Asymptotic approximations from quadrature rules

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We examine the ability of one- and two-point Gauss-Laguerre quadratures in correctly describing the asymptotic behavior of Fourier transforms. We illustrate the effectiveness of this method with the example of the neon atomic form factor and compare it to the results obtained from the familiar expansion in terms of inverse powers of the independent variable and the derivatives of the charge density at the origin.

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I. INTRODUCTION

The atomic form factor $F(k)$ remains one of the most important quantities in structure determination and is accessible from x-ray and electron scattering experiments [1]. This quantity is defined as a Fourier-Bessel transform

$$F(k)=4\pi\int_0^\infty r^2\rho(r)j_0(kr)dr \tag{1}$$

where j_0 is a zero-order spherical Bessel function and $\rho(r)$ is the spherically averaged charge density of the system. For our purposes, we choose to work with the alternative formulation

$$F(k)=\frac{4\pi}{k}\int_0^\infty r\rho(r)\sin(kr)dr \tag{2}$$

which may be expressed as

$$F(k)=\frac{4\pi}{k}\mathrm{Im}\left[\int_0^\infty r\rho(r)e^{ikr}dr\right] . \tag{3}$$

However, experimental data are only attainable for a limited range of small k which necessitates a knowledge of the asymptotic behavior of $F(k)$, in order to perform a correct analysis of these data.

For an *infinitely differentiable* density [2] $\rho(r)$, the asymptotic behavior of $F(k)$ for large k has been shown [3,5] to be

$$F(k)\simeq 8\pi\sum_{n=1}^{\infty}(-1)^n n\rho^{(2n-1)}(0)k^{-2n-2} \tag{4}$$

and the first two terms of the expansion in Eq. (4) have been given for the heliumlike ions by computing $\rho'(0),\rho^{(3)}(0)$ from highly accurate wave functions [6,7]. [The result of Eq. (4) may be derived [3,6] using the method of integration by parts.] If we truncate the expansion in Eq. (4) after the first term and use the cusp condition [4], the asymptotic behavior may be expressed as [8]

$$F(k)\simeq 16\pi Z\rho(0)k^{-4}+\eta_1(k) \tag{5}$$

where η_j is the error introduced by truncating the infinite series in Eq. (4) and the subscript is an index to denote the number of terms retained. In order to estimate the error resulting from this truncation, it has been proposed [7] to subtract half of the smallest term from the result. Thus the maximum error would be plus or minus half the smallest term retained. However, this proposal lacks in its ability to express η_j in an analytical form.

II. QUADRATURE RULES

We have recently shown [9] that Gauss-Laguerre quadratures may be used to compute the Fourier transforms of functions with an exponential-type *behavior*. This type of method was suggested by Wong [3,10] and is based on a transformation into the complex plane as follows. Let us consider the general Fourier transform

$$T(k)=\int_0^\infty g(r)f(r)e^{ikr}dr . \tag{6}$$

The three variations of the method discussed in Ref. [9] consisted of considering the following: $g(r)=r^m$, $m>-1$ and the variable change $z=-ikr$ (method I) [10]; imposing an exponential behavior, $g(r)=e^{-r}$ and the variable change $z=(1-ik)r$ (method II) [11]; and finally $g(r)=r^m e^{-\alpha r}$, α a positive, real parameter and the variable change $z=(\alpha-ik)r$ (method III) [9]. Substituting these, respectively, into Eq. (6) yields

$$T^{\mathrm{I}}(k)=\left[\frac{i}{k}\right]^{m+1}\int_0^\infty f\left[\frac{iz}{k}\right]z^m e^{-z}dz \quad (\text{method I}), \tag{7}$$

$$T^{\mathrm{II}}(k)=\frac{1}{1-ik}\int_0^\infty f\left[\frac{z}{1-ik}\right]e^{-z}dz \quad (\text{method II}), \tag{8}$$

$$T^{\mathrm{III}}(k)=\left[\frac{1}{\alpha-ik}\right]^{m+1}\int_0^\infty f\left[\frac{z}{\alpha-ik}\right]z^m e^{-z}dz \quad (\text{method III}), \tag{9}$$

which may be treated with Gauss-Laguerre quadratures. In this manner, Eqs. (7)–(9) may be expressed as

$$T^{\mathrm{I}}(k)=\left[\frac{i}{k}\right]^{m+1}\sum_{j=1}^{N}f\left[\frac{iz_j}{k}\right]\omega_j+E_N^{\mathrm{I}}(f,k) , \tag{10}$$

$$T^{\mathrm{II}}(k)=\frac{1}{1-ik}\sum_{j=1}^{N} f\left[\frac{x_j}{1-ik}\right]t_j+E_N^{\mathrm{II}}(f,k)\ , \tag{11}$$

$$T^{III}(k)=\left[\frac{1}{\alpha-ik}\right]^{m+1}\sum_{j=1}^{N} f\left[\frac{z_j}{\alpha-ik}\right]\omega_j+E_N^{\mathrm{III}}(f,k) \tag{12}$$

where x_j,t_j in Eq. (11) are the abscissas and weights of the N-order Gauss-Laguerre quadratures and the z_j,ω_j in Eqs. (10) and (12) are the abscissas and weights of *generalized* Gauss-Laguerre quadratures, i.e., those derived from polynomials orthogonal with respect to the weight function, $r^m e^{-z}$. The error terms $E_N^M(f,k)$ may be estimated as

$$E_N^{\mathrm{I}}(f,k)=\frac{N!\Gamma(N+m+1)}{(2N)!}\left[\frac{i}{k}\right]^{2N+m+1}\times f^{(2N)}\left[\frac{i\epsilon}{k}\right],\quad 0<\epsilon<\infty\ , \tag{13}$$

$$E_N^{\mathrm{II}}(f,k)=\frac{N!\Gamma(N+1)}{(2N)!}\left[\frac{1}{1-ik}\right]^{2N+1}\times f^{(2N)}\left[\frac{\epsilon}{1-ik}\right],\quad 0<\epsilon<\infty\ , \tag{14}$$

$$E_N^{\mathrm{III}}(f,k)=\frac{N!\Gamma(N+m+1)}{(2N)!}\left[\frac{1}{\alpha-ik}\right]^{2N+m+1}\times f^{(2N)}\left[\frac{\epsilon}{\alpha-ik}\right],\quad 0<\epsilon<\infty \tag{15}$$

where the superscript M on $E_N^M(f,k)$ labels the method used. The form factor may be computed from the charge density via Eq. (3) using the three different methods, i.e., the imaginary parts of Eqs. (10)–(12),

$$F(k)=\frac{4\pi}{k}\mathrm{Im}[T^M(k)]+E_{N,F}^M(f,k) \tag{16}$$

where the error of the form factor is

$$E_{N,F}^M(f,k)=\frac{4\pi}{k}\mathrm{Im}[E_N^M(f,k)]\ . \tag{17}$$

We use $f(z)=\rho(z)$, $m=1$ in Eq. (10), $f(z)=z\rho(z)e^z$ in Eq. (11), and $f(z)=\rho(z)e^{\alpha z}$, $m=1$ in Eq. (12). The results [9] obtained from a judicious choice of the parameter α illustrated that method III was the superior method for the whole range of k. In fact, all three methods were shown to perform better as k became larger [9].

The purpose of this paper is to examine the ability of these methods in yielding effective asymptotic approximations. Indeed, the ability of method I to yield good asymptotic approximations to simple test cases has already been demonstrated [3,10]. We hope to examine the applicability of this method along with methods II and III, for a more complex physical property such as the atomic form factor. We will compare the quality of results obtained from one- and two-point quadratures in Eqs. (10)–(12) with those obtained from the one- and two-term expansions in Eq. (4), i.e., we will compare η_1 and η_2 with $E_{1,F}^M$ and $E_{2,F}^M$, respectively, to determine which method yields the best approximation to $F(k)$ at large k. Such a numerical investigation is required since the question of whether the error of quadrature is smaller than the error of termwise integration is difficult to answer for the general case [12].

III. RESULTS AND DISCUSSION

We have computed $\rho'(0),\rho^{(3)}(0)$ for the neon atom from the near-Hartree-Fock wave functions of Clementi and Roetti [13], which are given in terms of Slater-type one-particle functions. We chose not to use the cusp condition [Eq. (5)] for the one-term expansion since the wave function only satisfies this condition approximately [14]. These values are then used to compute one- and two-term asymptotic approximations to the form factor from Eq. (4). Likewise, we have used the respective one- and two-point Gauss-Laguerre quadratures to compute the form factor for large k from Eqs. (10)–(12). Formulas are available to calculate $F(k)$ analytically [6]. Thus we may use these analytical results as a basis for the comparison of the results obtained from Eq. (4) with those obtained from Eqs. (10)–(12). We have presented the relative errors (deviations from the analytical results) from the one-term results of Eqs. (4) and (10)–(12) in Table I and the two-term results in Table II. All calculations were performed in double precision on a SUN 3/50 computer which yields about 15 figures of accuracy. The real parameter α in Eq. (12) was chosen to be seven in method III since the normalization condition $F(0)=N$ (number of electrons) was quite closely held for this value as k approached zero. However, it should be noted [9] that there is no universal value of α that is the best for all values of k.

In Table I we present errors resulting from the one-term expansion in Eq. (4) and the one-point quadrature rules of methods I–III along with the $F(k)$ values for various values of k. Note that the independent variable k and the relative errors in the tables are given on a logarithmic scale to make the behavior of the errors as functions of k more clear. We have included values of k that cannot be considered strictly asymptotic, to illustrate that these methods perform better as k becomes larger. However, it has been shown [9] that correct values may be attained for the small k regions with the use of higher-order quadratures than the ones considered in this paper. The results show that methods I and III perform the best with method III yielding about a half order of magnitude better results than the conventional one-term expansion of Eq. (4). All methods with the exception of method II are seen to perform better as k gets larger and the asymptotic limit is approached. On the other hand, method II does not converge to the analytical values and is the least effective of all the methods presented.

For large values of k one can see the k-dependent relationship of $F(k)$ and the errors resulting from the various methods used. The second column illustrates that $F(k)$ has a $\sim k^{-4}$ behavior for large k in accordance with the leading term in Eq. (4). Since the logarithms of the *rela-*

TABLE I. $F(k)$ and the logarithm of the relative errors[a] of the one-term approximations to $F(k)$ at various values of k. Numbers in square brackets denote powers of 10.

$\log_{10}(k/a_0^{-1})$	$F(k)$ (anal.)	$\eta_1/F(k)$	$E^{\mathrm{I}}_{1,F}/F(k)$	$E^{\mathrm{II}}_{1,F}/F(k)$	$E^{\mathrm{III}}_{1,F}/F(k)$
0.00	8.6362[0]	4.5582[0]	3.0067[0]	−2.9740[−1]	−1.0864[−1]
0.50	3.7614[0]	2.9187[0]	1.2058[1]	7.6825[−1]	−1.4176[−2]
1.00	1.2144[0]	1.3930[0]	7.1800[−1]	5.4179[−1]	−1.3312[−1]
1.50	1.5750[−1]	−7.5730[−3]	−3.2409[−1]	−1.2402[0]	−7.8737[−1]
2.00	2.8764[−3]	−1.0672[0]	−1.2564[0]	−3.6085[−1]	−1.5639[0]
2.50	3.0966[−5]	−2.0732[0]	−2.2506[0]	−3.2686[−1]	−2.5419[0]
3.00	3.1201[−7]	−3.0738[0]	−3.2500[0]	−3.2362[−1]	−3.5397[0]
3.50	3.1225[−9]	−4.0739[0]	−4.2500[0]	−3.2330[−1]	−4.5395[0]
4.00	3.1227[−11]	−5.0739[0]	−5.2500[0]	−3.2327[−1]	−5.5395[0]
4.50	3.1228[−13]	−6.0739[0]	−6.2500[0]	−3.2327[−1]	−6.5395[0]
5.00	3.1228[−15]	−7.0739[0]	−7.2500[0]	−3.2327[−1]	−7.5395[0]
5.50	3.1228[−17]	−8.0739[0]	−8.2500[0]	−3.2327[−1]	−8.5395[0]
6.00	3.1228[−19]	−9.0739[0]	−9.2500[0]	−3.2327[−1]	−9.5395[0]
6.50	3.1228[−21]	−1.0074[1]	−1.0250[1]	−3.2327[−1]	−1.0539[1]
7.00	3.1228[−23]	−1.1074[1]	−1.1250[1]	−3.2327[−1]	−1.1540[1]
7.50	3.1228[−25]	−1.2074[1]	−1.2251[1]	−3.2327[−1]	−1.2539[1]
8.00	3.1228[−27]	−1.307[1]	−1.325[1]	−3.2327[−1]	−1.352[1]
8.50	3.1228[−29]	−1.40[1]	−1.42[1]	−3.2327[−1]	−1.5[1]
9.00	3.1228[−31]	−1.5[1]	−1.5[1]	−3.2327[−1]	−1.5[1]
9.50	3.1228[−33]	−1.5[1]	−1.5[1]	−3.2327[−1]	−1.5[1]
10.0	3.1228[−35]	−1.5[1]	−1.5[1]	−3.2327[−1]	−1.5[1]

[a]Note that the logarithms of all relative errors with an absolute value $\leq 10^{-14.5}$ are reported as −1.5[1].

tive errors, i.e., $\log_{10}[\eta_j/F(k)]$, $\log_{10}[E^M_{N,F}/F(k)]$ are reported, we may surmise that the error η_1 taken from the expansion in Eq. (4) is k^{-6} dependent, i.e., the order of magnitude of the first neglected term. This same k^{-6} dependence is observed for methods I and III which may be explained via Eqs. (13) and (15). Take, for example, the error term for method I in Eq. (13). For very large k, we may consider the Taylor (MacLaurin) expansion of $f^{(2N)}$ around zero argument. Since the remaining factors in Eq. (13) are real we are only interested in the imaginary terms of the expansion. It is easy to show that the imaginary terms are odd inverse powers of k starting with k^{-1}. Since we are in the large k regime it is a good assumption that the first (k^{-1}) term will dominate over

TABLE II. $F(k)$ and the logarithm of the relative errors[a] of the two-term approximations to $F(k)$ at various values of k. Numbers in square brackets denote powers of 10.

$\log_{10}(k/a_0^{-1})$	$F(k)$ (anal.)	$\eta_2/F(k)$	$E^{\mathrm{I}}_{2,F}/F(k)$	$E^{\mathrm{II}}_{2,F}/F(k)$	$E^{\mathrm{III}}_{2,F}/F(k)$
0.00	8.6362[0]	7.4838[0]	2.9179[0]	4.1619[−1]	−4.0667[−1]
0.50	3.7614[0]	4.8401[0]	1.3709[1]	8.9624[−1]	−2.9527[−1]
1.00	1.2144[0]	2.2838[0]	3.4973[−1]	2.1905[−1]	−1.3367[0]
1.50	1.5750[−1]	−1.6123[−1]	−1.1755[0]	−1.0952[0]	−2.3941[0]
2.00	2.8764[−3]	−2.2272[0]	−2.7925[0]	−2.0182[0]	−3.4147[0]
2.50	3.0966[−5]	−4.2334[0]	−4.7605[0]	−2.9258[0]	−5.3431[0]
3.00	3.1201[−7]	−6.2340[0]	−6.7573[0]	−3.9174[0]	−7.3360[0]
3.50	3.1225[−9]	−8.2341[0]	−8.7570[0]	−4.9165[0]	−9.3353[0]
4.00	3.1227[−11]	−1.0234[1]	−1.0757[1]	−5.9164[0]	−1.1335[1]
4.50	3.1228[−13]	−1.2235[1]	−1.2752[1]	−6.9164[0]	−1.331[1]
5.00	3.1228[−15]	−1.42[1]	−1.5[1]	−7.9164[0]	−1.5[1]
5.50	3.1228[−17]	−1.5[1]	−1.5[1]	−8.9164[0]	−1.5[1]
6.00	3.1228[−19]	−1.5[1]	−1.5[1]	−9.9164[0]	−1.5[1]
6.50	3.1228[−21]	−1.5[1]	−1.5[1]	−1.0916[1]	−1.5[1]
7.00	3.1228[−23]	−1.5[1]	−1.5[1]	−1.1916[1]	−1.5[1]
7.50	3.1228[−25]	−1.5[1]	−1.5[1]	−1.2912[1]	−1.5[1]
8.00	3.1228[−27]	−1.5[1]	−1.5[1]	−1.386[1]	−1.5[1]
8.50	3.1228[−29]	−1.5[1]	−1.5[1]	−1.5[1]	−1.5[1]
9.00	3.1228[−31]	−1.5[1]	−1.5[1]	−1.5[1]	−1.5[1]
9.50	3.1228[−33]	−1.5[1]	−1.5[1]	−1.5[1]	−1.5[1]
10.0	3.1228[−35]	−1.5[1]	−1.5[1]	−1.5[1]	−1.5[1]

[a]Note that the logarithms of all relative errors with an absolute value $\leq 10^{-14.5}$ are reported as −1.5[1].

the remaining terms. Thus the overall behavior of $E^{\mathrm{I}}_{1,F}(f,k)$ for large k would be k^{-6} dependent. A similar argument holds for $E^{\mathrm{III}}_{1,F}(f,k)$ in Eq. (15) if we assume that for large k, $[1/(\alpha-ik)]$ behaves as (i/k). Analogously to method I, the Taylor expansion of $f^{(2N)}$ around zero would yield a dominant k^{-1} imaginary term which would give an overall k^{-6} behavior to Eq. (15).

For method II in Eq. (14) the situation is different. As in the case of method III, we assume that $[1/(1-ik)]$ behaves as (i/k). Note that this factor in Eq. (14) is raised to the $(2N+1)$ power which is always odd, thus yielding imaginary values. Therefore we are interested in the real terms that occur in the Taylor expansion of $f^{(2N)}$ around zero. It is again easy to show that the first real term is k independent with subsequent real terms having an even inverse power dependence on k. With the assumption that the k-independent term dominates at large k, we can see that $E^{\mathrm{II}}_{1,F}(f,k)$ will have a k^{-4} dependence. Since $F(k)$ also exhibits a k^{-4} behavior, the relative error should give a constant dependence on k as is indeed the case in Table I. [Note that $f(r)$ in method I differs from $f(r)$ in methods II and III by a factor of e^{r} and $e^{\alpha r}$, respectively.]

The relative performances of the three different methods may be explained in a similar manner. Consider the Taylor expansion around zero, of the integrands $f(iz/k)$, $f(i/(1-ik))$, $f(1/(\alpha-ik))$ as defined in Eqs. (10)–(12) for the three different methods, assuming that $1/1-ik$, $1/\alpha-ik$ behave as i/k for large k. For $f(z)=\rho(z)$ and k large,

$$f\left[\frac{iz}{k}\right]\simeq\rho(0)+\rho'(0)\left[\frac{iz}{k}\right]-\frac{\rho^{(2)}(0)}{2!}\left[\frac{z}{k}\right]^2+\cdots\quad\text{(method I)}\,. \tag{18}$$

For $f(z)=r\rho(z)e^{z}$ and k large,

$$f\left[\frac{iz}{k}\right]\simeq\rho'(0)\left[\frac{iz}{k}\right]-\left[\frac{2\rho(0)+\rho'(0)+\rho^{(2)}(0)}{2!}\right]\times\left[\frac{z}{k}\right]^2+\cdots\quad\text{(method II)}\,. \tag{19}$$

For $f(z)=\rho(z)e^{\alpha z}$ and k large,

$$f\left[\frac{iz}{k}\right]\simeq\rho(0)+[\alpha\rho(0)+\rho'(0)]\left[\frac{iz}{k}\right]-\left[\frac{\alpha^2\rho(0)+2\alpha\rho'(0)+\rho^{(2)}(0)}{2!}\right]\times\left[\frac{z}{k}\right]^2+\cdots\quad\text{(method III)}\,. \tag{20}$$

Also, substitution of the imaginary terms of the expansion in Eq. (18) into Eq. (7), and multiplication by $4\pi/k$, yields the same result as the familiar expansion in Eq. (4). This is equivalent to Watson's technique for asymptotic expansions [3] by expanding the integrand in a power series.

The construction of Gaussian quadrature defines these rules to be exact for polynomials of order $(2N-1)$. This may easily be seen by noting that the error terms in Eqs. (13)–(15) will vanish for a polynomial of order $(2N-1)$ or less. Thus the one-point Gauss-Laguerre rule is exact for polynomials of order one. In this manner consider the Taylor expansions around zero [Eqs. (18)–(20)] up to the linear term including only the imaginary terms for methods I and III and real terms for method II. Clearly since we are using a one-point quadrature we should be able to integrate up to the linear term exactly. For methods I and III, the first imaginary term is linear so we are able to integrate this exactly. On the other hand, the first real term in method II is the quadratic term which falls outside the precision of the one-point quadrature rule. Hence the superiority of methods I and III over method II.

The superiority of method III over method I may be explained by considering the linear term in Eqs. (20) and (18), respectively, which are represented exactly by the one-point rule. The additional $\alpha\rho(0)$ term present in method III may be considered as approximately representing the numerical values of the higher-order terms that lie outside the precision of the quadrature rule. Thus method III is superior to method I. Both methods I and III are seen to perform better as k becomes larger since we are approaching zero and the approximation to $f(i/k)$ by a Taylor series up to the linear term becomes better. It is interesting to note that substitution of the linear term of the Taylor expansion for method I into Eq. (10) and noting that $z_1=2$, $\omega_1=1$ for $N=1$, will give the same result for the asymptotic form factor as the first term in the familiar expansion in Eq. (4). Method I is superior to the traditional method of Eq. (4) since we are integrating over $f(iz/k)$ and not just the linear term of its expansion, i.e., we consider all terms of the expansion. This implicit integration of all higher-ordered terms, although not necessarily exact by definition of the quadrature rule, is the source of superiority of method I over the traditional expansion since the error in the quadrature rule would be less than the complete neglect of the integral.

Similar results are observed from the two-term expansion and two-point quadratures in Table II. It is again methods I and III that are shown to yield the least error with method III showing about one order of magnitude superiority over the two-term expansion of Eq. (4) for smaller values of k. For these methods the correct values of $F(k)$ are approached at smaller values than in the one-point case since the integrals of the third-order terms of the Taylor expansions are exact, which makes the approximation to $f(iz/k)$ better at smaller values of k. Thus the superiority of these methods over Eq. (4) is even greater for the two-point case. For very large values of k, the superiority diminishes as we approach the machine precision. Note also that the absolute errors exhibit $\sim k^{-8}$ behavior in accordance with the magnitude of the first neglected term in Eq. (4) and the expressions in Eqs. (13) and (15). The two-point rule of method II, while the

least effective of the three methods, yields better results and does converge to the analytical results, in contrast to the one-point rule, as we go farther into the asymptotic regions. This method performs better for the two-point rule since the quadratic term of the Taylor expansion in Eq. (17) is now within the precision of this rule. It is inferior to the traditional method since its absolute error exhibits $\sim k^{-6}$-dependent behavior as expected from Eq. (14) in contrast to the k^{-8} behavior of the traditional method.

It is interesting to compare the one-point rule of methods I and III in Table I with the two-point rule of method II in Table II. The linear term of method I has a contribution from $\rho'(0)$ while method III has a contribution from $\rho(0)$ as well. However, the quadratic term of method II has contributions from $\rho^{(2)}(0)$ as well. In a sense, the two-point rule of method II is thus able to describe the behavior of the density at the origin better than the one-point rules of the other two methods due to the inclusion of $\rho^{(2)}(0)$ in the quadratic term which is treated exactly by the two-point rule. Thus we would expect it to perform better than the other two methods as is evident from a comparison of the two tables.

Methods I and III are better than the traditional method for the two-point case since we implicitly include all terms of the Taylor expansion by integrating over $f(iz/k)$, $f(iz/(\alpha-ik))$ instead of just considering a truncated expansion as is the case of the traditional method of Eq. (4). This relative performance of the traditional method to methods I and III should also hold for the higher-order quadratures since the traditional method only considers a finite number of terms while methods I and III implicitly consider all terms.

IV. CONCLUSIONS

We have shown the superiority of one- and two-point Gauss-Laguerre quadratures over the familiar expansion [Eq. (4)] in terms of inverse powers of k and derivatives of the charge density at zero, in yielding asymptotic approximations to the atomic form factor. The quality of the two-point quadratures is even better than the one point, in relation to the familiar one- and two-term expansions, suggesting that methods I and III are converging to the true answer at a faster rate than the corresponding one- and two-term versions of the familiar expansions.

Furthermore, these methods have error formulas which may be formulated in an analytical manner in contrast to the expansion in Eq. (4). Moreover, they do not necessitate the evaluation of higher-order derivatives of the density at zero, but the evaluation of the density at points in the complex plane. On the other hand, it must be mentioned that if one is interested in higher-order terms in Eq. (4) one can simply add the new terms to the ones previously calculated. This is not the case for the methods presented here since the quadrature abscissas and weights are different for different orders of quadratures. Thus one would have to evaluate all new terms in Eqs. (10)–(12).

The restrictions on these methods are that $f(r)$ be readily evaluable at complex arguments and be analytic in the respective complex domain. Furthermore, the Fourier transform to be evaluated has to possess an asymptotic behavior analogous to Eq. (4). This excludes functions whose odd-order derivatives vanish at zero, e.g., Gaussian-type functions. Another class for which Eq. (4) is invalid are those functions that do not have a simple expansion in r around the origin [2]. However, for the large class of trial functions of exponential type, such as the one used in this work, Eq. (4) is valid. The applicability of method III to functions with nonexponential behavior depends on the extent with which a Gauss-Laguerre quadrature is able to effectively perform integrations over such functions, and would have to be evaluated individually. The demonstrated effectiveness coupled with the availability of useful error formulas makes these methods attractive for the asymptotic approximation of Fourier transforms.

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