DEFORMED RELATIVISTIC HARTREE-BOGOLIUBOV MODEL
FOR EXOTIC NUCLEI

S. G. Zhou∗
Institute of Theoretical Physics, Chinese Academy of Sciences, Beijing 100080, China
Center of Theoretical Nuclear Physics, National Laboratory of Heavy Ion Accelerator,
Lanzhou 730000, China
∗E-mail: sgzhou@itp.ac.cn

J. Meng
School of Physics, Peking University, Beijing 100871, China
Institute of Theoretical Physics, Chinese Academy of Sciences, Beijing 100080, China
Center of Theoretical Nuclear Physics, National Laboratory of Heavy Ion Accelerator,
Lanzhou 730000, China

P. Ring
Physikdepartment, Technische Universität München, 85748 Garching, Germany

A deformed relativistic Hartree-Bogoliubov (DRHB) model is developed aiming at a
proper description of exotic nuclei, particularly deformed ones with large spatial exten-
sion. In order to give an adequate description of both the contribution of the continuum
and the large spatial distribution in exotic nuclei, the DRHB equations are solved in a
Woods-Saxon basis in which the radial wave functions have proper asymptotic behaviors
at large distance from the nuclear center which is crucial for the formation of halo. The
formalism and the numerical procedure of the DRHB model in a Woods-Saxon basis are
briefly presented.

Keywords: Relativistic mean field model; Bogoliubov transformation; Deformed halo;
Woods-Saxon basis.

1. Introduction

One of the exotic phenomena observed in nuclei close to drip lines is the halo in
which the extremely weakly binding property leads to many new features, e.g., the
coupling between the bound states and the continuum due to pairing correlations
and the large spacial density distribution. In order to give an adequate theoretical
description of the halo phenomenon, the asymptotic behavior of nuclear densities
at large \( r \) must be considered properly and the discrete bound states, the contin-
umum and the coupling between them must be treated self consistently. This could
be achieved by solving the non-relativistic Hartree-Fock-Bogoliubov (HFB)\(^1-3\) or
relativistic Hartree-Bogoliubov (RHB)\(^4-6\) equations in coordinate space which can
fully take into account the mean-field effects of the coupling to the continuum.
In Refs.\textsuperscript{2–6} the spherical symmetry is assumed. Since most of the known nuclei are deformed, whether or not there exist deformed halos and what new features are expected in deformed exotic nuclei are very interesting questions\textsuperscript{7–12} which could be answered by the deformed counterparts of the HFB or RHB models. Nevertheless for deformed nuclei, to solve the HFB or RHB equations in coordinate space becomes much more sophisticated and numerically very time consuming. Although many efforts have been made to develop non-relativistic HFB models either in (discretized) coordinate space or in a basis with improved asymptotic behavior,\textsuperscript{13–20} the deformed relativistic Hartree-Bogoliubov model has been developed only in conventional harmonic oscillator basis.\textsuperscript{21–24}

The deformed relativistic Hartree equations have been solved in a basis in which the basis wave functions are calculated from solving the Dirac equation with spherical Hartree potentials.\textsuperscript{25,26} In Ref.\textsuperscript{27} the Woods-Saxon basis was proposed as a reconciler between the harmonic oscillator basis and the coordinate space. The Woods-Saxon wave functions have more realistic asymptotic behavior at large \( r \).

One can also use a box boundary condition to discretize the continuum. It has been shown that to solve the spherical relativistic Hartree equations in a Woods-Saxon basis is almost equivalent to do it in coordinate space.\textsuperscript{27} The Woods-Saxon basis may be used in more complicated situations, e.g., for the description of exotic nuclei where both deformation and pairing have to be taken into account.\textsuperscript{28} In this proceeding paper we will present briefly the formalism, numerical procedure and some preliminary results of the deformed relativistic Hartree Bogoliubov model in a Woods-Saxon basis. Throughout the paper, this model will be labeled as the DRHBWS model.

The paper is organized as follows. In Sec. 2 we give the formalism of the DRHBWS model. The numerical procedure and some preliminary results are presented in Sec. 3. A summary is given in Sec. 4.

### 2. Formalism

The starting point of the relativistic Hartree theory is a Lagrangian density where nucleons are described as Dirac spinors which interact via the exchanges of several mesons (\( \sigma, \omega, \) and \( \rho \)) and the photon,\textsuperscript{29–33}

\[
\mathcal{L} = \bar{\psi}_i \left( i\gamma \cdot \partial - M \right) \psi_i + \frac{1}{2} \partial_\mu \sigma \partial^\mu \sigma - U(\sigma) - g_\sigma \bar{\psi}_i \sigma \psi_i \\
- \frac{1}{4} \Omega_{\mu\nu} \Omega^{\mu\nu} + \frac{1}{2} m_\omega^2 \omega_\mu \omega^\mu - g_\omega \bar{\psi}_i \gamma_5 \omega \psi_i \\
- \frac{1}{4} \bar{R}_{\mu\nu} R^{\mu\nu} + \frac{1}{2} m_\rho^2 \rho_\mu \rho^\mu - g_\rho \bar{\psi}_i \gamma_5 \rho \psi_i \\
- \frac{1}{4} F_{\mu\nu} F^{\mu\nu} - e \bar{\psi}_i \left( 1 - \frac{\sigma_3}{2} \right) A \psi_i,
\]

(1)

with the summation convention used, \( \not{x} \equiv \gamma^\mu x_\mu = \gamma_\mu x^\mu \), \( M \) the nucleon mass, and \( m_\sigma, g_\sigma, m_\omega, g_\omega, m_\rho, g_\rho \) masses and coupling constants of the respective mesons. The nonlinear self-coupling for the scalar mesons is crucial for a satisfactory description
of the surface properties,

\[
U(\sigma) = \frac{1}{2} m^2 \sigma^2 + \frac{g_2}{3} \sigma^3 + \frac{g_3}{4} \sigma^4,
\]

and field tensors for the vector mesons and the photon fields are defined as

\[
\begin{align*}
\Omega_{\mu\nu} &= \partial_{[\mu} \omega_{\nu]} - \partial_{[\nu} \omega_{\mu]}, \\
F_{\mu\nu} &= \partial_{\mu} \rho_{\nu} - \partial_{\nu} \rho_{\mu} - g_{\rho} (\vec{\rho}_{\mu} \times \vec{\rho}_{\nu}), \\
F_{\mu\nu} &= \partial_{\mu} A_{\nu} - \partial_{\nu} A_{\mu}.
\end{align*}
\]

For the ground state of nuclei with time reversal symmetry, the nucleon spinors are the eigenvectors of the stationary Dirac equation,

\[
[\mathbf{\alpha} \cdot \mathbf{p} + V(\mathbf{r}) + \beta(M + S(\mathbf{r}))] \psi_i(\mathbf{r}) = \epsilon_i \psi_i(\mathbf{r}),
\]

and equations of motion for the mesons and the photon are

\[
\begin{align*}
(-\Delta + \partial_\mu U(\sigma)) \sigma(\mathbf{r}) &= -g_\rho \rho_\sigma(\mathbf{r}), \\
(-\Delta + \omega^2) \omega^0(\mathbf{r}) &= g_\omega \rho_\omega(\mathbf{r}), \\
(-\Delta + \rho^2) \rho^0(\mathbf{r}) &= g_\rho \rho_3(\mathbf{r}), \\
-\Delta A^0(\mathbf{r}) &= \epsilon_i \rho_i(\mathbf{r}),
\end{align*}
\]

where \(\omega^0\) and \(A^0\) are time-like components of the vector \(\omega\) and the photon fields and \(\rho^0\) the 3-component of the time-like component of the iso-vector component \(\rho\) meson. Equations (4) and (5) are coupled by the vector and scalar potentials,

\[
\begin{align*}
V(\mathbf{r}) &= g_\omega \omega^0(\mathbf{r}) + g_\rho \tau_3 \rho^0(\mathbf{r}) + \epsilon \frac{1 - \tau_3}{2} A^0(\mathbf{r}), \\
S(\mathbf{r}) &= g_\sigma \sigma(\mathbf{r}),
\end{align*}
\]

and various densities

\[
\rho_\sigma(\mathbf{r}) = \sum_{i=1}^A \bar{\psi}_i(\mathbf{r}) \psi_i(\mathbf{r}), \\
\rho_\omega(\mathbf{r}) = \sum_{i=1}^A \bar{\psi}_i(\mathbf{r}) \psi_i(\mathbf{r}), \\
\rho_3(\mathbf{r}) = \sum_{i=1}^A \bar{\psi}_i(\mathbf{r}) \tau_3 \psi_i(\mathbf{r}), \\
\rho_\omega(\mathbf{r}) = \sum_{i=1}^A \bar{\psi}_i(\mathbf{r}) \frac{1 - \tau_3}{2} \psi_i(\mathbf{r}).
\]

The pairing correlation is included via the Bogoliubov transformation and the relativistic Hartree-Bogoliubov equation reads,

\[
\sum_{\sigma'p'} \int d^3 \mathbf{r}' \left( \begin{array}{c}
h_D(\mathbf{r} \sigma p, \mathbf{r} \sigma' p') - \lambda \\
\Delta(\mathbf{r} \sigma p, \mathbf{r} \sigma' p') - \frac{\Delta^*}{2}(\mathbf{r} \sigma p, \mathbf{r} \sigma' p') \end{array} \right) \left( \begin{array}{c} U_k(\mathbf{r} \sigma' p') \\
V_k(\mathbf{r} \sigma' p') \end{array} \right) = E_k \left( \begin{array}{c} U_k(\mathbf{r} \sigma p) \\
V_k(\mathbf{r} \sigma p) \end{array} \right),
\]

where \(E_k\) is the quasiparticle energy, \(h_D\) the Dirac Hamiltonian in (3), and \(\lambda\) the Fermi energy. Here \(p = 1, 2\) (or \(\pm\)) is used to represent the particle-antiparticle degree of freedom.

If in the pp channel, we use a zero range density dependent force,

\[
V_{p_1p_2p_3p_4}(\mathbf{r}_1, \mathbf{r}_2; \sigma_1 \sigma_2 \sigma_1' \sigma_2') = \frac{1}{4} V_0 \delta(\mathbf{r}_1 - \mathbf{r}_2) \left[ 1 - 4 \vec{\sigma}_1' \cdot \vec{\sigma}_2' \right] \left[ \mathbf{I}_{11'} \cdot \mathbf{I}_{22'} \right],
\]

where \(\vec{\sigma}_i\) are the Pauli matrices, and \(\mathbf{I}_{ij}\) are the identity matrices.
for axially deformed nuclei with spacial reflection symmetry, we may expand the potentials, \( S(r), V(r), \) and \( \Delta(r) \), and various densities in terms of the Legendre polynomials,
\[
f(r) = \sum_{\lambda} f_\lambda(r) P_\lambda(\cos \theta), \quad f_\lambda(r) = \frac{2\lambda + 1}{2} \int d\cos \theta f(r) P_\lambda(\cos \theta), \quad \lambda = 0, 2, 4, \ldots .
\]

The quasi particle wave function is expanded in the Woods-Saxon basis \( \{ \epsilon_{i\kappa m}, \varphi_{i\kappa m}(r\sigma) \} \) as,
\[
U_k(r\sigma) = \sum_{i\kappa} \left( \begin{array}{c} u^{(m)}_{i\kappa}(r\sigma) \\ v^{(m)}_{i\kappa}(r\sigma) \end{array} \right),
\]
\[
V_k(r\sigma) = \sum_{i\kappa} \left( \begin{array}{c} v^{(m)}_{i\kappa}(r\sigma) \\ u^{(m)}_{i\kappa}(r\sigma) \end{array} \right),
\]

where the single particle energy \( \epsilon_{i\kappa m} \) and wave function \( \varphi_{i\kappa m}(r\sigma) \) are obtained from solving the spherical Dirac equation with Woods-Saxon-like potentials,
\[
\varphi_{i\kappa m}(r\sigma) = \frac{1}{r} \left( \begin{array}{c} iG_{i\kappa m}(r)Y_{jm}(\theta, \phi, \sigma) \\ \tilde{F}_{i\kappa m}(r)Y_{jm}(\theta, \phi, \sigma) \end{array} \right), \quad j = l \pm \frac{1}{2},
\]

with \( G_{i\kappa m}(r)/r \) and \( \tilde{F}_{i\kappa m}(r)/r \) the radial wave functions for the upper and lower components and \( Y_{jm}(\theta, \phi, \sigma) \) the spin spherical harmonics where \( \kappa = (-1)^{l+j+1/2}(j+1/2) \) and \( \tilde{l} = l + (-1)^{l+j-1/2} \). The states both in the Fermi sea and in the Dirac sea should be included in the basis for the completeness. In the Woods-Saxon basis, for each \( m \)-block the RHB equation (10) turns out to be,
\[
\begin{bmatrix} A & B \\ C & D \end{bmatrix} \begin{bmatrix} U \\ V \end{bmatrix} = E \begin{bmatrix} U \\ V \end{bmatrix},
\]

where
\[
A = \left( \begin{array}{c} u^{(m)}_{i\kappa}(r\sigma) \\ v^{(m)}_{i\kappa}(r\sigma) \end{array} \right), \quad B = \left( \begin{array}{c} u^{(m)}_{i\kappa}(r\sigma) \\ \tilde{v}^{(m)}_{i\kappa}(r\sigma) \end{array} \right),
\]
\[
C = \left( \begin{array}{c} v^{(m)}_{i\kappa}(r\sigma) \\ \tilde{u}^{(m)}_{i\kappa}(r\sigma) \end{array} \right), \quad D = \left( \begin{array}{c} v^{(m)}_{i\kappa}(r\sigma) \\ -\tilde{u}^{(m)}_{i\kappa}(r\sigma) \end{array} \right).
\]

The derivation of the matrix elements will be given in a detailed paper.\(^{37}\)

3. Numerical procedure and results

There are several parameters which have to be introduced for numerical reasons, e.g., the mesh size \( \Delta r \), the box size \( R_{\text{max}} \), and the cut off parameter on \( \lambda \) in the expansion (10), \( \lambda_{\text{max}} \). Instead of a cut off on the radial quantum number \( n \) in the
Fig. 1. The total binding energy $E$ (the lower panel), the proton pairing energy $E_{\text{pair}}^p$ (the middle panel), and the rms radius $R$ (the upper panel) of $^{20}$Mg versus the cutoff energy $E_{\text{cut}}^+$ in the Woods-Saxon basis for the DRHBWS model (solid circles). The spherical RCHB results (dashed lines) are also included for comparison.

expansion [11], an energy cutoff $E_{\text{cut}}^+$ is introduced for positive energy states in the Woods-Saxon basis and in each $\kappa$-block, the number of negative energy states in the Dirac sea is the same as that of positive energy states in the Fermi sea. We have investigated the dependence of our results on some of these parameters in spherical and deformed relativistic Hartree models. It’s found that a box of the size $R_{\text{max}} = 4r_0A^{1/3}$ with $r_0 = 1.2$ fm, a step size $\Delta r = 0.1$ fm, $\lambda_{\text{max}} = 4$, and $E_{\text{cut}}^+ = 100$ MeV give relative deviations of the binding energy, the rms radius, and the quadrupole moment from the standard ones smaller than 0.1 % for light nuclei. In order to reduce the computational time, a small cutoff $\lambda_{\text{max}} = 3$ is used which would not introduce sizable errors. The parameter set NL3 is used for the Lagrangian density.

There are two parameters ($\rho_0$ and $V_0$) in the phenomenological pairing force [9]. Since we are using a zero range force, a cutoff $E_{\text{cut}}^{q,p}$ must be introduced to define the pairing window. We take the empirical value 0.152 fm$^{-3}$ for the saturation density $\rho_0$. The pairing strength $V_0 = 374$ MeV fm$^3$ and the cutoff $E_{\text{cut}}^{q,p} = 60$
MeV reproduce the proton pairing energy in the spherical nucleus $^{20}\text{Mg}$ from the spherical relativistic Hartree Bogoliubov theory in a harmonic oscillator basis in which the Gogny force is used in the pp channel.

As the first application of the DRHBWS method, we study a spherical nucleus $^{20}\text{Mg}$ so that a comparison can be made between the DRHBWS and the spherical RCHB results. The ground state properties of $^{20}\text{Mg}$ are calculated with the DRHBWS and the RCHB codes. The total binding energy $E$, the proton pairing energy $E_{\text{pair}}^p$, and the rms radius $R$ of $^{20}\text{Mg}$ are plotted versus $E_{\text{cut}}^+$ in the lowest, middle and top panels of Fig. 1 respectively. The spherical RCHB results, regarded as exact ones, are shown as horizontal dashed lines. When the basis size increases, $E$, $E_{\text{pair}}^p$, and $R$ all converge to the corresponding exact values. In practical calculations, one can choose $E_{\text{cut}}^+$ according to the balance between the desired accuracy and the computational cost. For light nuclei, one can safely use $E_{\text{cut}}^+=100\ \text{MeV}$ which results in accuracies in the total binding energy and the proton pairing energy of about a hundred keV and in the rms radius of around 0.002 fm.

We are investigating some light deformed nuclei close to the neutron drip line by using the DRHBWS model. The results will be presented elsewhere.37

4. Summary

In order to give a proper description of exotic nuclei, particularly deformed ones with large spatial extension, the deformed relativistic Hartree-Bogoliubov (DRHB) equations are solved in a Woods-Saxon basis in which the radial wave functions have proper asymptotic behaviors at large distance from the nuclear center which is crucial for the formation of halo.

In this contribution, the formalism and the numerical procedure of the DRHB model in a Woods-Saxon basis are briefly presented. Some preliminary results, namely, the results for a spherical nucleus $^{20}\text{Mg}$ is also given and compared with the spherical relativistic Hartree-Bogoliubov model.

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