Novel ansatz for charge radii in density functional theories

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Charge radii are one of the most fundamental properties of atomic nuclei characterizing their charge distributions. Though the general trend as a function of the mass number is well described by the $A^{1/3}$ rule, some fine structures, such as the evolution along the calcium isotopic chain and the corresponding odd-even staggerings, are notoriously difficult to describe both in density functional theories and ab initio methods. In this letter, we propose a novel ansatz to describe the charge radii of calcium isotopes, by adding a correction term, proportional to the number of Cooper pairs, and determined by the BCS amplitudes and a single parameter, to the charge radii calculated in the relativistic mean field model with the pairing interaction treated with the BCS method. The new ansatz yields results consistent with data not only for calcium isotopes, but also for ten other isotopic chains, including oxygen, neon, magnesium, chromium, nickel, germanium, zirconium, cadmium, tin, and lead. It is remarkable that this ansatz with a single parameter can describe nuclear charge radii throughout the periodic table, particularly the odd-even staggerings and parabolic behavior. We hope that the present study can stimulate more discussions about its nature and relation with other effects proposed to explain the odd-even staggerings of charge radii.

Introduction: Charge radii [1], just as masses [2], are among the most fundamental quantities to characterize the ground states of atomic nuclei. On the other hand, compared to masses, they seem to be harder to describe theoretically. For instance, ab initio calculations have been able to describe masses (or binding energies) of light (or even medium mass) nuclei reasonably well for quite some time (see, e.g., Ref. [3]), but failed to do so for charge radii until quite recently (see, e.g., Refs. [4] and references therein). Nowadays, various semi-microscopic mass models [4] or mean field theories [7, 8] are able to describe known nuclear binding energies with an accuracy of less than 3 MeV, with a discrepancy of much less than 1%. As for charge radii, the discrepancy is still at the level of 5% [7, 8]. In particular, there are a few longstanding discrepancies in the theoretical description of charge radii. One of the most intricate is about calcium isotopes, which show a parabolic behavior between $^{39}$Ca and $^{48}$Ca and strong odd-even staggerings [10]. Furthermore, $^{52}$Ca has a radius larger than that of $^{48}$Ca [9], though $N = 32$ [11] and 34 [12] are found to be new magic numbers. All these features have remained a challenge for better theoretical understanding.

Conventional density functional theories, such as the relativistic mean field (RMF) model (see below) or the Hartree-Fock-Bogoliubov method (see, e.g., Fig. 6 of Ref. [13]), can not describe the peculiar features of calcium isotopes. The DF3-a EDF model can describe the charge radii of $^{39–49}$Ca, but then fails to do so for $^{50–52}$Ca [14]. The extended DF3-a+ph model, in which the particle-phonon coupling effects are taken into account [13], improves the description of $^{50–52}$Ca. The Fayans EDF model, with a novel density-gradient term added to the pairing interaction [15], can somewhat reproduce the odd-even staggerings below $N = 28$ [10], but not so satisfactorily (see Fig. 1). Ab initio calculations with chiral EFT interactions, such as NNLOsat [17], SRG1 and SRG2 [13], fail to reproduce experimental data as well [3].

It is clear that none of the existing theoretical models can describe the charge radii of calcium isotopes satisfactorily, which implies that some important physics is missing in all these models. In the present work, we propose a novel ansatz based on the RMF model and we show that it can describe the charge radii of calcium isotopes rather well. Such an ansatz is then extended to study ten other isotopic chains, and is shown to work remarkably well. How can such a term is derived in a more microscopic way in the RMF model is not clear yet, but its origin is very clear, i.e., the neutron proton pairing, as the evolution of charge radii along an isotopic chain can only come from the interaction between neutrons and protons. The odd-even staggering then clearly shows that this effect is from the pairing channel.

Novel ansatz for charge radii: The RMF model within non-linear Lagrangian densities is used in this study (see Refs. [14, 21] for some latest reviews). The corresponding Dirac equation for nucleons and Klein-Gordon equations for mesons and the photon are solved by the expansion method with the harmonic oscillator basis [22, 23]. In the present work, 12 shells are used to expand the fermion fields and 20 shells for the meson fields. The
mean-field effective force used is NL3[24]. In order to describe the pairing correlation, the state-dependent BCS method with a delta force is employed[23], with its strength tuned for each isotopic chain. The odd-A nuclei are treated with the blocking approximation. A detailed description of the deformed RMF(BCS) method can be found in Refs. [23].

In the RMF(BCS) method, conventionally charge radii are calculated in the following way [22, 23]:

\[ R_{ch}^2 = \frac{\int r^2\mathcal{A}n_p(r)}{\int d^3n_p(r)} + 0.64 \text{ fm}^2, \]

where the first term represents the charge distribution of point-like protons and the second term accounts for the finite size of the proton.

As can be seen from Fig. 1, the RMF(BCS) method cannot describe the charge radii of calcium isotopes, particularly, the parabolic behavior between \( N = 20 \) and \( N = 28 \) and the odd-even staggerings. We have checked that neither the point coupling version of the RMF model, or the deformed relativistic Hartree Bogoliubov theory in continuum [27], can describe calcium isotopes. As discussed in the introduction, the Skyme Hartree-Fock methods also fail to describe calcium isotopes. This is also the case for ab initio methods. See Refs. [4, 10] for more discussions.

A closer inspection of the experimental data reveals the following: the charge radius of \(^{40}\text{Ca}\) and that of \(^{48}\text{Ca}\) are almost the same, which can be understood due to the closed shell at \( N = 20 \) and \( N = 28 \). In between, the charge radii are larger, but more interestingly, show odd-even staggerings, similar to those more familiar in the binding energies of atomic nuclei. All these strongly point to the fact that such features are related to the pairing interaction. As the proton number is fixed, the evolution of the charge radius along the calcium isotopic chain should be attributed to neutron-proton correlations. Inspired by the above observation, we propose to add a correction term to the charge radius of Eq. (1), such that it becomes:

\[ R_{ch}^2 = \frac{\int r^2\mathcal{A}n_p(r)}{\int d^3n_p(r)} + 0.64 \text{ fm}^2 + \frac{a_0}{\sqrt{A}} \cdot \Delta \mathcal{D} \text{ fm}^2 \]  

(2)

In the above expression, \( A \) is the mass number, the constant \( a_0 = 0.834 \) is a normalization constant fixed by fitting to the charge radius of \(^{44}\text{Ca}\), and the quantity \( \Delta \mathcal{D} = |\mathcal{D}_n - \mathcal{D}_p| \) is defined as

\[ \mathcal{D}_{n,p} = \sum_{k > 0} u_k v_k, \]

(3)

where \( v_k \) and \( u_k \) are the BCS amplitudes, with \( v_k^2 \) the occupation probability of single particle orbital \( k \), and the summation is over all the occupied single particle levels. It should be emphasized in the present work that all the quantities appearing in the correction term are obtained self-consistently in the RMF(BCS) method.

It is interesting to note that \( u_k v_k \) represents a measure of the number of correlated pairs (Cooper pairs) \( \langle \text{Cooper pairs} \rangle \) in the BCS wave function \[29\]

\[ u_k v_k = \langle \text{BCS}|a_k^\dagger a_k^\dagger \text{BCS} \rangle. \]

(4)

Therefore, \( \Delta \mathcal{D} \) represents the difference of the fractions of Cooper pairs between neutrons and protons. In a recent work, Miller et al. has shown that in ab initio calculations, charge radii might be influenced by short range correlations missing in soft nucleon-nucleon interactions \[30\]. Our proposed ansatz [Eq. (2)] somewhat resembles Eq. (9) of Ref. [30].

![Fig. 1](image_url)  
**FIG. 1.** Charge radii of calcium isotopes obtained by the RMF(BCS) method and our new ansatz, denoted by RMF(BCS)*. The experimental data are taken from Refs. [1, 3, 10]. For comparison the Fayans EDF results [10] are also shown.

**Results and discussions:** In Fig. 1, we compare the charge radii of calcium isotopes calculated in the RMF(BCS) method with and without the correction term. It is clear that without the correction term, the RMF(BCS) results cannot describe experimental data, particularly, the parabolic behavior, the odd-even staggerings, as well as the fast increase beyond \( N = 28 \). On the other hand, with the correction term, the RMF(BCS)* results describe the data quite well. In fact, the results are even better than those of the Fayans EDF model, particularly for those nuclei with \( N > 20 \) \[10\]. Although the RMF(BCS)* method overestimates the

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1 Using other effective forces such as TM1[28] and PK1[24] does not change essentially any of our conclusions, but does affect the description of charge radii at a quantitative level.

2 The BCS coherent pairs mix correlated and uncorrelated pairs over the whole system, and therefore they cannot be interpreted as Cooper pairs except in the extreme strong-coupling and dilute limits where all the pairs are bounded and non-overlapping [29].
charge radii of $^{16,17,18}$Ca, it does correctly yield the odd-even staggerings (see also the lower panel of Fig. 2). It will be interesting to see how future experimental data compare with our predictions for calcium isotopes with $N \geq 53$.

| Neutron Number (A-Z) | $\Delta E$ (MeV) |
|----------------------|------------------|
| 16                  | Exp              |
| 18                  | RMF(BCS)         |
| 20                  | RMF(BCS)*        |
| 22                  |                  |
| 24                  |                  |
| 26                  |                  |
| 28                  |                  |
| 30                  |                  |
| 32                  |                  |
| 34                  |                  |
| 36                  |                  |
| 38                  |                  |
| 40                  |                  |

FIG. 2. Odd-even staggerings in the binding energies (upper panel) and charge radii (lower panel) of calcium isotopes. The experimental data of binding energies are taken from Ref. 2, while those of charge radii are from Refs. 1-3.

To highlight effects of the pairing correlation (and eliminating a smooth background from the mean field part), for bulk properties, such as masses and charge radii, one can define the so-called “double odd-even staggerings” for either an isotopic chain or an isotonic chain. For binding energies, one can use the following three-point formula $^{31,32}$:

$$\Delta E = \frac{1}{2} [B(N-1,Z) - 2B(N,Z) + B(N+1,Z)],$$  \hspace{1cm} (5)

where the $B(N,Z)$ is the binding energy for a nucleus of neutron number $N$ and proton number $Z$. Similarly, one can define a three-point formula to extract odd-even staggerings for charge radii $^{16}$:

$$\Delta r = \frac{1}{2} [R(N-1,Z) - 2R(N,Z) + R(N+1,Z)],$$  \hspace{1cm} (6)

where $R(N,Z)$ is the root-mean-square charge radius.

In Fig. 2 the odd-even staggerings of nuclear masses (upper panel) and charge radii (lower panel) are compared with experimental data. It is clear the RMF(BCS)/RMF(BCS)$^*$ method reproduces the odd-even staggerings of the masses quite well (as expected), but fails miserably for charge radii, while the new ansatz is able to describe charge radii remarkably well. We note that around the magic number $N=28$, the odd-even staggering effects seem to slightly overestimated.

The new ansatz can describe the charge radii of calcium isotopes very well, implying that it must have captured some important physics. Naturally, one would like to see whether it works for other nuclei. For such a purpose, we study the charge radii of oxygen, nickel, germanium, and zirconium, whose proton number is either magic or semi-magic, and neon, magnesium, chromium, and cadmium isotopes.

In Fig. 3 the charge radii of oxygen, nickel, germanium, and zirconium isotopes are compared with experimental data. For oxygen isotopes, the new ansatz yields results in agreement with the experimental data, especially, the sharp increase from $^{17}$O to $^{18}$O. For nickel isotopes, the new ansatz can reproduce the experimental data except for $^{56}$Ni, with $N=28$ a magic number (see discussions below). For germanium isotopes, the charge radii are also better reproduced by the new ansatz, notably those of $N=38,40,41$. While for zirconium isotopes, the new ansatz barely change the results, in agreement with data.

FIG. 3. Charge radii of oxygen, nickel, germanium, and zirconium isotopes obtained by the RMF(BCS) method and our new ansatz RMF(BCS)$^*$. The experimental data are taken from Refs. 1-3.

In Fig. 3 the charge radii of neon, magnesium, chromium, and cadmium isotopes are shown. The charge

$^3$ They give the same results for masses.
radii of neon isotopes are better described by the new ansatz, especially the odd-even staggerings of $^{24-26}\text{Ne}$. For magnesium isotopes, the new ansatz barely changes the results of the RMF(BCS) method. For chromium isotopes, the results from the new ansatz are in better agreement with the experimental data, particularly for $^{52}\text{Cr}$. For most cadmium isotopes, the new ansatz again yields better results. Only around $A = 120$, the charge radii are overestimated. One should note that the normalization factor of the correction term is fixed by $^{44}\text{Ca}$. It is interesting to point out that here once more we see a clear parabolic behavior between $N = 50/64$ and $N = 82$, similar to calcium isotopes.

Next, we investigate whether the new ansatz works for heavy nuclei with $Z \geq 50$. More specifically, we study tin and lead isotopes, whose $\Delta E$, $\Delta r$, and charge radii are shown in Fig. 5. The theoretical results agree well with the experimental data for both binding energies and charge radii. It should be noted that for tin and lead isotopes we have to use a smaller $a_0 = 0.22$ fixed by the charge radius of $^{120}\text{Sn}$ to better produce the odd-even staggerings in the charge radii. This reflects that the strength of the correction term might need to be adjusted for different isotopes. Or in other words, its mass dependence is not completely captured in the $1/\sqrt{A}$ factor. In addition, we note that the discontinuities across $N = 82$ and $N = 126$ are well reproduced in the RMF method (which has been attributed to the rather small isospin dependence of the spin-orbit term in the RMF method\(^\text{a}\)). A peculiar observation regarding lead isotopes is that the theoretical odd-even staggerings of charge radii around $N = 126$ is larger than its experimental counterpart, though they are smaller than data for those nuclei away from $N = 126$. It seems for nuclei with either magic proton or neutron numbers, the new ansatz behaves relatively worse. This is true also for those calcium isotopes nearby $N = 28$. Such a feature might be related to non-conservation of particle number in the BCS method.

**Summary and outlook:** Motivated by the peculiar features exhibited in the charge radii of calcium isotopes and the fact mean-field calculations failed to describe most (if not all) of the fine structures, we proposed a novel ansatz to correct the charge radii obtained from the RMF(BCS) method. With a single parameter fixed by the charge radius of $^{44}\text{Ca}$, we were able to reproduce the charge radii of calcium isotopes from $^{40}\text{Ca}$ up to $^{54}\text{Ca}$ in topic chains to better reproduce the odd-even staggerings of binding energies. 

\(^4\) It should be noted that for lead isotopes, the RMF(BCS) results already overestimate the charge radii but underestimated the corresponding odd-even staggerings.

\(^5\) This is understandable because even for the pairing strength of the delta force one has to re-tune it a little bit for different isotopes.
a way comparable or even better than most refined existing calculations. This ansatz was then applied to study ten more isotopic chains, i.e., oxygen, neon, magnesium, chromium, nickel, germanium, zirconium, cadmium, tin, and lead. Overall remarkable improvements are achieved, though for tin and lead isotopes we had to use a smaller normalization constant. In particular, we noted that the parabolic behavior of cadmium isotopes is also reasonably reproduced.

The more microscopic origin of the new ansatz remains to be identified. The most plausible factor is the short-range neutron-proton pairing correlation, which is missing in (most) mean-field calculations. Regardless of its microscopic nature, the phenomenological successes demonstrated in the present work hints that it must have captured relevant physics. In the future, one may further test such an ansatz by studying all the isotopic chains for which experimental data exist. In doing so, slight readjustment of the mean-field parameters might be needed as well. Furthermore, as the ansatz is based on the BCS theory, where particle number is not conserved, one may wish to study how its restoration affects the description of charge radii using, e.g., the FBCC method [38]. The fact that our ansatz performed slightly worse for nuclei with magic numbers, such as $N = 28$ and $N = 126$, indeed indicates such an necessity. Last but not the least, the new ansatz is also expected to work for Skyme Hartree-Fock models and therefore explicit studies are strongly encouraged.

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