HFB equation

$$
\left\{\begin{array}{l}
U^{\prime}=U+V^{*} Z^{*}  \tag{7}\\
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$$

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\end{equation*}
$$

Since one should have the relation between $U$ and $V$ as

$$
\begin{align*}
U^{\dagger} U+V^{\dagger} V=1, & U U^{\dagger}+V^{*} V^{T}=1  \tag{10}\\
U^{T} V+V^{T} U=0, & U V^{\dagger}+V^{*} U^{T}=0 \tag{11}
\end{align*}
$$

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

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

## Gradient method to solve the Hartree-Fock-Bogoliubov equation

## * Comparison between the Gradient and ITS evolution

$$
\left(\begin{array}{cc}
h-\lambda & \Delta  \tag{12}\\
-\Delta^{*} & -h^{*}+\lambda
\end{array}\right)\binom{U}{V}=\binom{U}{V} E,
$$

## Gradient evolution

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

ITS evolution

$$
\binom{U^{\prime}}{V^{\prime}}=\left\{1-\eta\left(\begin{array}{cc}
h-\lambda & \Delta \\
-\Delta^{*} & -h^{*}+\lambda
\end{array}\right)\right\}\binom{U}{V},
$$

## Gradient method to solve the Hartree-Fock-Bogoliubov equation

## $\star$ Details for evolution

- $V(r)$ : Harmonic oscillator potential for ${ }^{12} \mathrm{C}$ neutron

$$
\begin{equation*}
V(r)=\frac{1}{2} m \omega^{2} r^{2}=\frac{1}{2} \frac{m c^{2}}{\hbar^{2} c^{2}}(\hbar \omega)^{2} r^{2}, \quad \text { where } \quad \hbar \omega=\frac{41}{A^{1 / 3}} \mathrm{MeV} \tag{15}
\end{equation*}
$$

- Pairing potential:

$$
\begin{equation*}
\Delta\left(r, r^{\prime}\right)=-V_{p} e^{-\frac{\left(r-R_{0}\right)^{2}}{a^{2}}} \delta\left(r-r^{\prime}\right) \tag{16}
\end{equation*}
$$

$-V_{p}=0 \mathrm{MeV}$
$-R_{0}=r_{0} A^{1 / 3}$, with $r_{0}=1.04 \mathrm{fm}$
$-a=0.65 \mathrm{fm}$

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## 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 $\Delta \neq 0\left(V_{p}=10 \mathrm{MeV}\right)$


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 $\left|\Phi_{0}\right\rangle$ 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 $N^{20}$

$$
\begin{equation*}
Z=-\eta\left(H^{20}-\lambda N^{20}\right) . \tag{17}
\end{equation*}
$$

The parameter $\lambda$ is determined in such a way that $\Phi\left(Z_{1}\right)$ has the right particle number $N$ up to linear order in $Z$. This gives

$$
\begin{equation*}
N-N_{0}=\sum_{k<k^{\prime}} Z_{k k^{\prime}}^{*} N_{k k^{\prime}}^{20}+c . c .=Z \cdot N^{20}=-\eta\left(H^{20}-\lambda N^{20}\right) \cdot N^{20} . \tag{18}
\end{equation*}
$$

Therefore, one could have

$$
\begin{equation*}
\lambda=\frac{H^{20} \cdot N^{20}}{N^{20} \cdot N^{20}}+\frac{N-N_{0}}{\eta N^{20} \cdot N^{20}}, \tag{19}
\end{equation*}
$$

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

## Gradient evolution to solve the Hartree-Fock-Bogoliubov equation

Gradient evolution for $\Delta \neq 0\left(V_{p}=10 \mathrm{MeV}\right)$


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


Figure: Gradient evolution of the particle number expectation

## Gradient evolution to solve the Hartree-Fock-Bogoliubov equation

$\star$ Gradient evolution for $\Delta \neq 0\left(V_{p}=10 \mathrm{MeV}\right)$



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.

## Gradient evolution to solve the Hartree-Fock-Bogoliubov equation

Gradient evolution for $\Delta \neq 0\left(V_{p}=10 \mathrm{MeV}\right)$


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

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(2) My adventure

- ITS method to solve the Dirac equation
- ITS method to solve the Hartree-Fock-Bogoliubov equation
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(3) Summary and Perspectives


## 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...


## Summary and Perspectives

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