Folded potentials in cluster physics—a comparison of Yukawa and Coulomb potentials with Riesz fractional integrals

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Abstract
In cluster physics, a single-particle potential to determine the microscopic part of the total energy of a collective configuration is necessary to calculate the shell and pairing effects. In this paper, we investigate the properties of the Riesz fractional integrals and compare their properties with the standard Coulomb and Yukawa potentials commonly used. It is demonstrated that Riesz potentials may serve as a promising extension of standard potentials and may be reckoned as a smooth transition from Coulomb- to Yukawa-like potentials, depending on the fractional parameter $\alpha$. For the macroscopic part of the total energy, the Riesz potentials treat the Coulomb, symmetry and pairing contributions from a generalized point of view, since they turn out to be similar realizations of the same fractional integral at distinct $\alpha$ values.

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1. Introduction

Convolution integrals of the type

$$F(x) = \int_{-\infty}^{\infty} d\xi \, f(x - \xi) w(\xi) = \int_{-\infty}^{\infty} d\xi \, f(\xi) w(x - \xi)$$

(1)

play a significant role in the areas of signal and image processing or in obtaining the solutions of differential equations.

In classical physics, the first contact with the 3D generalization of a convolution integral occurs within the framework of gravitation and electromagnetic theory in terms of a volume integral to determine the potential $V$ of a given charge density distribution $\rho$:

$$V(\vec{x}) = \int_{\mathbb{R}^3} d^3\xi \frac{\rho(\vec{\xi})}{|\vec{x} - \vec{\xi}|},$$

(2)

where the weight $w$

$$w(|\vec{x} - \vec{\xi}|) = \frac{1}{|\vec{x} - \vec{\xi}|}$$

(3)
is interpreted as the gravitational or electromagnetic field of a point charge (Jackson 1998, Kibble and Berkshire 2004).

In nuclear physics, collective phenomena, such as fission or cluster-radioactivity, where many nucleons are involved, are successfully described by introducing the concept of a collective single-particle potential, based on folded potentials of, e.g., Woods–Saxon type. Several weight functions have been investigated in the past.

In this paper, we will demonstrate that the fractional Riesz potential (Riesz 1949, Podlubny 1999, Ortigueira 2006) which extends the weight function by introducing the fractional parameter $\alpha$

$$w(|x - \xi|) = \frac{1}{|x - \xi|^{\alpha}}$$

serves as a serious alternative for commonly used Nilsson (Nilsson 1955, Nilsson et al. 1969), Woods–Saxon (Eisenberg and Greiner 1987) and folded Yukawa potentials (Bolsterli et al. 1972, Möller and Nix 1981), modelling the single-particle potential widely applied in nuclear physics as well as in electronic cluster physics.

Hence, we give a direct physical interpretation of a multi-dimensional fractional integral within the framework of fragmentation theory (Fink et al. 1974, Sandulescu et al. 1976, Maruhn et al. 1980, Depta et al. 1985, Iwamoto and Herrmann 1991), which is the fundamental tool to describe the dynamic development of clusters in nuclear (Möller et al. 1993, Greiner et al. 1995, Poenaru et al. 2010) and atomic (Knight et al. 1984, Clemenger 1985, Martin et al. 1991, Brack 1993, de Heer 1993, Engel et al. 1993, Reinhard and Suraud 2004, Chowdhury et al. 2006) physics.

2. Folded potentials in fragmentation theory

The use of collective models for the description of collective aspects of nuclear motion has proven considerably successful over the past decades.

Calculating life-times of heavy nuclei (Myers and Swiatecki 1966, Grumann 1969, Sobiczewski and Pomorski 2007, Krappe and Pomorski 2012), fission yields (Lustig et al. 1980, Greiner and Maruhn 1997, Kruppa et al. 2000, Staszczak et al. 2013), giving insight into phenomena such as cluster-radioactivity (Poenaru and Greiner 2010), bimodal fission (Herrmann et al. 1988) or modelling the ground state properties of triaxial nuclei (Möller et al. 2008), remarkable results have been achieved by introducing an appropriate set of collective coordinates, such as length, deformation, neck or mass asymmetry (Scharnweber et al. 1970, Gneuss and Greiner 1971, Maruhn and Greiner 1972, Vasak et al. 1983, Troltenier et al. 1991) for a given nuclear shape and investigating its dynamic properties.

As an example, in figure 1, the parametrization of the 3-sphere model is sketched. It determines the geometry of a given cluster shape by two intersecting spheres, which are smoothly connected via a third sphere, which models a neck depending on the size of the radius $r_3$.

The corresponding set of collective coordinates $\{q^i, i = 1, ..., 4\}$ is given by Depta et al. (1990):

- the two centre distance $\Delta z = z_2 - z_1$,
- the mass asymmetry $\eta_A = (A_1 - A_2)/(A_1 + A_2)$,
- the charge asymmetry $\eta_Z = (Z_1 - Z_2)/(Z_1 + Z_2)$,
- the neck $c_3 = 1/r_3$,

where $A_1, Z_1$ and $A_2, Z_2$ are the numbers of nucleons and protons in the two daughter nuclei.

This choice of collective coordinates allows us to describe a wide range of nuclear shapes involved in collective phenomena from a generalized point of view (Herrmann et al. 1986),
e.g., a simultaneous description is made possible of general fission properties and the cluster-
radioactive decay of radium

\[ ^{223}\text{Ra} \rightarrow ^{14}\text{C} + ^{209}\text{Pb} \]  

which was predicted by Sandulescu, Poenaru and Greiner in 1980 and later experimentally
verified by Rose and Jones in 1984 (Sandulescu et al. 1980, Rose and Jones 1984).

In order to describe the properties and dynamics of such a process, we start with the
classical Hamiltonian function

\[ H = T + V_0, \]  

introducing a collective potential \( V_0 \), depending on the collective coordinates,

\[ V_0(q') = E_{\text{macro}}(q') + E_{\text{mic}}(q') \]  

with a macroscopic contribution \( E_{\text{macro}} \) based on, e.g., the liquid drop model and a microscopic
contribution \( E_{\text{mic}} \), which mainly contains the shell and pairing energy based on a single-particle
potential \( V_{s.p.} \) and the classical kinetic energy \( T \):

\[ T = \frac{1}{2} B_{ij}(q') \dot{q}_i \dot{q}_j \]  

with collective mass parameters \( B_{ij} \).

There are several common methods to generate the collective mass parameters \( B_{ij} \), e.g.,
the cranking model (Inglis 1954, Schneider et al. 1986, Ring and Schuck 2008) or irrotational
flow models (Werner and Wheeler 1958, Kelso 1964, Davies et al. 1976, Wu et al. 1985).

Quantization of the classical Hamiltonian (Podolsky 1928) results in the collective
Schrödinger equation

\[ \hat{S}_0 \Psi(q', t) = \left( -\frac{\hbar^2}{2} \frac{1}{\sqrt{B}} \frac{\partial}{\partial q} B^{ij} \frac{1}{\sqrt{B}} \frac{\partial}{\partial q} \right) \Psi(q', t) = 0 \]  

with \( B = \det B_{ij} \) being the determinant of the mass tensor. This is the central starting point for
a discussion of nuclear collective phenomena.

For a specific realization of the single-particle potential \( V_{s.p.} \), for protons and neutrons
respectively, a Woods–Saxon-type potential may be used. The advantages of such a potential
are a finite potential depth and a given surface thickness. Furthermore, arbitrary geometric
shapes may be treated similarly by a folding procedure, which yields smooth potential values for such shapes.

For the 3-sphere model, in order to define a corresponding potential, a Yukawa function is folded with a given volume $V$, which is uniquely determined within the model:

$$
V_Y(\vec{r}) = -\frac{V_0}{4\pi a^4} \int_V d^3\vec{r}' \frac{\exp(-|\vec{r}-\vec{r}'|/a)}{|\vec{r}-\vec{r}'|/a}
$$

(10)

with the parameter potential depth $V_0$ and surface thickness $a$.

For protons, in addition, the Coulomb potential has to be considered, which is given for a constant density $\rho_0$:

$$
V_C(\vec{r}) = \rho_0 \frac{1}{a} \int_V d^3\vec{r}' \frac{1}{|\vec{r}-\vec{r}'|/a},
$$

(11)

where the charge density is given by

$$
\rho_0 = \frac{Ze}{4\pi R_0^3}.
$$

(12)

Both potentials may be written as general convolutions in $R^3$ of type

$$
V_{\text{type}}(\vec{r}) = C_{\text{type}} \int_{R^3} d^3\vec{r}' \rho(\vec{r}) w_{\text{type}}(|\vec{r}-\vec{r}'|)
$$

(13)

with the weights

$$
w_Y(d) = \exp(-d/a)
$$

(14)

$$
w_C(d) = \frac{1}{d/a},
$$

(15)

where $d = |\vec{x}-\vec{\xi}|$ is a measure of distance on $R^3$ and a density, which is constant inside the nucleus

$$
\rho(\vec{r}) = \begin{cases} 
\rho_0 & \text{inside the nucleus} \\
0 & \text{outside the nucleus} 
\end{cases}
$$

(16)

Therefore the single-particle potential $V_{s.p.}$ is given by

$$
V_{s.p.} = V_Y + \left(1 + t_3\right) V_C + \kappa \vec{\sigma} (\nabla V_Y \times \vec{p})
$$

(17)

where $t_3$ is the eigenvalue of the isospin operator with $+\frac{1}{2}$ for protons and $-\frac{1}{2}$ for neutrons, which guarantees that the Coulomb potential $V_C$ only acts on protons. The last term is the spin–orbit term with the Pauli matrices $\vec{\sigma}$, $\vec{p}$ is the momentum operator and the strength is parametrized with $\kappa$. This term is necessary to split up the degeneracy of energy levels with different angular momentum and to generate the experimentally observed magic shell closures (Elsasser 1933).

In the original Nilsson oscillator potential, an additional $\vec{l}\cdot\vec{\sigma}$ term was necessary to lower the higher angular momentum levels in agreement with experiment (Strutinsky 1967a, 1967b, 1968, Mosel and Greiner 1969, Tajima and Suzuki 2001). For Woods–Saxon-type potentials, such a term is not necessary. Whether Riesz potentials are a realistic alternative, will be investigated in the next section.

The solutions of the single-particle Schrödinger equation with the potential $V_{s.p.}$ yield single-particle energy levels, which are used to calculate the microscopic part of the total potential energy and contain two major parts, the shell and pairing corrections:

$$
E_{\text{mic}}(q') = E_{\text{shell}}(q') + E_{\text{pair}}(q').
$$

(18)
3. The Riesz potential as smooth transition between Coulomb and folded Yukawa potential

Let us reinterpret the Riesz potential
\[ V_{\text{RZ}}(\vec{r}) = C_{\text{RZ}} \int_{R^3} d^3r' \rho(|\vec{r} - \vec{r}'|) w_{\text{RZ}}(|\vec{r} - \vec{r}'|) \] (19)

with the weight
\[ w_{\text{RZ}}(d) = \frac{1}{(d/a)^\alpha} \quad 0 < \alpha < 3 \] (20)
as the 3D version of the one-dimensional Riesz integral (Riesz 1949) applied to a scalar function \( \rho(\vec{r}) \), where the Riesz integral is given as a symmetric superposition of the right \( (L^+_{\alpha}) \) and left \( (L^-_{\alpha}) \) Liouville integrals (Miller and Ross 1993, Podlubny 1999, Herrmann 2011):
\[ R_{\text{RZ}} f(x) = \frac{L^+_{\alpha} + L^-_{\alpha}}{2} f(x) \] (21)
\[ = \frac{1}{2 \cos(\pi \alpha/2)} \left( \frac{1}{\Gamma(\alpha)} \int_x^{+\infty} (\xi - x)^{\alpha-1} f(\xi) \, d\xi + \frac{1}{\Gamma(\alpha)} \int_{-\infty}^x (x - \xi)^{\alpha-1} f(\xi) \, d\xi \right) \] (22)
\[ = \frac{1}{2 \Gamma(\alpha) \cos(\pi \alpha/2)} \int_{-\infty}^{+\infty} |x - \xi|^{\alpha-1} f(\xi) \, d\xi, \quad 0 < \alpha < 1 \] (23)
and with the fractional parameter \( \alpha \in \mathbb{R} \), which allows a smooth transition between \( 0 < \alpha < 3 \) and consequently we may treat and interpret the Coulomb \( (\alpha = 1) \), Riesz and Yukawa potentials similarly from a generalized point of view.

In the following, we will investigate the behaviour of the Riesz potential with varying \( \alpha \) and compare its properties with the cases of Coulomb and Yukawa weight functions. In a way, the parameter \( \alpha \) in the Riesz potential may be interpreted as a global screening of the Coulomb weight, such that the effect of the Yukawa exponential is partly modelled:
\[ w_{\text{C}}(d) = \frac{1}{d/a} \] (24)
\[ w_{\text{RZ}}(d) = \frac{1}{(d/a)^{\alpha-1}} \frac{1}{d/a} \] (25)
\[ w_{\text{Y}}(d) = \exp^{-d/a} \frac{1}{d/a} \] (26)

Therefore, the Riesz potential could be an interesting alternative to the Yukawa potential in the case \( \alpha \gg 1 \). In a way, we expect the screening properties of the Riesz potential for increasing \( \alpha \) to result in an interpolation between the Coulomb and Yukawa limit.

Hence, the fragmentation potentials used in the dynamic description of fission or cluster emission processes are an ideal framework to discuss and understand the properties of the Riesz integral.

The integral (13) with the weights (24)–(26) may be evaluated analytically for a spherical nucleus with radius \( R_0 \) and
\[ \rho(r) = \rho_0 H(R_0 - r) \] (27)
with the Heaviside step function \( H \).
In this case, we have
\[ V_{\text{sphere}}^\text{type}(r) = C_{\text{type}} \rho_0 \int_0^{R_0} r'^2 \, dr' \int_0^\pi \sin(\theta') \, d\theta' \int_0^{2\pi} d\phi' u_{\text{type}}(|\vec{r} - \vec{r}'|) \] (28)
with
\[ |\vec{r} - \vec{r}'| = \sqrt{r^2 + r'^2 - 2rr' \cos(\theta')} \] (29)

With the substitution \( u = \sqrt{r^2 + r'^2 - 2rr' \cos(\theta')} \),
we end up with a double integral for spherical shapes:
\[ V_{\text{sphere}}^\text{type}(r) = 2\pi C_{\text{type}} \rho_0 \int_0^{R_0} dr' \int_0^{\sqrt{(r+r')^2}} du \, u \, u_{\text{type}}(u) \] (31)
\[ = 2\pi \rho_0 C_{\text{type}} \int_0^{R_0} dr' \int_{|r-r'|}^{r+r'} \, du \, u \, u_{\text{type}}(u). \] (32)

This integral is valid for any analytic weight \( w(u) \) and may be easily solved for the Coulomb, Riesz and Yukawa weight functions. We obtain
\[ V_{\text{C}}^\text{sphere}(r) = a_C C \begin{cases} \frac{Ze}{R_0} & r \leq R_0 \\ \frac{Ze}{r} & r \geq R_0 \end{cases} \] (33)
\[ V_{\text{RZ}}^\text{sphere}(r) = 4\pi a^2 C_{\text{RZ}} \frac{2\pi}{(\alpha - 2)(\alpha - 3)(\alpha - 4) r} \] \[ \times \begin{cases} (r + R_0)^{3-\alpha} & r \leq R_0 \\ (r - R_0)^{3-\alpha} & r \geq R_0 \end{cases} \] (34)
\[ V_{\text{Y}}^\text{sphere}(r) = 4\pi a^3 C_Y \begin{cases} 1 - \left( 1 + \frac{R_0}{\alpha} \right) e^{-R_0/\alpha} \frac{\sinh(r/\alpha)}{r/\alpha} & r \leq R_0 \\ \frac{e^{-r/\alpha}}{r/\alpha} \left( \frac{R_0}{\alpha} \cosh \left( \frac{R_0}{\alpha} \right) - \sinh \left( \frac{R_0}{\alpha} \right) \right) & r \geq R_0 \end{cases} \] (35)

In figure 2, a sequence of these potentials is plotted for a spherical nucleus, ranging from the Coulomb (\( \alpha = 1.00 \)) and Riesz potential with increasing \( \alpha \) up to the Yukawa potential with parameter settings according to Bolsterli et al. (1972).

For large \( \alpha > 2.00 \), the Riesz potential as well as the Yukawa potential models a finite surface thickness.

A remarkable difference between both potentials follows for small \( z \). In this area, the Yukawa potential models a more Woods–Saxon-type potential, while the Riesz potential may be compared with a harmonic oscillator potential. But this behaviour is restricted only to the lowest energy levels; for realistic calculations the energy region near the Fermi level is much more relevant. In this region, both potential types show similar behaviour for \( 2.00 < \alpha < 2.50 \).

Hence, both potentials seem to be interesting candidates for the generation of realistic single-particle energy levels.

For cylinder symmetric configurations, the integral (13) cannot be solved analytically. Instead, we switch to cylinder coordinates \( \{\rho, z, \phi\} \). With the distance
\[ d_{\text{cyl}} = \sqrt{\rho^2 + \rho'^2 - 2\rho\rho' \cos(\phi')} + (z - z')^2, \] (36)
Figure 2. For a spherical assumed shape (here $^{232}\text{U}$) the potential for different weight functions is drawn. From top to bottom: Coulomb ($\alpha = 1.00$), Riesz ($\alpha = 1.25, 1.75, 2.25, 2.50$) and Yukawa (with $a = 0.9$ (fm)) weight. In order to compare the plots with cylinder symmetric shapes, potential is drawn in cylinder coordinates ($z, \rho$) for a sequence of $\rho = 0.00, 0.25, 0.50, 0.75, 1.00 \times R_0$. $R_0(^{232}\text{U}) = 8.26$ (fm).

we have to solve the integral

$$V_{\text{type}}(\rho, z) = C_{\text{type}} \int_V d\rho' \rho' dz' d\phi' \rho(\rho', z') w_{\text{type}}(d_{\text{cyl}})$$

numerically.

In figure 3, we have solved (37) and compared the three different weights for the strong asymmetric cluster decay

$$^{232}\text{U} \rightarrow ^{208}\text{Pb} + ^{24}\text{Ne}. \quad (38)$$

The Riesz potential allows for a smooth transition between the Coulomb case and the Yukawa limit by varying $\alpha$. Hence, we obtain a direct geometric interpretation of the fractional parameter $\alpha$.

Up to now, we discussed the properties of the single-particle potential, which is the starting point for a calculation of the microscopic part of the collective potential.
Figure 3. For the configuration $^{232}\text{U} \rightarrow ^{208}\text{Pb} + ^{24}\text{Ne}$, the Coulomb, Riesz ($\alpha = 2.50$) and Yukawa ($\alpha = 0.9$ (fm)) potentials are plotted for $\Delta z = 0.75R_0$ (left column) and $\Delta z = 1.375R_0$ (right column). $R_0(^{232}\text{U}) = 8.26$ (fm).

The self-energy of a given configuration contributes to the macroscopic part of the nuclear potential as the Coulomb and surface or more sophisticated Yukawa energy term in a macroscopic energy formula, historically first used in Weizsäcker’s famous liquid drop mass formula (Weizsäcker 1935):

$$E_{\text{macro}} = a_vA + a_sA^{2/3} - a_cZA^{-1/3} + a_{\text{sym}}(N-Z)A^{-1} + a_{\text{pair}}A^{-1/2}$$

as a function of the nucleon number $A = r_0R_0^3$ containing a volume, surface, Coulomb, symmetry and pairing term.

The self-energy for a given charge type $E_{\text{type}}$ is defined as the volume integral over the potential restricted on the volume of a given shape:

$$E_{\text{type}}(\vec{r}) = \frac{1}{2}C_{\text{type}} \int_V d^3\rho(\vec{r}) \int_{R_0} d^3\rho'(\vec{r}') w_{\text{type}}(|\vec{r} - \vec{r}'|)$$

8
For a spherical shape, the self-energy as a function of the sphere radius $R_0$(fm) is plotted for the Coulomb, the Riesz ($\alpha = 1.49, 1.98, 2.47, 2.96$) and the Yukawa ($\alpha = 0.9$ (fm)) potentials. To compare all different types, all energies are normalized to $E_{type}(R_0 = 1) = 1$. Depending on $R_0$, the Yukawa self-energy behaviour is covered by the Riesz self-energy within a range of $2.0 \leq \alpha \leq 2.5$ values.

\begin{equation}
E_{type}(\vec{r}) = \frac{1}{2} C_{type} \int \int_V d^3r d^3r' \rho(\vec{r})\rho(\vec{r}')w_{type}(|\vec{r} - \vec{r}'|). \tag{41}
\end{equation}

For the three different weights (24)–(26), we obtain for the simplest case of a sphere with radius $R_0$, a unit charge ($Z = 1$) and with a thickness parameter $a > 0$:

$$E_C = \frac{3}{5} \frac{a}{R_0}$$ \tag{42}
$$E_{RZ} = \frac{9 \times 2^{1-\alpha} a^\alpha}{(3 - \alpha)(4 - \alpha)(6 - \alpha)} \frac{1}{R_0^\alpha}, \quad 0 \leq \alpha < 3 \tag{43}$$
$$E_Y = \frac{3a^3 - 3aR_0^2 + 2R_0^3 - 3ae^{-2R_0/a}(a + R_0)^2}{4R_0^6}. \tag{44}$$

We obtain the important result that the Riesz self-energy behaves like

$$E_{RZ} \sim \frac{1}{R_0^\alpha} \tag{45}$$

which scales with the nucleon number $A \sim R_0^3$ as

$$E_{RZ} \sim A^{-\alpha/3} \tag{46}$$

and therefore allows us to model the influence of a screened Coulomb-like charge contribution to the total energy.

In figure 4, we compare the $R_0$ dependence for the three different types of self-energies. Depending on the size of the spherical nucleus, e.g. $R_0(208\text{Pb}) = 7.25$ (fm), the behaviour of the Yukawa self-energy is covered by the Riesz self-energy for $\alpha$ within the range $2 \leq \alpha \leq 2.5$ and therefore the Riesz self-energy covers the full range of relevant categories.
In addition, it should be mentioned that for the case $\alpha = 3/2$, the Riesz self-energy behaves like $A^{-1/2}$, which emulates the pairing term, and for $\alpha = 3$ the Riesz self-energy behaves like $A^{-1}$, which is equivalent to the behaviour of the proton–neutron symmetry term in the Weizsäcker mass formula.

Therefore, the macroscopic pairing, symmetry and Coulomb contributions to the total energy content of a nucleus may be treated from a generalized point of view as different realizations of the same Riesz potential are all determined in the same way for a given shape.

As a consequence, there is a one-to-one correspondence between a given change in the shape geometry and the dynamic behaviour of these energy contributions. On the other hand, the hitherto abstract fractional coefficient $\alpha$ now may be interpreted within the context of cluster physics as a smooth order parameter with a well-defined physical meaning for distinct $\alpha$ values.

The combination of concepts and methods developed in different branches of physics, here demonstrated for the case of fractional calculus and cluster physics, has always led to new insights and improvements. As an additional step based on this concept, which marks the direction for future research, we may emphasize the convolution aspect of the Riesz integral, which may be interpreted within the framework of linear system theory, leading to new insights into large amplitude collective motion.

4. Conclusion

From all these presented results, we may draw the conclusion that the Riesz potential may be considered as a promising alternative approach to folded potentials, which are widely used to describe nuclear dynamics within the framework of a collective shell model.

Of course, these potentials are only an alternative starting point to calculate fragmentation potentials based on a fractional integral definition, but it is indeed remarkable that the Coulomb, pairing and symmetry parts of the macroscopic energy contribution may be considered as specific realizations of the fractional Riesz integral with the fractional parameters $\alpha \in \{1, 3/2, 3\}$ and therefore develop dynamically in a similar way for a given shape configuration.

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