Binding energies and modelling of nuclei in semiclassical simulations

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Abstract

We study the binding energies of spin-isospin saturated nuclei with nucleon number $8 \leq A \leq 100$ in semiclassical Monte Carlo many-body simulations. The model Hamiltonian consists of, (i) nucleon kinetic energy, (ii) a nucleon-nucleon interaction potential, and (iii) an effective Pauli potential which depends on density. The basic ingredients of the nucleon-nucleon potential are, a short-range repulsion, and a medium-range attraction. Our results demonstrate that one can always expect to obtain the empirical binding energies for a set of nuclei by introducing a proper density dependent Pauli potential in terms of a single variable, the nucleon number, A. The present work shows that in the suggested procedure there is a delicate counterbalance of kinetic and potential energetic contributions allowing a good reproduction of the experimental nuclear binding energies. This type of calculations may be of interest in further reproduction of other properties of nuclei such as radii and also exotic nuclei.

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In our exploratory work [1], we studied the nuclear binding energies for medium mass nuclei with nucleon number $8 \leq A \leq 44$ in semiclassical simulations via Monte Carlo many-body techniques. The purpose of that work was to study the role of an effective Pauli potential, which is often adopted in semiclassical simulations of many-nucleon systems. It was demonstrated that the empirical binding energies for these nuclei can be reproduced satisfactorily using the Pauli potential, where the density dependence is parameterized by one variable, the Fermi momentum. The agreement with the empirical binding energies was excellent in spite of the simplicity of the model. The conclusion of our previous work is rather general, it does not depend on the detail of the NN potential provided a short-range repulsion and medium-range attraction are included. One can always expect to find a proper counter balancing density dependent Pauli potential to reproduce the empirical binding energies. Although the model is not based on the fundamental physics of strong interaction QCD, it gives a possible guidance for treating complicated many-nucleon systems in a simple, practical manner in semiclassical simulations. This may be very helpful to study the many-nucleon systems such as the pasta phase [2, 3, 4, 5] and neutron halo nuclei [6].

In this study, we are able to extend our previous work [1] to treat a wider range of nuclei with $8 \leq A \leq 100$ for spin-isospin saturated $Z = N$ (even $Z$ and $N$) nuclei. We show that the density dependence of the Pauli potential can be well parameterized in the whole range in terms of one single variable, the nucleon number $A$. The Fermi momentum is no longer a good parameter due to the fact that the average Fermi momenta in nuclei with $A > 50$ saturate to a value $\simeq 260$ MeV/c (e.g., 265 MeV/c for a $^{208}$Pb nucleus) [7]. The present result generalizes our previous conclusion that the density dependence of the Pauli potential is crucial to reproduce the empirical nuclear binding energies. It is important to explore heavier systems since stability of this type of procedures must be tested with respect to increasing number of nucleons. We have shown in Ref. [1] that in the limit of infinite symmetric nuclear matter in these many-body simulations one should obtain the corresponding binding energy around $-16$ MeV. Also in other simulations as in heavy-ion or pasta phases one usually has a wide mass distribution of clusters. In addition, we explicitly show that it is possible to reproduce the empirical binding energies using different NN interaction potentials. Thus, it suggests a simple and pragmatic procedure in modelling a set of nuclei calibrated by the empirical binding energies for a given NN interaction potential. Then, the evaluation of further experimental observables of nuclei such as radii and also
exotic systems such as hypernuclei could be attempted with this type of procedure [8].

In the present approach, nucleons are treated as classical, structureless particles. The model Hamiltonian consists of nucleon kinetic energy, NN ($V_{NN}$), Coulomb ($V_{Coul}$) and Pauli ($V_{Pauli}$) potentials. The Pauli potential simulates nucleon fermionic nature using the Gaussian form introduced by Dorso et al. [9], but we allow for a density dependence. In this study, we use a simplified NN interaction potential keeping only S-wave interactions without isospin nor spin dependence [1]. The model Hamiltonian is given by,

$$H = \sum_{i=1}^{A} \frac{p_i^2}{2m_N} + \sum_{i=1,j>i}^{A} \left[ V_{NN}(r_{ij}) + V_{Coul}(r_{ij}) + V_{Pauli}(r_{ij}, p_{ij}) \right],$$  

(1)

where $p_i$ is the 3-momentum of $i$-th nucleon and $r_{ij} = |r_i - r_j|$ ($p_{ij} = |p_i - p_j|$) the relative distance (momentum) of the $i$-th and $j$-th nucleons. Explicit expressions for the potentials in Eq. (1) are as follows.

- **NN interaction potential:**

  $$V_{NN}(r_{ij}) = \begin{cases} V_{Core}, & \text{for } 0 \leq r_{ij} < a, \\ -V_0, & \text{for } a \leq r_{ij} < b, \\ 0, & \text{for } a + b \leq r_{ij}. \end{cases}$$  

(2)

The potential consists of a repulsive core of strength $V_{Core}$ of width $a$ and an attractive well of strength $V_0$ and width $b$. The values used are, $V_{Core} = 10$ MeV, $a = 1$ fm and $b = 2$ fm. For $V_0$, we use two values, $V_0 = 3$ MeV and $V_0 = 5$ MeV.

- **Coulomb potential:**

  $$V_{Coul}(r_{ij}) = \frac{e^2}{4\pi r_{ij}}(1/2 + \tau_i)(1/2 + \tau_j),$$  

(3)

where $\tau_i$ ($\tau_j$) is the isospin third-component of $i$-th ($j$-th) nucleon ($+1/2$ for protons, $-1/2$ for neutrons), and $e$ the proton electric charge.

- **Pauli potential:**

  $$V_{Pauli}(r_{ij}, p_{ij}) = V_P \exp \left( -\frac{r_{ij}^2}{2\sigma_0^2} - \frac{p_{ij}^2}{2P_0^2} \right) \delta_{\tau_i \tau_j} \delta_{\sigma_i \sigma_j},$$  

(4)

where $\delta_{\tau_i \tau_j}$ ($\delta_{\sigma_i \sigma_j}$) is the Kronecker’s delta for the isospin (spin) third-component. It prevents nucleons from occupying the same phase space volume when they have the same quantum numbers. (See Ref. 10 for other approaches.) As demonstrated in Ref. 1, it is crucial to allow a density dependence for this Pauli potential if one wants to reproduce the empirical
binding energies. Thus, we discuss next the density dependence of the Pauli potential before presenting results.

First, we show in Fig. 1 the average Fermi momentum versus the nucleon number $A$ obtained by interpolating the values given in Ref. [7]. One can see that the Fermi momenta $(p_F)$ increase as the nucleon number $A$ increases up to $A \simeq 50$. For heavier nuclei with $A > 50$ they saturate to a value of $p_F \simeq 260 \text{ MeV}/c$ (e.g., 265 MeV/c for a $^{208}\text{Pb}$ nucleus) [7]. Thus, including also heavy nuclei with $A > 50$, it is more convenient to use the nucleon number $A$ to characterize the density dependence of the Pauli potential, although the Fermi momentum was used previously [1] for nuclei with $8 \leq A \leq 44$. In this work, we need to extend the parametrization to heavier systems to parameterize the density dependent strength $V_P$ in the Pauli potential Eq. (4).

For $q_0$ and $p_0$ in the Pauli potential, the density dependence can be determined as follows. In a nucleus, a typical nucleon sphere radius $r$ may be given by

$$r = \left( \frac{3}{4\pi \rho} \right)^{1/3},$$

(5)

where $\rho = 2p_F^3/3\pi^2$ is the nucleon density and $p_F$ the nucleon Fermi momentum. Then, the average inter-nucleon distance $2r$ may be estimated as $(2r/\sqrt{2}q_0) \simeq 1$, where $q_0$ is "an
effective range” of the Pauli potential. With the uncertainty principle, \( q_0 p_0 \simeq \hbar \), this leads to:

\[
q_0 \simeq \frac{(9\pi)^{1/3}\hbar}{\sqrt{2}p_F}, \tag{6}
\]

\[
p_0 \simeq \frac{\hbar}{q_0} = \frac{\sqrt{2}}{(9\pi)^{1/3}p_F}. \tag{7}
\]

For the Fermi momentum \( p_F \) appearing in Eqs. (6) and (7), we use the value as shown in Fig. 1 for the nuclei with \( 8 \leq A \leq 44 \), while for \( 48 \leq A \leq 100 \), we use the saturated value, \( p_F = 260 \text{ MeV/c} \).

By performing simulations to reproduce the empirical binding energies for the nuclei with \( 8 \leq A \leq 100 \) for \( V_0 = 3 \text{ MeV} \) in Eq. (2), we get the \( A \) dependence for \( V_P \) in the Pauli potential as shown in Fig. 2 (the blobs). This justifies that the density dependence of

![Graph showing Pauli potential strength vs. nucleon number A](image)

**FIG. 2:** Pauli potential strength \( V_P \) vs. nucleon number \( A \) obtained with \( V_0 = 3 \text{ MeV} \) in the NN potential Eq. (2). Simulations are performed for nuclei with \( A = 8, 12, 16, ..., 100 \) (even \( Z \) and \( N \)) spin-isospin saturated nuclei. This applies for all results treated in this study. The solid line corresponds to the parameterization given by Eq. (5).

the Pauli potential may be parameterized well by the nucleon number \( A \). As expected, the strength \( V_P \) of the Pauli potential increases with \( A \). This behaviour may be analogous to
that of the vector potential in Hartree approximation in relativistic mean field models \[11\].

Then, for \( V_0 = 3 \text{ MeV} \), we get the parameterization:

\[
V_P(A) = -25.645 + 2.9596A + 0.0551A^2 \text{ (MeV)},
\]

while for \( V_0 = 5 \text{ MeV} \), we get:

\[
V_P(A) = -1088.2 + 140.55A + 0.9809A^2 \text{ (MeV)}.
\]

Both cases reproduce the empirical binding energies well. Note that the parameterizations are approximate and are given as a guidance. Thus, this suggests that, for a given reasonable NN interaction potential, we can model a set of nuclei which are calibrated by the empirical binding energies. Then, we can use them to study other properties of these nuclei, such as charge distribution, proton and neutron density distributions, and proton and neutron r.m.s. radii \[8\]. Although this procedure may be simple, one can regard that all complicated many-body effects are condensed into a density dependent effective Pauli potential. The present approach is not based on the fundamental theory of strong interaction QCD, but we would like to emphasize, a simple, pragmatic aspect for treating complicated, many-nucleon systems in semiclassical simulations.

Now, we are in a position to discuss the results. In the present study, all simulations are performed with a fixed temperature \( T = 1 \text{ MeV} \). In the simulation a nucleus is constructed by initially placing \( A \) nucleons uniformly inside a sphere of radius \( R_0 \) of range 2-3 fm within a cubic box of volume \( V = L^3 \) and impose \( L >> r_{ij} \). Then, using the Metropolis algorithm \[12\], the ground state configuration is searched by thermal relaxation. The Pauli potential should be gradually turned on to avoid instabilities. After this, we sample the configurations in order to calculate the statistical average for its binding energy.

In Fig. 3 we show the binding energy per nucleon \((-E/A)\) as calculated with the model with \( V_0 = 3 \text{ MeV} \) versus nucleon number \( A \). The central bars show the calculated values of nuclei considered in this work and match those in Ref. \[13\]. The dotted line is a guidance for eyes. The statistical uncertainties are shown by error-bars, and they are less than 5 %. The empirical values are well reproduced with the density dependent Pauli potential. Thus, for this NN interaction potential with \( V_0 = 3 \text{ MeV} \) in Eq. (2), we have obtained a set of nuclei which reproduce the empirical binding energies. Let us note that shell effects are partially included through the \( A \) dependence in the Pauli potential strength parameterization. Next,
we discuss the dependence on the NN interaction potentials by comparing the results with $V_0 = 3$ MeV and $V_0 = 5$ MeV. We show contributions from the kinetic and potential energies in Fig. 4 for the nuclei with $8 \leq A \leq 56$. The solid and dashed lines are the results for $V_0 = 3$ and $V_0 = 5$ MeV, respectively. For each case, the upper (lower) line corresponds the contribution from the kinetic (potential) energy per nucleon. The dotted-line is the sum of the two contributions, for both $V_0 = 3$ MeV and $V_0 = 5$ MeV cases. This suggests that the empirical binding energies can be always reproduced by introducing a proper counter balancing Pauli potential, once a NN interaction is specified.

Further, we analyze how the empirical binding energy can be achieved by considering the $^{20}\text{Ne}$ nucleus case as an example. In Fig. 5 we show kinetic ($K/A$), potential ($V/A$) and total ($E/A$) energies per nucleon for a $^{20}\text{Ne}$ nucleus versus the Pauli potential strength $V_P$. The empirical value is indicated by the cross. As increasing the Pauli potential strength $V_P$, the kinetic energy contribution increases, while the potential energy contribution stays nearly constant. The increase of the kinetic energy contribution originates from the momentum dependence in the Pauli potential, due to the modification in the canonical momenta (or

FIG. 3: Binding energy per nucleon, $-E/A$, for the set of nuclei considered in this work. (See also caption of Fig. 2)
FIG. 4: Kinetic and potential energy contributions to the binding energy per nucleon. The solid and dashed lines are the results obtained with $V_0 = 3$ and $V_0 = 5$ MeV, respectively. For each case, the upper (lower) line corresponds to the contribution from the kinetic (potential) energy per nucleon. The dotted line is the sum of the two contributions for both cases, and goes through the empirical values. (See also caption of Fig. 2)

the effective masses) of the interacting nucleons via the Pauli potential. Because of this positively increasing kinetic energy, the empirical binding energy is finally achieved. This example is for a fixed nucleon number nucleus. In order to be able to reproduce the empirical binding energies for a set of nuclei, the similar procedure must be repeated for all the nuclei in the set. Thus, one can naturally understand why $A$ (or density) dependence in the Pauli potential is necessary.

For the first time we have demonstrated that the density dependence of the Pauli potential, crucial to reproduce the empirical binding energies in semiclassical simulations, can be parametrized in terms of a single variable: the nucleon number $A$. Such results overcomes previous hypothesis describing the density dependence in terms of the Fermi momentum. Once the correct density dependence is included through the Pauli potential, the only other necessary ingredient is a reasonable nucleon-nucleon interaction. The procedure presented is robust, the simulation remaining stable when increasing the number of particles. The
The validity of the parametrization of the Pauli potential in terms of the nucleon number $A$ is made manifest by the counterbalance between the growing repulsion coming from the kinetic energy and the increasing attraction of the potential energy. This result opens the door to study properties of wider sets of nuclei with a correct parametrization of the Pauli potential. Although the procedure presented in this work is not based on the fundamental theory of strong interaction QCD, we would like to emphasize that, it suggests a simple, pragmatic procedure in modelling a set of nuclei calibrated by the empirical binding energies for a given NN interaction potential. Then, using this procedure one may think of further testing asymmetric systems by studying other properties of nuclei such as radii or other exotic nuclei in semiclassical simulations.

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