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The symmetrized Fermi function and its transforms

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Abstract. The Fermi function is a useful model in many branches of physics, from statistical mechanics to nuclear physics to astrophysics. The *symmetrized* Fermi function has the advantage that with it, many useful integrals can be evaluated *exactly*. Strangely, this does not seem to be well known in the physics community.

1. Introduction

The Fermi function

$$F((r-R)/d) = \frac{1}{1+e^{(r-R)/d}} \tag{1}$$

is used in many areas of physics. Recently we found it useful in a study of quantum dots. In statistical mechanics it describes the occupation of states by fermions, with $R = E_F$ and $d = k_B T$. In nuclear physics, it is commonly used as a shape for the radial density distribution, or for the single-nucleon potential-energy function, with R the half-density radius and d the surface-thickness parameter. In this context it is usually called the Woods–Saxon potential. It is a convenient function with a more or less flat interior and a narrow surface. There has always been some mild embarrassment concerning the fact that it puts a cusp at the centre of the nucleus, $r = 0$, but because in most cases the radius R is large compared to the surface thickness d, this cusp is ignored.

Recently it came to our attention that a perfectly reasonable alternative function exists that removes this embarrassment: it is the symmetrized Fermi function

$$\rho_S(r) = \frac{\sinh(R/d)}{\cosh(r/d)+\cosh(R/d)} = \rho_S(r/d, R/d) \tag{2}$$

which was used by Buck and Pilt [1] as the shape of a nuclear potential. They ascribed it to Burov *et al* [2], who in turn cite Eldyshev *et al* [3]. Grammaticos [4] appears to have independently discovered it in variational calculations on the density distribution in nuclei. Behrens and Bühring [5] used it as one of their models for computing β-decay matrix elements; another recent reference is Grypeos *et al* [6]. Thus, the symmetrized Fermi function has been known to some experts, but the least one can say is that it is not 'well known' generally. None of the text books on nuclear physics refers to it.

When $R \gg d$, the symmetrized function is indistinguishable on a graph from the usual Fermi function, so the cusp seems more a difficulty of principle than a practical matter.

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However, if R and d are comparable, this is not at all so. In any case, it is an advantage to deal with a function for which one can derive analytic results.

The model appears to have been invented by Eldyshev *et al* [3], to describe the nuclear-charge distribution. They gave the *exact* form factor

$$G(q) = \frac{4\pi}{Nq}\int_0^\infty \sin(qr)\rho_S(r)r\,\mathrm{d}r = \frac{3}{q^3}\frac{\pi qd}{\sinh\pi qd}\left[\frac{\pi qd}{\tanh\pi qd}\sin(qR) - qR\cos(qR)\right]\frac{1}{R(R^2+\pi^2d^2)} \tag{3}$$

where $1/N$ is the normalization factor that gives a volume integral of unity:

$$N = \frac{4\pi}{3}R(R^2+\pi^2d^2). \tag{4}$$

These results can be checked easily by contour-integral methods (see section 4). By expanding $G(q)$ in powers of q^2 one can extract the values of all the even moments of the charge distribution. One wonders why this has not been common knowledge up until now? Further, one wonders what is the relation between these exact results and the well known Sommerfeld lemma [7] which has traditionally been used to evaluate moments of the Fermi function?

The purpose of this note is to explore these questions. It is convenient to start with a paper of Blankenbecler [8], who derived a clever operator expression for integrals over the Fermi function. We see that when this is applied to the symmetrized Fermi function equation (2), Blankenbecler's derivation becomes exact. Otherwise, he had dropped a term which generates a complicated series of small corrections, that were explored at length by Maximon and Schrack [9]. In Elton's famous book on nuclear sizes [10] the same corrections were dropped. Therefore the 'approximate' results obtained by many authors for the usual Fermi function are in fact exact results for the symmetrized Fermi function. As a result, many calculations have actually used the latter, without knowing what they were doing.

2. Blankenbecler's method

First we check that equation (2) can be written as a symmetrized Fermi function.

$$\rho_S(r) = \frac{1}{1+\mathrm{e}^{(r-R)/d}} + \frac{1}{1+\mathrm{e}^{-(r+R)/d}} - 1 = \frac{1}{1+\mathrm{e}^{(r-R)/d}} - \frac{1}{1+\mathrm{e}^{(r+R)/d}} = \frac{\sinh(R/d)}{\cosh(r/d)+\cosh(R/d)}. \tag{5}$$

Note that when $r = 0$, the value is $\tanh(R/2d)$, while when $r = R$, it is $0.5\tanh(R/d)$. The ratio is

$$\frac{\rho_S(R)}{\rho_S(0)} = \frac{1}{1+\tanh^2(R/2d)} \tag{6}$$

which is close to 0.5 when $R \gg 2d$. Hence R is the 'half-density radius' at least as much as it is for the usual Fermi function. Being an even function of r, $\rho_S(r)$ has zero slope at the origin, and therefore no cusp, avoiding the defect of the usual Fermi function.

In general,

$$\frac{-1}{\rho_S(r)}\frac{\mathrm{d}\rho_S(r)}{\mathrm{d}r} = \frac{\rho_S(r)}{d}\frac{\sinh r/d}{\sinh R/d} \tag{7}$$

which is approximately $1/2d$ at $r = R$, when $R \gg d$. Therefore, it is still reasonable to refer to d as the 'surface thickness parameter'.

In Blankenbecler's approach, integrals over the usual Fermi function equation (1) are put in dimensionless form, with $x = r/d$, and $y = R/d$.

$$F(x-y) = \frac{1}{1+\mathrm{e}^{x-y}} \qquad \frac{\mathrm{d}F(x)}{\mathrm{d}x} \equiv f(x). \tag{8}$$

Take a general weight function $h(x)$ and consider the integral

$$I = \int_0^\infty h(x)F(x-y)\,\mathrm{d}x. \tag{9}$$

This we integrate by parts, writing

$$H(x) = \int_0^x h(x')\,\mathrm{d}x' \tag{10}$$

so that

$$\begin{aligned} I &= -\int_0^\infty H(x)f(x-y)\,\mathrm{d}x \\ &= -\int_{-y}^\infty H(x'+y)f(x')\,\mathrm{d}x'. \end{aligned} \tag{11}$$

The boundary term vanishes at the origin by choice of H, and at ∞ due to the Fermi function. Blankenbecler then made the usual approximation of extending the lower limit to $-\infty$, considering that $y = R/d$ is generally a large value. In the case of the symmetrized Fermi function, this approximation is unnecessary, because there is a second piece of $\rho_S(x, y) = F(x-y) - F(x+y)$ to be considered. In it the sign of y is reversed so one has the additional contribution

$$\begin{aligned} J &= -\int_y^\infty H(x'-y)f(x')\,\mathrm{d}x' \\ &= \int_{-y}^{-\infty} H(-x'-y)f(-x')\,\mathrm{d}x' \\ &= \int_{-\infty}^{-y} H(x'+y)f(x')\,\mathrm{d}x'. \end{aligned} \tag{12}$$

In the third line we have used the fact that the derivative of the Fermi function is even: $f(-x) = f(x)$, and we have taken $h(x)$ to be *even* so that $H(x)$ is *odd*. For this restricted class of weight functions

$$\int_0^\infty h(x)\rho_S(x, y)\,\mathrm{d}x = I - J = -\int_{-\infty}^\infty H(x'+y)f(x')\,\mathrm{d}x'. \tag{13}$$

Hence, Blankenbecler's argument is exact, but it applies to the symmetrized Fermi function, and only for *even* weight functions. The trick now is to write Taylor's theorem in the form $H(y+x') = \mathrm{e}^{x'D}H(y)$, where D is the derivative operator acting on $H(y)$. Changing variables to $\eta = \mathrm{e}^{x'}$ gives

$$I_S = \int_0^\infty \frac{\eta^D}{(1+\eta)^2}\,\mathrm{d}\eta H(y). \tag{14}$$

The integral may be evaluated formally by supposing that D is a small number $|D| < 1$, putting a branch point at the origin. The integrand then has a cut along the positive real axis and a double pole at -1. Choosing the keyhole contour to exclude the cut, and using Cauchy's theorem gives

$$I_S = \frac{\pi D}{\sin \pi D} H(y). \tag{15}$$

This is a very compact result, which is completely equivalent to Sommerfeld's method (see appendix A).

More generally, when the weight function $h(x)$ is odd, the neglected 'small correction terms' (see appendix B) due to the integral J will be doubled in size when applied to the symmetrized Fermi function, as compared with the usual Fermi function. However, providing that they really are negligible, the result is still useful.

3. Applications

The simplest case is for the normalization integral, for which we choose

$$H(y) = \frac{y^3}{3} \qquad \text{with } H''(y) = 2y. \tag{16}$$

When we expand the operator in equation (15) in powers of D, only even powers occur. Hence only these two derivatives contribute, giving

$$\int_0^\infty \rho_S(x) x^2 \, \mathrm{d}x = \frac{R}{3d^3}[R^2 + \pi^2 d^2]. \tag{17}$$

The d^3 is removed as a common factor on both sides of the equation, and a 4π is added for integration over angles, which then verifies equation (4). Similarly, using

$$H(y) = \frac{y^5}{5} \qquad H''(y) = 4y^3 \qquad H^{(4)}(y) = 24y \tag{18}$$

we obtain the mean square radius

$$\langle r^2 \rangle = \tfrac{1}{5}[3R^2 + 7\pi^2 d^2]. \tag{19}$$

Finally, the choice

$$H(y) = \frac{1}{\lambda} \sin \lambda y \qquad H'(y) = \cos \lambda y, \ldots \tag{20}$$

allows us to evaluate the form factor (here, $\lambda = qd$). Unlike the first two examples, we can evaluate the operator in closed form, rather than by the series expansion. We continue this in the next section.

4. Form factor

The nuclear form factor is the Fourier transform of the density distribution (2):

$$\begin{aligned} G(q) &= \frac{1}{N} \int_0^\infty \mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}} \rho_S(r) \, \mathrm{d}^3 r \\ &= \frac{4\pi}{Nq} \int_0^\infty \sin(qr) \rho_S(r) r \, \mathrm{d}r \\ &= \frac{-4\pi}{Nq} \frac{\partial}{\partial q} \int_0^\infty \cos(qr) \rho_S(r) \, \mathrm{d}r \end{aligned} \tag{21}$$

where N normalizes $G(q = 0) = 1$. We therefore wish to evaluate

$$K = \int_0^\infty \cos(\lambda x)\rho_S(x, y)\,\mathrm{d}x \tag{22}$$

where $x = r/d$, $y = R/d$ and $\lambda = qd$. Since the integrand is even, we can write

$$K = \tfrac{1}{2}\Re \int_{-\infty}^{\infty} \mathrm{e}^{\mathrm{i}\lambda x}\rho_S(x)\,\mathrm{d}x. \tag{23}$$

The integrand has poles at the complex points $z = \pm y + \mathrm{i}\pi$. Consider, therefore, the contour integral over a rectangle consisting of the real line $z = x$, the line $z = x + 2\mathrm{i}\pi$, and two ends which will be allowed to recede to $\pm\infty$. Using Cauchy's theorem, we find

$$(1 - \mathrm{e}^{-2\lambda\pi})K = \pi\mathrm{i}[\mathrm{e}^{\mathrm{i}\lambda(-y+\mathrm{i}\pi)} - \mathrm{e}^{\mathrm{i}\lambda(y+\mathrm{i}\pi)}]. \tag{24}$$

Hence,

$$K = \frac{\pi}{\sinh \pi qd}\sin qR \tag{25}$$

where we have reverted to physical units. By taking the derivative with respect to q we recover the result given in equation (3).

Now we apply Blankenbecler's method to the case of equation (20) to obtain the same result. Only even-order derivatives of $H(y) = \sin\lambda y/\lambda$ are required, and one sees that

$$D^{2k}H(y) = (-)^k\lambda^{2k}H(y) \tag{26}$$

so that the operator D in equation (15) can be consistently replaced by $\mathrm{i}\lambda$. This avoids having to sum a series that would otherwise converge only for $|\lambda| < 1$. We have

$$K = \frac{\mathrm{i}\pi\lambda}{\sin \mathrm{i}\pi\lambda}H(y) = \frac{\pi}{\sinh\pi qd}\sin qR \tag{27}$$

in agreement with the direct evaluation in equation (25).

5. Other Bessel transforms

In considering models of quantum dots, we have had to deal with the problem of constructing the potential inside a semiconductor, knowing its form at the exposed surface. For cases of cylindrical symmetry the use of Fourier–Bessel expansions has some advantages over the more conventional Poisson formula. This lead us to consider the integral

$$v(q) \equiv \int_0^\infty \rho_S(r/d, R/d)J_0(qr)r\,\mathrm{d}r. \tag{28}$$

As before, we use dimensionless variables $x = r/d$, $y = R/d$ and $\lambda = qd$. Then

$$q^2 v(q) = \lambda^2 \int_0^\infty \rho_S(x, y)J_0(\lambda x)x\,\mathrm{d}x \tag{29}$$

for which the function $H(x) = \lambda x J_1(\lambda x)$. Note that this is an *even* function of x, so Blankenbecler's method is no longer exact. In fact, the so-called small corrections are twice as large as for the usual Fermi function, which can be seen from equations (11) and (12). But so long as they are negligible this has little importance (see appendix B for more discussion). Equation (29) can be evaluated by Blankenbecler's method as above but requires a little more ingenuity. The result will be expressed using variables $z = \lambda y = qR$, and $\alpha = \lambda\pi = \pi q d$ (in this section, z is real). Using now $D = \mathrm{d}/\mathrm{d}z$, equation (15) becomes

$$q^2 v(q) = \frac{\alpha D}{\sin\alpha D} H(z). \tag{30}$$

Expanding in powers of $\alpha = \pi q d$, and taking the derivatives, one finds for the first few terms

$$\begin{aligned} q^2 v(q) = q R J_1(qR) &- \frac{(\pi q d)^2}{6}[q R J_1(qR) - J_0(qR)] \\ &+ \frac{7(\pi q d)^4}{360}\left[q R J_1(qR) - 2J_0(qR) + \frac{J_1(qR)}{qR}\right] \\ &- \frac{31(\pi q d)^6}{360(42)}\left[q R J_1(qR) - 3J_0(qR) + \frac{3}{qR}J_1(qR) - \frac{3}{(qR)^2}J_2(qR)\right] + \cdots. \end{aligned} \tag{31}$$

As noted in appendix A, this series diverges for large $|\alpha|$, so one would like to know its sum. Further study reveals that the coefficients involve functions

$$y_p(z) \equiv (-)^{p+1}(2p-1)!!\frac{J_p(z)}{z^p} \tag{32}$$

with $y_0 = -J_0(z)$ and $y_{-1} \equiv z J_1(z)$. Differentiation is facilitated by the relation

$$y_p'' = -y_p - y_{p+1}. \tag{33}$$

For example, one has

$$(z J_1(z))'' = -z J_1(z) + J_0 = -y_{-1} - y_0. \tag{34}$$

At large z, the J_0 term is of relative order $1/z$. If we could neglect it altogether, then we could replace the derivative operator in equation (30) by i since only even powers of D occur in the expansion. The result would be $z J_1(z)\alpha/\sinh\alpha$, as in equation (27).

Taking the derivatives systematically leads to the tableau

$$\begin{aligned} -(z J_1)^{(2)} &= z J_1 + y_0 \\ (z J_1)^{(4)} &= z J_1 + 2y_0 + y_1 \\ -(z J_1)^{(6)} &= z J_1 + 3y_0 + 3y_1 + y_2 \\ (z J_1)^{(8)} &= z J_1 + 4y_0 + 6y_1 + 4y_2 + y_3 \\ -(z J_1)^{(10)} &= z J_1 + 5y_0 + 10y_1 + 10y_2 + 5y_3 + y_4. \end{aligned} \tag{35}$$

One sees that the rule for carrying out the derivatives generates coefficients according to Pascal's triangle, so they are the binomial coefficients ${}_\ell C_p$. The general case is therefore

$$(-)^\ell D^{2\ell} z J_1(z) = \sum_{p=0}^{\ell} {}_\ell C_p\, y_{p-1}. \tag{36}$$

Following equation (A.3), with $c_0 = \frac{1}{2}$, we have

$$\frac{\alpha D}{\sinh\alpha D} = 2\sum_{\ell=0}^{\infty}(-)^\ell c_{2\ell}\alpha^{2\ell}D^{2\ell}. \tag{37}$$

This gives

$$q^2 v(q) = 2\sum_{\ell=0}^{\infty}(-)^\ell c_{2\ell}\alpha^{2\ell}\sum_{p=0}^{\ell} {}_\ell C_p\, y_{p-1}. \tag{38}$$

By reversing the order of summations we have

$$q^2 v(q) = 2\sum_{p=0}^{\infty} y_{p-1} \sum_{\ell=p}^{\infty} (-)^{\ell}\, {}_{\ell}C_p c_{2\ell} \alpha^{2\ell}. \tag{39}$$

The coefficient of y_{p-1} can be expressed in closed form if we note from equation (37) (with $D = 1$) that

$$\frac{\alpha^{2p}}{p!}\left(\frac{\partial}{\partial\alpha^2}\right)^p \frac{\alpha}{\sinh\alpha} = \sum_{\ell=p}^{\infty} (-)^{\ell} c_{2\ell}\, {}_{\ell}C_p \alpha^{2\ell}. \tag{40}$$

Thus,

$$\begin{aligned} q^2 v(q) - zJ_1(z)\frac{\alpha}{\sinh\alpha} &= \sum_{p=1}^{\infty} y_{p-1}\frac{1}{p!}\alpha^{2p}\frac{\partial^p}{\partial(\alpha^2)^p}\frac{\alpha}{\sinh\alpha} \\ &= \sum_{p=1}^{\infty} y_{p-1}\frac{1}{2^p p!}\alpha^{2p}\left(\frac{1}{\alpha}\frac{\partial}{\partial\alpha}\right)^p \frac{\alpha}{\sinh\alpha} \\ &= \sum_{p=1}^{\infty} (-)^p \frac{(2p-3)!!}{2^p p!}\frac{J_{p-1}(z)}{z^{p-1}}\alpha^{2p}\left(\frac{1}{\alpha}\frac{\partial}{\partial\alpha}\right)^p \frac{\alpha}{\sinh\alpha}. \end{aligned} \tag{41}$$

We worked out the first few terms of this series explicitly, with the result

$$\begin{aligned} q^2 v(q) = \frac{\pi q d}{\sinh \pi q d}\Bigg[& qRJ_1(qR) + \frac{1}{2}\left(\frac{\pi q d}{\tanh\pi q d} - 1\right) J_0(qR) \\ & + \frac{1}{8}\left[\left(\frac{2\pi q d}{\tanh \pi q d} + 1\right)\left(\frac{\pi q d}{\tanh\pi q d} - 1\right) - (\pi q d)^2\right]\frac{J_1(qR)}{qR} \\ & + \frac{1}{16}\left[3\left(\frac{2(\pi q d)^2}{\tanh^2\pi q d} + \frac{2\pi q d}{\tanh\pi q d} + 1\right)\left(\frac{\pi q d}{\tanh \pi q d} - 1\right) - \frac{5(\pi q d)^3}{\tanh\pi q d}\right] \\ & \times \frac{J_2(qR)}{(qR)^2} + \cdots \Bigg]. \end{aligned} \tag{42}$$

It is seen that $\alpha/\sinh\alpha$ is a common factor, and the remaining coefficients become polynomials in α at large qd, so $q^2 v(q)$ decreases exponentially. The coefficients of y_p become more and more complicated but one can certainly work them out systematically. The result is an asymptotic series in z, where the dependence on α has been summed. One is not limited to small qd, as for the Sommerfeld expansion, or equation (31). On the other hand, if equation (42) is expanded in powers of α, it reproduces exactly equation (31).

In figure 1 we show a log plot of $|v(q)|$ versus q for the case $R = 30$, $d = 1$. The maxima of $|v(q)|$ vary by 20 orders of magnitude over the range considered, and on this scale the exact (numerical) values cannot be distinguished from expression (42). In figure 2, we have expanded a small portion of the drawing, for $2.2 < q < 2.4$. In this case, the zeroth order approximation, $zJ_1(z)\alpha/\sinh\alpha$ is shown as a broken curve. Adding successive terms from equation (42) quickly brings one to complete overlap with the full curve. The mean square deviation between the exact and approximate curves drops by a factor of more than 100 as each successive term is added, in figure 2.

6. Conclusion

For the symmetrized Fermi function one can evaluate many moments and integrals exactly in closed form. This simplification should allow numerous arguments to be simplified. For

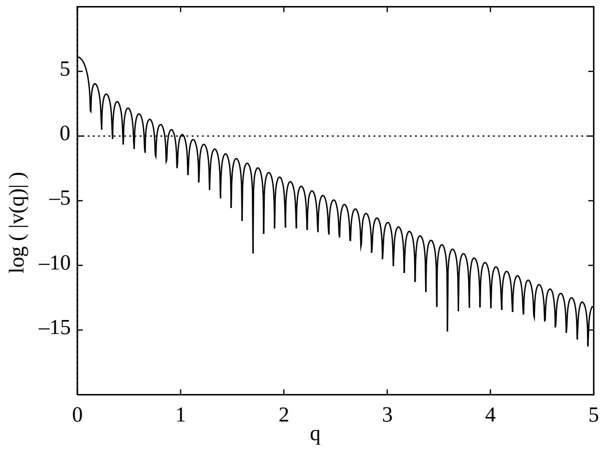

Figure 1. A log plot of $|v(q)|$ for the case $R = 30$, $d = 1$.

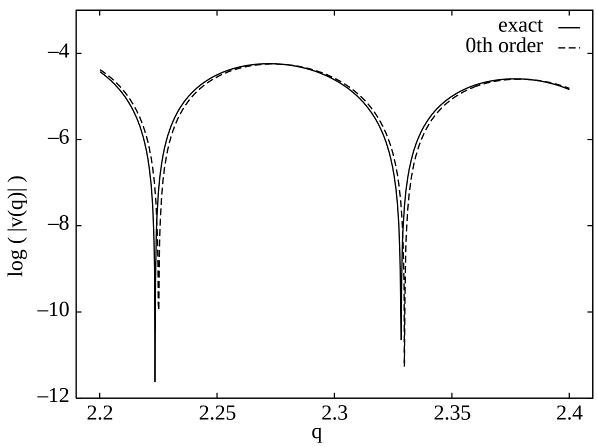

Figure 2. Expanded plot of a portion of figure 1. Full curve, exact; broken curve, leading term of equation (42).

example, in a very instructive paper, Amado and collaborators [11] discussed the Fermi function as a strong nuclear form factor for nucleon–nucleus scattering. Their approach closely parallels our direct evaluation, and they obtained K of equation (25) by summing the contributions from the poles of the Fermi function as we did implicitly in equation (24). Having a closed form would have simplified their discussion.

In two-dimensional problems such as quantum dots, one requires transforms involving cylinder functions. We have given an example where the resulting series works well. By extending the definition of the y_p to negative p, one can do similar integrals involving any odd power of x times J_0. The dependence on the 'small' parameter $\alpha = \pi q d$ is summed exactly, while the dependence on the large parameter $z = qR$ is given by an asymptotic series, but one which reproduces the Taylor series at small α. Calculations presented show that very good results were obtained in our example.

We therefore expect that this method can be useful in a variety of different contexts, wherever the Fermi function finds application.

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Appendix A. Relation to Sommerfeld's lemma

Here we relate our results to the well known Sommerfeld lemma as outlined by Chandrasekhar [7], which expresses the integral of equation (9) (approximately) as a series of terms involving the function $H(y)$ of equation (10) and its even-order derivatives. $H(y)$ must be sufficiently smooth and $H(0) = 0$. One has

$$\int_0^\infty F(x-y)\frac{\mathrm{d}H(x)}{\mathrm{d}x}\,\mathrm{d}x \approx H(y) + 2\sum_{\nu=2,4,6,\ldots} c_\nu H^{(\nu)}(y). \tag{A.1}$$

The coefficients are (for $\nu \neq 0$)

$$c_\nu = 1 - \frac{1}{2^\nu} + \frac{1}{3^\nu} - \frac{1}{4^\nu} + \cdots. \tag{A.2}$$

The first few of these sums are

$$c_2 = \frac{\pi^2}{12} \qquad c_4 = \frac{7\pi^4}{720} \qquad c_6 = \frac{31\pi^6}{30\,240} \cdots. \tag{A.3}$$

For large ν the coefficients approach unity from below.

Comparing with Blankenbecler's formula, equation (15), we see that the coefficient c_ν of equation (A.2) can be computed as half the coefficient of D^ν in the Taylor expansion of $\pi D/\sin \pi D$. This is undoubtedly the easiest way to generate them. Through this relation they are closely related to the Bernoulli numbers. The general result may be found in Gradshtein and Ryzhik [12]:

$$\frac{\pi x}{\sinh \pi x} = 1 + 2\sum_{n=1}^\infty B_{2n}(2^{2n-1}-1)\frac{(\pi x)^{2n}}{(2n)!} \tag{A.4}$$

from which

$$c_{2n} = (-)^{n+1}B_{2n}(2^{2n-1}-1)\frac{(\pi)^{2n}}{(2n)!}. \tag{A.5}$$

For reference,

$$B_2 = \frac{1}{6} \qquad B_4 = \frac{-1}{30} \qquad B_6 = \frac{1}{42} \cdots. \tag{A.6}$$

Appendix B. Error term

If one deals with the unsymmetrized Fermi function, then the integral I of equation (9) lacks the second piece of $\rho_S(x, y) = F(x-y) - F(x+y)$. This induces an error (see equation (13))

$$\begin{aligned} J &= \int_0^\infty \frac{h(x)}{1+\mathrm{e}^{x+y}}\,\mathrm{d}x \\ &= -\sum_{p=1}(-)^p \mathrm{e}^{-py}\int_0^\infty \mathrm{e}^{-px}h(x)\,\mathrm{d}x. \end{aligned} \tag{B.1}$$

In the particular case at hand, $h(x) = xJ_0(\lambda x)$, the integral is known [12]

$$\int_0^\infty x\mathrm{e}^{-px} J_0(\lambda x)\,\mathrm{d}x = \frac{p}{(p^2+\lambda^2)^{3/2}}. \tag{B.2}$$

Hence,

$$\begin{aligned} J &= -\sum_{p=1}(-)^p \mathrm{e}^{-py} \frac{p}{(p^2+\lambda^2)^{3/2}} \\ &= -\sum_{p=1}(-)^p \mathrm{e}^{-pR/d} \frac{p}{(p^2+q^2d^2)^{3/2}}. \end{aligned} \tag{B.3}$$

Since this is an alternating series of positive terms, the sum is less than the first term, and greater than the difference of the first two.

$$\mathrm{e}^{-R/d}\frac{1}{(1+q^2d^2)^{3/2}} \geqslant J \geqslant \mathrm{e}^{-R/d}\frac{1}{(1+q^2d^2)^{3/2}}\left(1-\mathrm{e}^{-R/d}\frac{2(1+q^2d^2)^{3/2}}{(4+q^2d^2)^{3/2}}\right). \tag{B.4}$$

The magnitude of the error is set by $\mathrm{e}^{-R/d}$, and when $R \gg d$ this is bound to be small. However, as a function of qd, it decreases only as the inverse third power, so asymptotically this will overtake the expansion given in equation (42). For the values adopted in figure 1, this will only show up at much larger values of qd.

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