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# Evaluation of folding integrals using Fourier–Bessel expansions

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**Abstract.** The conditions are examined under which Fourier–Bessel expansions can be used correctly in the evaluation of multiple folding integrals. A proper formulation of the method is given.

## 1. Introduction

Many applications of physics require the evaluation of folding integrals. Typically, sources of two-body forces with a potential $U(s)$ are given that have specified density distributions of limited radial extent, $\rho_i(r_i)$, $i = 1, 2$, and one is faced with the task of calculating the potential energy $V(r)$ of a given configuration of the sources

$$V(r) = \int\int U(|r + r_1 - r_2|)\, \rho_1(r_1)\rho_2(r_2)\, \mathrm{d}r_1\, \mathrm{d}r_2 \tag{1}$$

where $r$ is the displacement of the source with density $\rho_1(r_1)$ from that with density $\rho_2(r_2)$. The potential $U(s)$ may be, for example, the familiar Coulomb potential [1], an effective nucleon–nucleon interaction (as in the folding model of the nuclear optical potential [2]), or the Uehling potential of the vacuum polarization in quantum electrodynamics [3].

The well known convolution theorem [4] reduces the evaluation of the six-dimensional folding integral (1) to the evaluation of the Fourier transforms of the density distributions $\rho_i(r_i)$

$$\tilde{\rho}_i(q) = \int \rho_i(r_i) \exp(\mathrm{i}q \cdot r_i)\, \mathrm{d}r_i \tag{2}$$

and of the two-body potential $U(s)$

$$\tilde{U}(q) = \int U(s) \exp(\mathrm{i}q \cdot s)\, \mathrm{d}s = 4\pi \int_0^\infty U(s) j_0(qs) s^2\, \mathrm{d}s \tag{3}$$

and to the evaluation of a three-dimensional Fourier integral whose integrand involves the product of these Fourier transforms or their complex conjugates:

$$V(r) = \frac{1}{(2\pi)^3} \int \tilde{U}(q)\, \tilde{\rho}_1{}^*(q)\, \tilde{\rho}_2(q) \exp(-\mathrm{i}q \cdot r)\, \mathrm{d}q. \tag{4}$$

While it is assumed that the densities themselves are real, $\rho_i^*(r_i) = \rho_i(r_i)$, their Fourier transforms are complex in general. Multipole expansions of the densities $\rho_i(r_i)$ further

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reduce the three-dimensional Fourier transforms (2) and the three-dimensional Fourier integral (4) to multipole sums of one-dimensional integrals (see, for example, [1]).

Much less well known and used is a discrete version of this momentum-space procedure, based on a Fourier–Bessel expansion of the two-body potential $U(s)$ and in which the evaluation of the Fourier integral (4) is replaced by a better-controlled and computationally more efficient summation of a series expansion. While the use of Fourier–Bessel expansions for the evaluation of folding integrals has been reported in the literature on several occasions [3, 5–8], it appears that the method itself and the conditions under which it is applicable have not yet been properly investigated and formulated. The present paper is an attempt to remedy that.

## 2. Fourier–Bessel expansions

Let us consider a potential $U(\boldsymbol{s})$ that is a function of not only the modulus $s = |\boldsymbol{s}|$, but also of the orientation of $\boldsymbol{s}$ with respect to some coordinate system. This would arise, for example, when the force acting between two particles is affected by the presence of other particles, i.e. when three(or more)-body forces are significant. Or, $U(\boldsymbol{s})$ may be an external non-central 'one-body' potential, and one needs to calculate the one-body potential energy of particles that are located in $U(\boldsymbol{s})$, apart from the potential energy arising from their two-body interactions.

The potential $U(\boldsymbol{s})$ is assumed to have a multipole expansion

$$U(\boldsymbol{s}) = \sum_{lm} U_{lm}(s)\, \mathrm{i}^l Y_{lm}(\hat{\boldsymbol{s}}). \tag{5}$$

General Fourier–Bessel expansions of the multipoles $U_{lm}(s)$ in terms of the spherical Bessel functions of order $l$, valid for $s$ in a range $s < R$,

$$U_{lm}(s) = \sum_{n=1}^{\infty} c_n^{(lm)}\, j_l\bigl(q_n^{(l)} s\bigr) \tag{6}$$

have coefficients $c_n^{(lm)}$ that are given by

$$c_n^{(lm)} = \frac{1}{w_n^{(l)}} \int_0^R U_{lm}(s)\, j_l\bigl(q_n^{(l)} s\bigr)\, s^2\, \mathrm{d}s \tag{7}$$

where $q_n^{(l)} R$ are the positive roots of the equations

$$a_l\, j_l(x) + b_l x\, j_l'(x) = 0 \tag{8}$$

where the prime denotes the first derivative and $a_l$ and $b_l$ are arbitrary constants, subject only to the obvious condition $a_l^2 + b_l^2 > 0$. The constants $w_n^{(l)}$ in (7) are the normalization integrals of the orthogonal systems $j_l\bigl(q_n^{(l)} s\bigr)$, $n = 1, 2, \ldots$,

$$\int_0^R j_l\bigl(q_m^{(l)} s\bigr)\, j_l\bigl(q_n^{(l)} s\bigr)\, s^2\, \mathrm{d}s = w_n^{(l)} \delta_{mn}$$

$$w_n^{(l)} = \begin{cases} \dfrac{R^3}{2}\bigl[j_l'\bigl(q_n^{(l)} R\bigr)\bigr]^2 & b_l = 0 \\[2ex] \dfrac{R^3}{2}\left[\bigl(q_n^{(l)} R\bigr)^2 - \left(l + \dfrac{1}{2}\right)^2 + \left(\dfrac{a_l}{b_l} - \dfrac{1}{2}\right)^2\right]\left[\dfrac{j_l\bigl(q_n^{(l)} R\bigr)}{q_n^{(l)} R}\right]^2 & b_l \neq 0\,. \end{cases} \tag{9}$$

Equations (6)–(9) are obtained by reformulating the standard Fourier–Bessel expansions [9], which use the Bessel functions $J_\nu(x)$, in terms of the spherical Bessel functions $j_l(x) =$

$(\pi/2x)^{1/2}J_{l+1/2}(x)$. A formal expression of the completeness of the systems of spherical Bessel functions that can be used in a Fourier–Bessel expansion of a function of $s$ is a closure relation, valid within the sphere $s = |s| < R$:

$$\sum_{lm}\sum_{n}\frac{1}{w_n^{(l)}}j_l\left(q_n^{(l)}s\right)j_l\left(q_n^{(l)}s'\right)\mathrm{i}^l Y_{lm}(\hat{s})\left[\mathrm{i}^l Y_{lm}(\hat{s}')\right]^* = \delta(s-s'). \tag{10}$$

Using the Fourier–Bessel expansions (6), the potential (5) can be now written for $|s| < R$ as

$$U(s) = \frac{1}{4\pi}\sum_{lm}\sum_{n=1}^{\infty}c_n^{(lm)}\int \exp\left(\mathrm{i}q_n^{(l)}\cdot s\right)Y_{lm}\left(\hat{q}_n^{(l)}\right)\mathrm{d}\hat{q}_n^{(l)} \tag{11}$$

where $q_n^{(l)}$ are vectors with discrete moduli $|q_n^{(l)}| = q_n^{(l)}$ and polar angles $\hat{q}_n^{(l)}$, and where the identity

$$j_l(qs)\,\mathrm{i}^l Y_{lm}(\hat{s}) = \frac{1}{4\pi}\int \exp(\mathrm{i}q\cdot s)Y_{lm}(\hat{q})\,\mathrm{d}\hat{q} \tag{12}$$

which follows from the expansion of $\exp(\mathrm{i}q\cdot s)$ in spherical harmonics, is employed.

## 3. Folding integrals

Let us generalize the double-folding integral (1), by using the potential $U(s)$ instead of $U(|s|)$, to

$$V(r) = \int\int U(r + r_1 - r_2)\,\rho_1(r_1)\rho_2(r_2)\,\mathrm{d}r_1\,\mathrm{d}r_2 \tag{13}$$

and assume that the densities $\rho_i(r_i)$ are negligible at distances $|r_i|$ greater than some radii $R_i$. Such an assumption can be always made for densities that represent the distribution of charge, mass, etc, of particles or other well localized sources. In order to be able to formulate the use of Fourier–Bessel expansions in (13) correctly, the densities $\rho_i(r_i)$ are cut off at the radii $R_i$:

$$\rho_i(r_i) = 0 \qquad \text{for} \qquad |r_i| > R_i. \tag{14}$$

By choosing the radii $R_i$ sufficiently large, the cut-offs change the original densities to an arbitrarily small degree, but, strictly speaking, under consideration from now on is the folding integral (13), where $\rho_i(r_i)$ are the cut-off densities (14).

Using in (13) the Fourier–Bessel expansion (11) of the potential $U(r + r_1 - r_2)$, with an expansion radius

$$R = r_{\max} + R_1 + R_2 \tag{15}$$

an expansion of $V(r)$, valid for $|r| < r_{\max}$, is obtained:

$$V(r) = \frac{1}{4\pi}\sum_{lm}\sum_{n=1}^{\infty}c_n^{(lm)}\int \tilde{\rho}_1\left(q_n^{(l)}\right)\tilde{\rho}_2^*\left(q_n^{(l)}\right)\exp\left(\mathrm{i}q_n^{(l)}\cdot r\right)Y_{lm}\left(\hat{q}_n^{(l)}\right)\mathrm{d}\hat{q}_n^{(l)}. \tag{16}$$

Here $\tilde{\rho}_i\left(q_n^{(l)}\right)$ are the Fourier transforms (2) of the densities $\rho_i(r_i)$, cut off as in (14), at points $q = q_n^{(l)}$. The expansion (16) is valid for distances $|r| < r_{\max}$ because with such values of $r$ the expansion of $U(r + r_1 - r_2)$ used is guaranteed to hold for all the values of the argument $r + r_1 - r_2$ that contribute to (13).

In order to be able to perform the angular integrations in (16) analytically, the Fourier transforms $\tilde{\rho}_i(q)$ are expanded in multipoles:

$$\tilde{\rho}_i(q) = \sum_{l_i m_i} \tilde{\rho}^{(i)}_{l_i m_i}(q) \mathrm{i}^{l_i} Y_{l_i m_i}(\hat{q}). \tag{17}$$

These multipoles can be expressed as

$$\tilde{\rho}^{(i)}_{l_i m_i}(q) = 4\pi \mathrm{i}^{l_i} \int_0^{R_i} \rho^{(i)}_{l_i m_i}(r_i) j_{l_i}(q r_i) r_i^2 \, \mathrm{d}r_i \tag{18}$$

where $R_i$ are the cut-off radii of the densities $\rho_i(r_i)$ and $\rho^{(i)}_{l_i m_i}(r_i)$ are their multipoles

$$\rho^{(i)}_{l_i m_i}(r_i) = \int \rho_i(\boldsymbol{r}_i) \left[\mathrm{i}^{l_i} Y_{l_i m_i}(\hat{\boldsymbol{r}}_i)\right]^* \mathrm{d}\hat{\boldsymbol{r}}_i. \tag{19}$$

The expansion (16) is then written as

$$V(r) = \frac{1}{4\pi} \sum_{lm} \sum_{\substack{l_1 m_1 \\ l_2 m_2}} \sum_{n=1}^{\infty} c_n^{(lm)} \tilde{\rho}^{(1)}_{l_1 m_1}\left(q_n^{(l)}\right) \tilde{\rho}^{(2)\,*}_{l2 m_2}\left(q_n^{(l)}\right)$$

$$\times \int \exp\left(\mathrm{i} q_n^{(l)} \cdot \boldsymbol{r}\right) \mathrm{i}^{l_1} Y_{l_1 m_1}\left(\hat{\boldsymbol{q}}_n^{(l)}\right) \left[\mathrm{i}^{l_2} Y_{l_2 m_2}\left(\hat{\boldsymbol{q}}_n^{(l)}\right)\right]^* Y_{lm}\left(\hat{\boldsymbol{q}}_n^{(l)}\right) \mathrm{d}\hat{\boldsymbol{q}}_n^{(l)}. \tag{20}$$

Expanding the products of three spherical harmonics above in terms of single spherical harmonics and using the identity (12), equation (20) is written finally as

$$V(r) = \frac{1}{4\pi} \sum_{lm} \sum_{\substack{l_1 m_1 \\ l_2 m_2}} \sum_{n=1}^{\infty} c_n^{(lm)} (-1)^{m+m_2} \hat{l}\hat{l}_1\hat{l}_2 \mathrm{i}^{l_1} \tilde{\rho}^{(1)}_{l_1 m_1}\left(q_n^{(l)}\right) \left[\mathrm{i}^{l_2} \tilde{\rho}^{(2)}_{l_2 m_2}\left(q_n^{(l)}\right)\right]^*$$

$$\times \sum_{\lambda' \lambda} (2\lambda' + 1) \hat{\lambda} \begin{pmatrix} l_1 & l_2 & \lambda' \\ m_1 & -m_2 & -\mu' \end{pmatrix} \begin{pmatrix} l_1 & l_2 & \lambda' \\ 0 & 0 & 0 \end{pmatrix}$$

$$\times \begin{pmatrix} \lambda' & l & \lambda \\ \mu' & m & -\mu \end{pmatrix} \begin{pmatrix} \lambda' & l & \lambda \\ 0 & 0 & 0 \end{pmatrix} j_\lambda\left(q_n^{(l)} r\right) \mathrm{i}^\lambda Y_{\lambda\mu}(\hat{\boldsymbol{r}}) \tag{21}$$

where $\hat{l} = (2l+1)^{1/2}$ etc, and the large parentheses denote 3-$j$ coefficients; $\mu' = m_1 - m_2$ and $\mu = m + m_1 - m_2$. Equation (21) is a Fourier–Bessel expansion of the folding integral (13) with a general, non-spherical potential $U(\boldsymbol{s})$ and densities $\rho_i(\boldsymbol{r}_i)$, holding within a sphere $r = |\boldsymbol{r}| < R - R_1 - R_2$, where $R$ is the Fourier–Bessel expansion radius of $U(\boldsymbol{s})$.

## 4. Special cases

The general formula (21) simplifies when the potential $U(\boldsymbol{s}) = U(|\boldsymbol{s}|)$, i.e. when it is a function of the modulus of the dispacement $\boldsymbol{s}$, as is the case with rotationally invariant two-body potentials. Then only the $l = 0$ term in (21) contributes, and the positive roots $q_n^{(l)} R$ of (8) for $l = 0$ are simply $n\pi$, $n = 1, 2, \ldots$ when $b_0 = 0$ in (8), or $(n - \frac{1}{2})\pi$, $n = 1, 2, \ldots$ when $a_0 = 0$, with the normalization constants (9) $w_n^{(0)} = R/\left[2\left(q_n^{(0)}\right)^2\right]$ in both these cases. Even if it could be under special circumstances advantageous not to take $a_0$ or $b_0$ in (8) as 0, those particular choices are adopted almost universally in the Fourier–Bessel expansions

that are based on the spherical Bessel function $j_0(x)$. Assuming then a spherical potential $U(s)$, and taking $q_n^{(0)} = n\pi/R$, the folding integral (13) is given for $r = |\mathbf{r}| < R$ by

$$V(r) = \frac{1}{\sqrt{4\pi}} \sum_{\substack{l_1 m_1 \\ l_2 m_2}} \sum_{n=1}^{\infty} c_n (-1)^{m_1} \hat{l}_1 \hat{l}_2 \mathrm{i}^{l_1} \tilde{\rho}_{l_1 m_1}^{(1)}\left(\frac{n\pi}{R}\right)\left[\mathrm{i}^{l_2} \tilde{\rho}_{l_2 m_2}^{(2)}\left(\frac{n\pi}{R}\right)\right]^* \times \sum_{\lambda} \hat{\lambda} \begin{pmatrix} l_1 & l_2 & \lambda \\ m_1 & -m_2 & -\mu \end{pmatrix} \begin{pmatrix} l_1 & l_2 & \lambda \\ 0 & 0 & 0 \end{pmatrix} j_\lambda\left(\frac{n\pi}{R} r\right) \mathrm{i}^{\lambda} Y_{\lambda\mu}(\hat{\mathbf{r}}) \tag{22}$$

where

$$c_n = \frac{1}{\sqrt{4\pi}} c_n^{(00)} = \frac{2}{R}\left(\frac{n\pi}{R}\right)^2 \int_0^R U(s)\, j_0\left(\frac{n\pi}{R} s\right) s^2 \, \mathrm{d}s. \tag{23}$$

An equally valid expansion is obtained by replacing the coefficients $n\pi/R$ in (22) and (23) by $(n - \frac{1}{2})\pi/R$.

Further simplification ensues when only one of the densities, say $\rho_2(r_2)$, is non-spherical. Then only the $l_1 = 0$ term in (22) contributes, and (22) reduces to

$$V(r) = \sum_{l_2 m_2} \sum_{n=1}^{\infty} c_n \tilde{\rho}_1\left(\frac{n\pi}{R}\right)(-1)^{l_2}\left[\mathrm{i}^{l_2} \tilde{\rho}_{l_2 m_2}^{(2)}\left(\frac{n\pi}{R}\right)\right]^* j_{l_2}\left(\frac{n\pi}{R} r\right)\left[\mathrm{i}^{l_2} Y_{l_2 m_2}(\hat{\mathbf{r}})\right]^* \tag{24}$$

where

$$\tilde{\rho}_1(q) = \frac{1}{\sqrt{4\pi}} \tilde{\rho}_{00}^{(1)}(q) = 4\pi \int_0^{R_1} \rho_1(r_1) j_0(q r_1) r_1^2 \, \mathrm{d}r \tag{25}$$

is the Fourier transform of the spherical density $\rho_1(r_1)$. Finally, the expansion formula for the fully spherically symmetric case, i.e. when the potential and both densities are spherically symmetric, is particularly simple

$$V(r) = \sum_{n=1}^{\infty} c_n \tilde{\rho}_1\left(\frac{n\pi}{R}\right) \tilde{\rho}_2\left(\frac{n\pi}{R}\right) j_0\left(\frac{n\pi}{R} r\right) \tag{26}$$

where $\tilde{\rho}_2(q)$ is the Fourier transform of the spherical density $\rho_2(r_2)$, defined as in (25).

Still more simplifications ensue when one of the density distributions is that of a point source, i.e. given by the Dirac $\delta$-function. The double-folding integral (13) then reduces to a single-folding one. The expansion formulae obtained here cover the single-folding case simply by noting that the Fourier transform of the three-dimensional $\delta$-function is a constant equal to unity. If then $\rho_i(r_i) = \delta(\mathbf{r}_i)$, $i = 1$ or 2, one would use

$$\frac{1}{\sqrt{4\pi}} \tilde{\rho}_{l_i m_i}^{(i)}(q) = \tilde{\rho}_i(q) \delta_{l_i 0} \delta_{m_i 0} = \delta_{l_i 0} \delta_{m_i 0} \qquad i = 1 \text{ or } 2 \tag{27}$$

for the single-folding case in the expansion formulae (21), (24) and (26). Single folding with a non-spherical 'one-body' potential $U(s)$ over the density $\rho_1(r_1)$, the expansion formula for which is qiven by equation (21) with equation (27), would qive the potential energy in the field $U(s)$ of a particle with density distribution $\rho_1(r_1)$.

## 5. Conclusions

The great advantage of using discrete Fourier–Bessel methods over the continuous Fourier-integral formulation is that the Fourier integral into which the folding integral can be transformed, and which invariably has to be evaluated numerically, is replaced by a series expansion in which, in principle, only the number of the terms included controls the degree

*of approximation to the exact value of the folding integral within a finite-radius sphere.* In other words, a procedure of numerical integration is replaced by an analytical method.

An essential aspect of the discrete Fourier–Bessel methods as they are formulated here is the use of finite-radius Fourier transforms for both the 'potential' and densities in question. As Fourier transforms usually have to be evaluated numerically, they are as such finite-radius transforms *de facto*. However, one should bear in mind a difference between the finite-radius transform of a potential that may have an infinite range, and that of a density that is assumed to be cut off at some finite radius. In the present formulation, the difference is that the latter transform is considered as the infinite-radius transform of a function that is defined to vanish beyond a certain finite radius.

A comment is made on the Fourier–Bessel procedures as they have been used in practice for the evaluation of folding integrals. It may happen that the infinite-radius Fourier transform of a density that decays rapidly at large distances is available analytically, but its finite-radius transform is not. It is then computationally advantageous to use the infinite-radius Fourier transform instead of a numerically evaluated transform of that density cut off at a radius $r_1 = R_1$. To approximate well the exact value of the folding integral within a sphere of radius $r_{\max}$, the Fourier–Bessel expansion radius $R$ of the potential must be *chosen sufficiently large so that the radius* $r_{\max} = R - R_1 - R_2$ *has the desired value, with* $R_1$ now a radius beyond which the density in question can be considered as negligible. The folding integral whose value is being approximated in such a procedure is one in which the full density, i.e. the density that is not cut off at any finite radius, appears. However, the degree of such an aproximation is governed not only by the number of terms in the Fourier–Bessel expansion, but also, in a less controllable manner, by the choice of the value for $R_1$, which, for a given value of $R$, affects the value of $r_{\max}$. While it may be argued that, strictly speaking, a procedure like that is no longer a rigorous analytical method, in practice it yields very accurate results with densities that are used to model the distribution of physical attributes of particles (see, for example, [8]). Such densities decay at large distances exponentially, and thus the choice of the radius $R_1$ beyond which they can be regarded as vanishing presents no practical difficulty.

In closing, this point is illustrated by the concrete example of a Yukawa potential

$$U(s) = \frac{\mathrm{e}^{-\mu s}}{s}. \tag{28}$$

The Coulomb potential $1/s$ can be treated as the special case $\mu = 0$ of the Yukawa potential. The coefficients (23) of the Fourier–Bessel expansion of $U(s)$ are then

$$c_n = \frac{2}{R}\left(\frac{n\pi}{R}\right)^2 \frac{1-(-1)^n \mathrm{e}^{-\mu R}}{(n\pi/R)^2 + \mu^2}. \tag{29}$$

The Fourier transform (25) with $R_1 \to \infty$ of a Fermi density $\rho_{\mathrm{F}}(r)$, normalized to unit volume,

$$\begin{aligned} \rho_{\mathrm{F}}(r) &= \rho_0 \left[1 + \mathrm{e}^{(r-c)/a}\right]^{-1} \\ \rho_0 &= \frac{3}{4\pi c^3}\left[1 + \left(\frac{\pi a}{c}\right)^2 - 6\left(\frac{a}{c}\right)^3 \sum_{n=1}^{\infty} (-1)^n \frac{\mathrm{e}^{-nc/a}}{n^3}\right]^{-1} \end{aligned} \tag{30}$$

is given by [1]

$$\tilde{\rho}_F(q) = 4\pi\rho_0 \left[ \frac{t}{q^3}(t\cosh\pi qa \sin qc - qc\cos qc) - 2a^3 \sum_{n=1}^{\infty}(-1)^n \frac{n\,e^{-nc/a}}{(n^2+a^2q^2)^2} \right] \tag{31}$$

$$t = \frac{\pi qa}{\sinh \pi qa}.$$

The Fermi density is often used to model the distribution of mass and charge of particles; the uniform density with radius $c$ is obtained as the limit $a \to 0$. A Fourier–Bessel expansion of the Coulomb potential due to two extended charge distributions described by the Fermi densities (30) is then given by equation (26), and equations (29) (with $\mu = 0$) and (31) for $c_n$ and $\tilde{\rho}_i(n\pi/R)$, respectively. Using double-precision (8-byte) arithmetic and the values $c_1 = 3$, $a_1 = 0.5$, $c_2 = 5$ and $a_2 = 0.5$ fm for the parameters of the two Fermi densities, which are typical for the charge distributions of light- and medium-mass atomic nuclei, an expansion radius $R$ of about 28 fm and 27 terms in the expansion (26), out of which only the odd ones happen to be non-zero, are needed to obtain the Coulomb potential to six-digit accuracy in the range $0.1 < r < 15$ fm. For ten-digit accuracy in the same range, an expansion radius of about 35 fm is required and the number of terms increases to 63, again including the zero-value terms. This was checked by recalculating this expansion using an extended, 16-byte precision arithmetic.

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