Effects of three-nucleon spin-orbit interaction on isotope shifts of Pb nuclei

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(Dated: February 5, 2015)

We investigate effects of the 3N interaction, which effectively adds a density-dependent term to the LS channel, on the isotope shifts of the Pb nuclei. With the strength so as to keep the $\ell s$ splitting of the single-nucleon orbits, the density-dependence in the LS channel tends to shrink the wave functions of the $j = \ell + 1/2$ orbits while makes the $j = \ell - 1/2$ functions distribute more broadly. Thereby the kink in the isotope shifts of the Pb nuclei at $N = 126$ becomes stronger, owing to the attraction from neutrons occupying $0i_{11/2}$ in $N > 126$. The density-dependence in the LS channel enables us to reproduce the data of the isotope shifts by the Hartree-Fock-Bogolyubov calculations in a long chain of neutron numbers, even without degeneracy between the $n1g_{9/2}$ and $n0i_{11/2}$ levels. We exemplify it by the semi-realistic M3Y-P6 interaction.

PACS numbers: 21.10.Ft, 21.30.Fe, 21.60.Jz, 27.80.+w

Introduction. As finite quantum many-body systems dominated by the strong interaction, atomic nuclei supply challenging problems for us. One of the important questions is whether we need many-nucleon interaction and, if so, how it affects the nuclear structure and reactions. In particular, the three-nucleon (3N) interaction is under current interest. The 3N interaction could become the more significant at the higher density, because its energy contribution depends on the nucleon density more strongly than that of the two-nucleon (2N) interaction. This indicates astrophysical importance of the 3N interaction, since energy of the nuclear matter at high density is quite relevant to the supernovae and the neutron stars. More and more evidence has been accumulated from the detailed analysis of the few-nucleon systems [1] that the 3N interaction is not negligible. It has also been argued that the saturation properties extracted from the mass systematics are difficult to be accounted for only by the 2N interaction, and can be improved by the 3N interaction [2]. In connecting the results in the few-nucleon systems to the saturation properties of the infinite nuclear matter and the astrophysical problems, it is desirable to reveal effects of the 3N interaction in medium-to heavy-mass nuclei. There have been arguments on structure of medium-mass nuclei, e.g. on the binding energies in the O and Ca nuclei [2]. However, since it is not an easy task to determine the 3N interaction with good precision, its effects on nuclear structure are not always transparent if arguments are based only on quantitative assessment of energies. Effects of the 3N interaction on the nuclear structure should be investigated further; particularly observable effects on wave functions of medium-to heavy-mass nuclei.

The spin-orbit ($\ell s$) splitting in the nucleonic single-particle (s.p.) orbitals is essential to the nuclear shell structure. Whereas the size of the $\ell s$ splitting has been known from the data, it has been questioned whether the 2N interaction is able to produce sufficient $\ell s$ splitting [4]. The LS channels of the nucleonic interaction, which contain $l_i l_j \cdot (s_i + s_j)$ as will be given in Eq. (1), determine overall size of the $\ell s$ splitting. Recently Kohno has found [3, 6] that the 3N interaction from the chiral effective-field theory ($\chi$EFT) [7] gives significant density-dependence in an LS channel when it is converted to an effective 2N interaction, and this sizably contributes to the $\ell s$ splitting. To confirm whether this picture is correct, it is intriguing to search effects of the density-dependence on observables other than the $\ell s$ splitting.

The isotope shifts of the Pb nuclei, in which a conspicuous kink has been observed at $N = 126$ when plotted as a function of the neutron number $N$, are significantly influenced by attraction from neutrons occupying the $0i_{11/2}$ orbital [8]. Since the density-dependence in the LS channel gives a broader $n0i_{11/2}$ function as illustrated below, it may affect the isotope shifts. In this paper we shall examine effects of the density-dependent LS channel connected to the 3N interaction on the isotope shifts of the Pb nuclei.

We mention that a density-dependent LS interaction was considered in Ref. [3]. However, its influence on physical quantities other than energies has not been explored sufficiently.

Framework. We implement the spherical Hartree-Fock-Bogolyubov (HFB) calculations for the Pb nuclei. The computational method is identical to that employed in Ref. [10]. We employ the M3Y-P6 semi-realistic interaction [10] except the LS channels. The Michigan-three-range-Yukawa (M3Y) type interactions, which were obtained from the $G$-matrix [12] with phenomenological modification [10, 11], have been applied in the mean-
Hartree-Fock energy is given by following form: 

\[ E_{\text{HF}}^{(\text{LS})} = \frac{1}{4} \int d^3r D[\rho(r)] \]

where \( D[\rho(r)] \) is a density-dependent term. The \( D[\rho(r)] \) introduces the density-dependence in the central channels, which plays a crucial role in reproducing the saturation properties. 

The M3Y-type interaction has the LS channels of the following form: 

\[ v_{ij}^{(\text{LS})} = \sum_n (v_n^{(\text{LS}E)} P_{\text{TE}} + v_n^{(\text{LSCO})} P_{\text{TO}}) f_n^{(\text{LS})}(r_{ij}) \mathbf{L}_{ij} \cdot (\mathbf{s}_i + \mathbf{s}_j) \]

where the subscripts \( i \) and \( j \) are indices of nucleons, \( L_{ij} = r_{ij} \times p_{ij} \) with \( r_{ij} = r_i - r_j \) and \( p_{ij} = (p_i - p_j)/2 \), \( s_i \) is the spin operator, \( r_{ij} = |r_{ij}| \), and \( f_n^{(\text{LS})}(r) = e^{-\mu_n^{(\text{LS})}} r / \mu_n^{(\text{LS})} r \). \( P_{\text{TE}} \) (\( P_{\text{TO}} \)) denotes the projection operator on the triplet-even (triplet-odd) two-particle states. In M3Y-P6, \( v^{(\text{LS})} \), the zero-range form of the 2\( N \)D, instead of enhancing \( v^{(\text{LS})} \), 

\[ \frac{1}{2} \delta D[\rho(r)] \frac{d}{dr} \left( \rho(r) + \rho_\tau(r) \right) \]

The rearrangement term that contains \( \delta D/\delta \rho = -\omega_1/(1 + d_1 \rho)^2 \) enhances effects of the 3N interaction on the \( \ell s \) splitting, as argued in Ref. [6].

In the MF calculations so far, the 2N LS interaction has been determined by fitting the \( \ell s \) splitting to the experimental data. To investigate effects of the density-dependent LS channel without influencing the \( \ell s \) splitting, we determine the parameter \( w_1 \) so as to reproduce the M3Y-P6 result of the \( n0i_{11/2} \) splitting at \( 208 \text{Pb} \). This LS-modified variant of M3Y-P6 will be called M3Y-P6a. As well as the \( n0i \) splitting, the s.p. energies do not change from those of M3Y-P6 significantly. Influence on the binding energy is insignificant as well; 0.4 MeV increase at \( /16O \) and decrease by 4.9 MeV at \( /208Pb \). The parameters in \( v^{(\text{LS})} \) and \( v^{(\text{LS}P)} \) are tabulated in Table I.

\begin{table}[h]
\centering
\caption{Parameters of the LS channels in M3Y-P6 and M3Y-P6a.}
\begin{tabular}{|c|c|c|}
\hline
\textbf{parameters} & \textbf{M3Y-P6} & \textbf{M3Y-P6a} \\
\hline
\( 1/\mu_1^{(\text{LS})} \) & 0.25 & 0.25 \\
\( \ell_{1}^{(\text{LSE})} \) & (MeV) & 11222.2 & -5101. \\
\( \ell_{1}^{(\text{LSCO})} \) & (MeV) & -4173.4 & -1897. \\
\( 1/\mu_2^{(\text{LS})} \) & (fm) & 0.40 & 0.40 \\
\( \ell_{2}^{(\text{LSE})} \) & (MeV) & -741.4 & -337. \\
\( \ell_{2}^{(\text{LSCO})} \) & (MeV) & -1390.4 & 632. \\
w_1 & (MeV-fm^2) & 0. & 742. \\
d_1 & (fm^3) & 1. & 1. \\
\hline
\end{tabular}
\end{table}

Results and discussions. We define the isotope shifts of the Pb nuclei by \( \Delta (r^2)_p(A^{\text{Pb}}) = (r^2)_p(A^{\text{Pb}}) - (r^2)_p(208\text{Pb}) \), where \( (r^2)_p(A^{\text{Pb}}) \) represents the proton mean-square (m.s.) radius in the \( A^{\text{Pb}} \) nucleus \( (A = N + 82) \). \( \Delta (r^2)_p \) has been measured precisely for a chain of the Pb nuclei [10, 20], disclosing a remarkable kink at \( N = 126 \).

We here note the finite-size effect of the constituent protons on the isotope shifts. In the convolution model which is customarily used for the charge density distribution, contribution of the charge radius of constituent protons is canceled out in \( \Delta (r^2)_p \) because the proton number \( Z \) is fixed.

The previous MF calculations indicate that the kink in \( \Delta (r^2)_p(A^{\text{Pb}}) \) at \( N = 126 \) occurs owing to occupation of the \( n0i_{11/2} \) orbit [5]. As the s.p. function of \( /0i_{11/2} \) has a larger radius than those of the neighboring orbits, the attraction between protons and neutrons makes \( /0i_{11/2} \)
larger as \(n_{0i_{11/2}}\) is occupied to greater degree. Because the neutron occupation on \(0i_{11/2}\) is negligible in \(N \leq 126\) while sizable in \(N > 126\), \(\Delta (r^2)_p\) has a kink at the magic number \(N = 126\). Although neutrons primarily occupy \(1g_{9/2}\) beyond \(N = 126\), the pair correlation allows them to occupy \(0i_{11/2}\). The s.p. energy difference \(\varepsilon_n(0i_{11/2}) - \varepsilon_n(1g_{9/2})\) was considered important in the previous studies, to which the occupation probability on \(n_{0i_{11/2}}\) is sensitive. On this basis, it was argued that the kink in \(\Delta (r^2)_p\) may derive the isospin-dependence of the \(ls\) potential \(21\). However, it has been difficult to give a kink comparable to the observed one unless \(n_{1g_{9/2}}\) and \(n_{0i_{11/2}}\) are nearly degenerate \(8\).

The density-dependence in the LS channel leads to an additional effect. The LS channels of the \(2N\) interaction may derive the \(ls\) potential whose strength is proportional to the derivative of the density, indicating that the \(ls\) splitting is a surface effect. Equation \(43\) gives the larger \(D[\rho]e\) for the higher \(\rho\). Therefore, when the size of the \(ls\) splitting is equated, \(D[\rho]\) in Eq. \(2\) makes the \(ls\) potential stronger in the interior and weaker in the exterior, as recognized from Eq. \(43\). Since the \(ls\) potential acts attractively on the \(j = \ell + 1/2\) orbits and repulsively on the \(j = \ell - 1/2\) orbits, variational calculations shrink the wave functions of the \(j = \ell + 1/2\) orbits while extend those of the \(j = \ell - 1/2\) orbits. This trend is confirmed by difference of the radial functions \(R_\ell(r)\) for \(j = n_{0i_{13/2}}\) and \(n_{0i_{11/2}}\) shown in Fig. \(1\) which are obtained by the HF calculations at \(^{208}\)Pb. We take the phase \(R_{n0}(r) \geq 0\) as usual. The m.s. radius of the s.p. function of \(n_{0i_{11/2}}\) increases by \(0.49\) fm \(^2\) as we switch the interaction from M3Y-P6 to M3Y-P6a. Note that the m.s. radius of \(n_{1g_{9/2}}\) does not differ much between M3Y-P6 and M3Y-P6a. The root-m.s. matter radius of the \(^{208}\)Pb nucleus changes by \(-0.03\) fm, and the neutron-skin thickness \(\sqrt{\langle r^2 \rangle_n} - \sqrt{\langle r^2 \rangle_p}\) by \(+0.001\) fm, both of which are basically irrelevant to the isotope shifts.

We depict \(\Delta (r^2)_p\) in Fig. \(2\). The HFB results with M3Y-P6a (red solid line) are compared to those with M3Y-P6 (green dashed line). The kink at \(N = 126\) takes place because of the \(n_{0i_{11/2}}\) occupation; indeed it becomes invisible if all the valence neutrons in \(N > 126\) occupy \(n_{1g_{9/2}}\), as shown by the thin brown dot-dashed line. The larger \(n_{0i_{11/2}}\) radius provides the more rapid increase of \(\Delta (r^2)_p\) in \(N > 126\). Thus the stronger kink is obtained with M3Y-P6a than with M3Y-P6, in better agreement with the experimental data \(19, 20\). The same trend is obtained with M3Y-P7 \(10\) and D1M \(22\) after replacing a part of the LS channel by \(v^{(LS)}\) of Eq. \(2\).

In the limit that \(n_{0i_{11/2}}\) has equal occupation probability to the lower-lying \(n_{1g_{9/2}}\) orbit, the s.p. functions obtained by M3Y-P6 give \(\Delta (r^2)_p\) indistinguishable from the red solid line in Fig. \(2\) and therefore comparable to the observed one in \(N > 126\). This is analogous to the results reported in the previous studies without density-dependence in the LS channels \(8, 23\). However, the energy difference between \(n_{1g_{9/2}}\) and \(n_{0i_{11/2}}\) is not negligible in the experimental data, being \(0.78\) MeV if extracted from the lowest states of \(^{209}\)Pb \(24\). With this difference it is unlikely that the occupation probabilities of these orbits are so close. In contrast, with M3Y-P6a \(n_{0i_{11/2}}\) lies higher than \(n_{1g_{9/2}}\) by \(0.72\) MeV at \(^{208}\)Pb, and the occupation probability on \(n_{0i_{11/2}}\) is substantially lower than that on \(n_{1g_{9/2}}\), as presented in Fig. \(3\). Nevertheless, owing to the density-dependence in the LS channel, the kink of \(\Delta (r^2)_p\) is reproduced to fair degree. If these orbits were equally occupied in \(N > 126\), \(\Delta (r^2)_p\) could increase further, providing the red dotted line in Fig. \(2\).
The even-odd staggering of $\Delta(r^2)_p(^{14}\text{Pb})$ observed in $N \geq 126$ is well reproduced by the HFB calculations. This originates from the staggering in the occupation probabilities in Fig. 3, which owes to a quasiparticle on $n1g_{9/2}$ in the ground states of the odd-$N$ isotopes. Thus the even-odd staggering supports the picture that $n0i_{11/2}$ is responsible for the kink of $\Delta(r^2)_p$.

In Fig. 2, we find that increase of $\Delta(r^2)_p(^{14}\text{Pb})$ in $N \leq 126$ is slower with M3Y-P6a than with M3Y-P6, which is linked to the smaller radius of $n0i_{13/2}$ with M3Y-P6a. The slope of $\Delta(r^2)_p$ in the M3Y-P6a results is in good agreement with the data in wide region of $N \leq 126$, although the even-odd staggering is not visible as in the data.

We thus confirm that the isotope shifts of the Pb nuclei can be described by the density-dependent LS interaction without the $n1g_{9/2}$-$n0i_{11/2}$ degeneracy. As such density-dependence is naturally derived from the 3N interaction as shown by Kohno, the strong kink in the isotope shifts may be regarded as an effect of the 3N interaction. Importance of the 3N interaction in the $\ell s$ splitting was pointed out also in Ref. [25]. On the contrary, it was suggested [26] that many-body correlations induced by the 2N interaction could enhance the $\ell s$ splitting. Although the many-body correlations do not yield significant density-dependence within the lowest-order Brueckner theory [5], their effects should be investigated further for complete understanding. We remark that the effects of the 3N interaction presented here are on the wave functions, not on the energies, and are therefore unrenormalizable with usual density-independent 2N interactions.

We finally comment on the strength of the LS interaction. As is important to nuclear structure, the $\ell s$ splitting should not change much even when density-dependence is introduced. All the effects of the density-dependent LS interaction presented in this paper become the stronger with the greater $w_1$ in Eq. (4), when keeping the $\ell s$ splitting by enhancing or reducing the $2N$ LS strength. In the present study, $w_1$ has been fixed so as not to alter the $\ell s$ splitting of M3Y-P6, which gives reasonable shell structure, while the $2N$ LS interaction is returned to that of the M3Y-Paris interaction. In Ref. [6], Kohno showed that the effective strength of the LS interaction at $\rho \approx \rho_0$ deduced from the chiral 3N interaction [7] is comparable to the empirical strength that reproduces the observed $\ell s$ splitting, though significantly weak at lower densities. However, we have found that the $\ell s$ splitting is better connected to the strength at $\rho \approx (2/3)\rho_0$, rather than at $\rho = \rho_0$. It should also be noted that the current $\chi$EFT [7] (so-called N$^3$LO) is not guaranteed to be fully convergent at $\rho \approx \rho_0$. We have therefore used the functional form of Eq. (2), which is consistent with the $\chi$EFT calculations [5, 6, 17], but have not taken the strength derived in Ref. [5, 6] seriously, emphasizing the qualitative effects of the 3N interaction.

Summary. We have investigated effects of the density-dependent LS interaction, which has been derived from the chiral 3N interaction by Kohno, on the isotope shifts of the Pb nuclei. As this LS interaction effectively comes stronger as the density grows, the wave functions of the $j = \ell + 1/2$ orbits shrink while those of the $j = \ell - 1/2$ orbits distribute more broadly. Since the attraction from neutrons occupying $0i_{11/2}$ produces the kink in the isotope shift of the Pb nuclei at $N = 126$, the broader $n0i_{11/2}$ function makes the kink stronger. By introducing density-dependence in the LS channel with the strength so as to keep the original $\ell s$ splitting, we can reproduce the data on the isotope shifts of the Pb nuclei with the Hartree-Fock-Bogolyubov calculations in a long chain of neutron numbers, as has been exemplified by an LS-modified variant of the semi-realistic M3Y-P6 interaction. It is remarked that the rapid increase of the radius in $N > 126$ can be described fairly well without degeneracy between the $n1g_{9/2}$ and $n0i_{11/2}$ levels, unlike previous studies.

Further exploration of effects of the density-dependent LS interaction will be desired, including application to the deformed MF calculations as well as to the RPA calculations.

Discussion with M. Kohno is gratefully acknowledged. This work is financially supported in part as KAKENHI No. 24105008 by The MEXT, Japan, and as No. 25400245 by JSPS. Numerical calculations are performed on HITAC SR16000s at IMAT in Chiba University, ITC in University of Tokyo, IIC in Hokkaido University, and YITP in Kyoto University.

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