# Deformation constrained relativistic mean－field approach with fixed configuration and time－odd component ${ }^{*}$ 

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#### Abstract

Deformation constrained relativistic mean－field（RMF）approach with fixed configuration and time－ odd component has been developed and applied to investigate magnetic moments of light nuclei near doubly－ closed shells．Taking ${ }^{17} \mathrm{O}$ as an example，the results and discussion are given in detail．


Key words relativistic mean field theory，deformation constrained，configuration－fixed，time－odd potential， magnetic moment

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## 1 Introduction

During the last two decades，the relativistic mean field（RMF）theory has achieved lots of success ${ }^{[1-4]}$ in describing not only stable nuclei，but also exotic nuclei ${ }^{[5,6]}$ and supernova as well as neutron stars ${ }^{[7]}$ ．

In odd－A or odd－odd nuclei，however，the dirac current due to the unpaired valence nucleon will lead to the time－odd component of vector fields，i．e．，the nuclear magnetic potential and the wave functions of nuclei are no longer time reversal invariant．In other words，the time－odd fields will give rise to the core polarization which will modify the nuclear current， single－particle spin，and angular momentum，and de－ scribe appropriately the magnetic moments．In fact， the time－odd fields are essential in describing the magnetic moments ${ }^{[8-10]}$ ，and rotating nuclei ${ }^{[11,12]}$ ， etc．With the time－odd nuclear magnetic potential in RMF theory，the magnetic moments in LS closed－ shell nuclei plus or minus one nucleon have been re－ produced well ${ }^{[8-10]}$ ．

In order to find the ground state of deformed nu－
cleus in mean field calculation，it is crucial to ob－ tain the potential energy surface（PES）as a function of deformation．There are two different ways to ob－ tain the PES，i．e．，adiabatic and configuration－fixed （diabatic）constrained approaches．On the energy surfaces obtained from adiabatic constrained calcu－ lations，there are some irregularities，and some local minima are too obscure to be recognized．In com－ parison，the configuration－fixed constrained calcula－ tion avoid these irregularities，thus yielding a con－ tinuous and smooth energy surface curve for each configuration ${ }^{[13,14]}$ ．

In Ref．［13］，the configuration－fixed constrained RMF approach has been developed．Although the time－odd triaxial RMF approach has been developed ${ }^{[10]}$ ，but the computation is too expensive for global study of nuclear properties．Here the de－ formation constrained RMF approach with fixed con－ figuration and time－odd component is applied to the investigate the magnetic moments of light nuclei near doubly－closed shells．

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## 2 Theoretical framework

The starting point of the RMF theory is the standard effective lagrangian density constructed with the degrees of freedom associated with the nucleon field $\psi$, two isoscalar meson fields $\sigma$ and $\omega$, the isovector meson field $\rho$ and the photon field $A^{[1-4]}$ :

$$
\begin{align*}
\mathcal{L}= & \bar{\psi}\left[\mathrm{i} \gamma^{\mu} \partial_{\mu}-m-g_{\sigma} \sigma-g_{\omega} \gamma^{\mu} \omega_{\mu}-g_{\rho} \gamma^{\mu} \tau \cdot \rho_{\mu}-\right. \\
& \left.e \gamma^{\mu} \frac{1-\tau_{3}}{2} A_{\mu}\right] \psi+ \\
& \frac{1}{2} \partial^{\mu} \sigma \partial_{\mu} \sigma-\frac{1}{2} m_{\sigma}^{2} \sigma^{2}-\frac{1}{3} g_{2} \sigma^{3}-\frac{1}{4} g_{3} \sigma^{4}- \\
& \frac{1}{4} \omega^{\mu \nu} \omega_{\mu \nu}+\frac{1}{2} m_{\omega}^{2} \omega^{\mu} \omega_{\mu}+\frac{1}{4} c_{3}\left(\omega^{\mu} \omega_{\mu}\right)^{2}- \\
& \frac{1}{4} \boldsymbol{R}^{\mu \nu} \cdot \boldsymbol{R}_{\mu \nu}+\frac{1}{2} m_{\rho}^{2} \boldsymbol{\rho}^{\mu} \cdot \boldsymbol{\rho}_{\mu}-\frac{1}{4} F^{\mu \nu} F_{\mu \nu} \tag{1}
\end{align*}
$$

From the classical variation principle, the equation of motion for nucleon can be obtained as:
$\left\{\boldsymbol{\alpha} \cdot[-\mathrm{i} \boldsymbol{\nabla}-\boldsymbol{V}(\boldsymbol{r})]+V_{0}(\boldsymbol{r})+\beta[M+S(\boldsymbol{r})]\right\} \psi_{\mathrm{i}}(\boldsymbol{r})=\varepsilon_{\mathrm{i}} \psi_{\mathrm{i}}(\boldsymbol{r})$.
The attractive scalar potential and the repulsive timelike vector potential are respectively $S(\boldsymbol{r})=g_{\sigma} \sigma(\boldsymbol{r})$ and $V_{0}(\boldsymbol{r})=g_{\omega} \omega(\boldsymbol{r})+g_{\rho} \tau_{3} \rho(\boldsymbol{r})+e \frac{1-\tau_{3}}{2} A(\boldsymbol{r})$. The time-odd nuclear magnetic potential: $\boldsymbol{V}(\boldsymbol{r})=g_{\omega} \boldsymbol{\omega}(\boldsymbol{r})$ is due to the spatial component of the vector fields and it will break the time-reversal invariance. Compared with $\boldsymbol{\omega}(\boldsymbol{r})$ field, $\boldsymbol{\rho}(\boldsymbol{r})$ and $\boldsymbol{A}(\boldsymbol{r})$ fields turned out to be small in $\boldsymbol{V}(\boldsymbol{r})$, so they were often neglected for light nuclei ${ }^{[8]}$.

The self-consistent symmetries imposed are axial symmetry and parity. Thus, only azimuthal current $j_{\varphi}\left(z, r_{\perp}\right)$ on circular lines around the symmetry axis is non-zero ${ }^{[8]}$. In particular, the space-like component of $\omega$ meson is determined by

$$
\begin{equation*}
\left\{-\Delta+m_{\omega}^{2}\right\} \omega_{\varphi}(\boldsymbol{r})=\sum_{\mathrm{i}} \bar{\psi}_{\mathrm{i}} \gamma_{\varphi} \psi_{\mathrm{i}} \tag{3}
\end{equation*}
$$

where the summation is taken over the particle states only, i.e., no-sea approximation. In odd- $A$ nuclei, the source term in Eq. (3) is due to the unpaired nucleon, which breaks time-reversal invariance and gives rise to core polarization effect.

The potential energy surface is obtained through the constrained calculation in which the binding energy at certain deformation is obtained by constraining the quadrupole moment $\langle\hat{Q}\rangle$ to a given value $\mu^{[15]}$, i.e.,

$$
\begin{equation*}
\left\langle H^{\prime}\right\rangle=\langle H\rangle+\frac{1}{2} C(\langle\hat{Q}\rangle-\mu)^{2} \tag{4}
\end{equation*}
$$

We use both adiabatic and configuration-fixed constrained calculation. "Adiabatic" means that the nu-
cleons always occupy the lowest single particle levels during the constraint process, while "configurationfixed" means that the nucleons must occupy the same combination of the single particle levels during the constraint process. This is required by the following equation:

$$
\begin{equation*}
\left\langle\psi_{\mathrm{i}}(q) \mid \psi_{\mathrm{j}}(q+\Delta q)\right\rangle \approx 1 \tag{5}
\end{equation*}
$$

where $i$ and $j$ run over all the single-particle states of two adjacent configurations and $q$ is corresponding deformation parameter.

## 3 Results and discussion

The single-nucleon Dirac spinor has the form

$$
\begin{equation*}
\psi_{\mathrm{i}}(\boldsymbol{r}, s, t)=\binom{f_{\mathrm{i}}(\boldsymbol{r}, \boldsymbol{s})}{\mathrm{i} g_{\mathrm{i}}(\boldsymbol{r}, \boldsymbol{s})} \chi_{t_{\mathrm{i}}}(t) \tag{6}
\end{equation*}
$$

The single-nucleon Dirac spinor and meson fields are solved by expanding in terms of harmonic oscillator basis with major shells chosen as $N_{\mathrm{f}}=N_{\mathrm{b}}=14$ for the nucleons and mesons respectively ${ }^{[4,16]}$. In odd- $A$ nuclei, as the time reversal invariance is broken by the unpaired valence neutron, Eq. (6) can be written as the linear combination of time reversal conjugate basis:

$$
\begin{align*}
& f(\boldsymbol{r}, s)=\sum_{\alpha} f_{\alpha}|\alpha\rangle+\sum_{\bar{\alpha}} f_{\bar{\alpha}}|\bar{\alpha}\rangle  \tag{7}\\
& g(\boldsymbol{r}, s)=\sum_{\tilde{\alpha}} g_{\tilde{\alpha}}|\tilde{\alpha}\rangle+\sum_{\tilde{\bar{\alpha}}} g_{\tilde{\alpha}}|\tilde{\bar{\alpha}}\rangle \tag{8}
\end{align*}
$$

and the dirac equation for the nucleons should be solved separately in two subspaces, which are related by time-reversal operator ${ }^{[10]}$

$$
\left(\begin{array}{cc}
A_{\alpha^{\prime} \alpha} & B_{\alpha^{\prime} \tilde{\alpha}}  \tag{9}\\
-B_{\beta^{\prime} \alpha} & C_{\tilde{\beta}^{\prime} \tilde{\alpha}}
\end{array}\right)\binom{f_{\alpha}}{g_{\tilde{\alpha}}}=\varepsilon_{\mathrm{i}}\binom{f_{\alpha^{\prime}}}{g_{\tilde{\beta}^{\prime}}}
$$

and

$$
\left(\begin{array}{cc}
A_{\bar{\alpha}^{\prime} \bar{\alpha}} & B_{\bar{\alpha}^{\prime} \tilde{\alpha}}  \tag{10}\\
-B_{\tilde{\bar{\beta}}^{\prime} \bar{\alpha}} & C_{\tilde{\bar{\beta}}^{\prime} \tilde{\alpha}}
\end{array}\right)\binom{f_{\bar{\alpha}}}{g_{\tilde{\alpha}}}=\varepsilon_{\overline{\mathrm{i}}}\binom{f_{\bar{\alpha}^{\prime}}}{g_{\tilde{\bar{\beta}}^{\prime}}} .
$$

The oscillator lengths parameters are $b_{z}=b_{\perp}=$ $\sqrt{\hbar / M \omega_{0}}$, where $M$ is the nucleon mass. The oscillator frequency is given by $\hbar \omega_{0}=41 A^{-1 / 3}$. The parameter set PK1 ${ }^{[17]}$ is adopted.

The magnetic moments for light nuclei near doubly-closed shells with $A=15,17,39$, and 41 are given in Table 1. Both PK1 and NL1 ${ }^{[8]}$ give the reasonable values compared with the data. The magnetic moment calculated by two parament sets are close to each other because two effective interaction have a small marginal effect on the single particle
wavefunction and configurations. It indicates that nuclear magnetic moments are not parameter sets dependent.

Table 1. Magnetic moments ( $\mu$ ) of light nuclei near closed shells in units of $\mu_{N}$. The results of NL1 are taken from Ref. [8] and the data is taken from Ref. [18].

| $\mu$ | ${ }^{15} \mathrm{O}$ | ${ }^{17} \mathrm{O}$ | ${ }^{39} \mathrm{Ca}$ | ${ }^{41} \mathrm{Ca}$ | ${ }^{15} \mathrm{~N}$ | ${ }^{17} \mathrm{~F}$ | ${ }^{41} \mathrm{Sc}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Exp. | 0.72 | -1.89 | 1.02 | -1.60 | -0.28 | 4.72 | 5.43 |
| PK1 | 0.65 | -2.01 | 1.01 | -2.15 | -0.22 | 4.95 | 6.14 |
| NL1 | 0.65 | -2.03 | 0.96 | -2.13 | -0.29 | 4.99 | 6.07 |

The energy surface for ${ }^{17} \mathrm{O}$ in configuration-fixed constrained calculation is presented with solid lines in Fig. 1, where the minima of each configuration are indicated by stars labeled by letters of the alphabet. It is shown obviously that state $A$ has the lowest energy with a prolate deformation $\beta=0.08$ and B is the second minima with oblate deformation $\beta=-0.07$. The energy difference between A and B is only 0.05 MeV . Moreover, it is noticed that the contribution of timeodd component to the binding energy of g.s. is about 0.2 MeV as found in Ref. [19]. The magnetic moment as function of quadrupole deformation is also plotted in Fig. 1 and for a fixed configuration, the magnetic moment is continuously variational. The main component of valence neutron wavefunction is $1 d_{5 / 2}$ for both state A and B. For state A, the parity and the third component of valence neutron spin is $1 / 2^{+}$and corresponding magnetic moment is $-0.51 \mu_{N}$. For state $B$, it is $5 / 2^{+}$and corresponding magnetic moment is $-2.01 \mu_{N}$. This value is well closed to the data $5 / 2^{+}$and $-1.89 \mu_{N}{ }^{[18]}$.


Fig. 1. Potential energy surfaces and magnetic moment in adiabatic(open circles) and configuration-fixed(solid lines) constrained deformed RMF calculation with time-odd component and PK1 parameter for ${ }^{17} \mathrm{O}$. The minima in the energy surfaces for fixed configuration are represented as stars and labeled respectively as A and B.

## 4 Summary and concluding remarks

The deformation constrained RMF approach with fixed configuration and time-odd component has been developed and applied to the investigation of the magnetic moment of light nuclei near doubly-closed shells. The nuclear magnetic moments are in good agreement with the data in light nuclei near doubly-closed shells. Taking ${ }^{17} \mathrm{O}$ as an example, the results and discussion are given in detail.

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