J Math Chem (2012) 50:17–81
DOI 10.1007/s10910-011-9914-4

REVIEW

On the mathematical nature of Guseinov's rearranged one-range addition theorems for Slater-type functions

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Received: 25 November 2010 / Accepted: 8 September 2011 / Published online: 6 October 2011

Abstract Starting from one-range addition theorems for Slater-type functions, which are expansion in terms of complete and orthonormal functions based on the generalized Laguerre polynomials, Guseinov constructed addition theorems that are expansions in terms of Slater-type functions with a common scaling parameter and integral principal quantum numbers. This was accomplished by expressing the complete and orthonormal Laguerre-type functions as finite linear combinations of Slater-type functions and by rearranging the order of the nested summations. Essentially, this corresponds to the transformation of a Laguerre expansion, which in general only converges in the mean, to a power series, which converges pointwise. Such a transformation is not necessarily legitimate, and this contribution discusses in detail the difference between truncated expansions and the infinite series that result in the absence of truncation.

Keywords Slater-type function · Addition theorem · Laguerre expansion · Power series

1 Introduction

Electronic structure theory is a highly interdisciplinary research topic which benefited greatly from interactions with related scientific disciplines. It is generally agreed that molecular electronic structure calculations only became feasible because of the spectacular advances in computer hard and software. But we must not forget that advances in pure and applied mathematics also played a crucial role.

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While mathematicians and theoretical physicists have a venerable tradition of a close and mutually beneficial collaboration, the same cannot be said about the interaction of mathematicians and theoretical chemists (my personal views on this topic are explained in [208]). This is highly deplorable. Theoretical chemists could—and should—learn more about new mathematical concepts or powerful numerical techniques. On the other hand, electronic structure theory offers quite a few challenging mathematical and computational problems which could serve as a valuable source of inspiration for mathematicians. A more extensive collaboration would certainly be mutually beneficial (see for example [208, Sect. 8] and references therein).

Advances in mathematics are particularly important for molecular multicenter integrals, which occur in molecular calculations on the basis of the Hartree–Fock–Roothaan equations [30,136,167] and also in other approximation schemes. The efficient and reliable evaluation of the three- and six-dimensional molecular integrals, which are notoriously difficult in the case of the physically better motivated exponentially decaying basis functions, is one of the oldest mathematical and computational problems of molecular electronic structure theory. In spite of heroic efforts of numerous researchers, no completely satisfactory solution has been found yet, and we have to continue searching for more powerful mathematical and computational techniques. A review of the older literature can be found in articles by Browne [18], Dalgarno [23], Harris and Michels [135], and Huzinaga [140].

Quantum mechanics only determines which types of molecular integrals we have to evaluate, but how we manipulate and ultimately evaluate them is a mathematical problem. Thus, for a researcher working on multicenter integrals, physical insight and a good knowledge of quantum mechanics is actually less important than the ability of skillfully manipulating complicated expressions involving special functions and a profound knowledge of advanced mathematical techniques with a special emphasis on numerics.

The evaluation of multicenter integrals is difficult because of the different centers occurring in their integrands. This effectively prevents the straightforward separation of the three- and six-dimensional integrals into products of simpler integrals. A promising computational strategy requires that we find a way of separating the integration variables at tolerable computational costs.

Principal tools, which can accomplish a separation of integration variables, are so-called addition theorems. These are special series expansions of a function $f(\boldsymbol{r} \pm \boldsymbol{r}')$ with $\boldsymbol{r}, \boldsymbol{r}' \in \mathbb{R}^3$ in terms of other functions that only depend on either $\boldsymbol{r}$ or $\boldsymbol{r}'$. The basic features of these fairly complicated series expansions are reviewed in Sect. 2. A much more detailed treatment will be given in my forthcoming review [211].

Infinite series expansions are among the most fundamental mathematical tools with countless applications not only in mathematics, but also in science and engineering. Nevertheless, a mathematically rigorous use of infinite series is not necessarily an easy thing. Many scientists have a highly cavalier attitude when it comes to questions of existence and convergence. Since mathematics is ultimately used to describe natural phenomena, it is tempting to believe that nature guarantees that all intermediate mathematical manipulations are legitimate. Needless to say that such an attitude is overly optimistic and can easily have catastrophic consequences.

Strictly speaking, an infinite series is a meaningless object unless we specify its convergence type—for example pointwise convergence, convergence in the mean, or even distributional or weak convergence—and provide convincing evidence that this series converges according to its specified type of convergence. It is important to take into account that different convergence types of series expansions imply different mathematical properties with different advantages and disadvantages. This applies also to addition theorems. As discussed in my forthcoming review [211], the different convergence types of addition theorems may well provide the most useful characterization of their properties.

Slater-type functions were originally introduced by Slater [178,179] to provide computationally convenient analytical approximations to numerically determined solutions of effective one-particle Schrödinger equations. In unnormalized form, they can be expressed as follows:

$$\chi_{N,L}^{M}(\beta, \boldsymbol{r}) = (\beta r)^{N-L-1}\, \mathrm{e}^{-\beta r}\, \mathcal{Y}_{L}^{M}(\beta \boldsymbol{r}) = (\beta r)^{N-1}\, \mathrm{e}^{-\beta r}\, Y_{L}^{M}(\boldsymbol{r}/r). \tag{1.1}$$

Here, $\beta > 0$ is a scaling parameter, $\mathcal{Y}_{L}^{M}(\beta \boldsymbol{r}) = (\beta r)^{L} Y_{L}^{M}(\boldsymbol{r}/r)$ is a regular solid harmonic and $Y_{L}^{M}(\boldsymbol{r}/r)$ is a surface spherical harmonic (in my own work, I have always used the phase condition of Condon and Shortley [21, Eqs. (6) and (9) on p. 115]). By a slight abuse of language, the index N is frequently called principal quantum number. In most, but not in all cases N is a positive integer satisfying $N \geq L + 1$.

Because of the importance of Slater-type functions as basis functions in atomic and molecular electronic structure calculations, it is not surprising that there is an extensive literature on their notoriously difficult multicenter integrals in general as well as on their addition theorems in special. A reasonably complete bibliography on their addition theorems would be beyond the scope of this article. Let me just mention two classic articles by Barnett and Coulson [6] and by Löwdin [153], respectively, which have inspired many other researchers.

As discussed in more detail in Sect. 3, Guseinov [41–44,46] derived so-called one-range addition theorems for Slater-type functions with integral and nonintegral principal quantum numbers. He expanded Slater-type functions $\chi_{N,L}^{M}(\beta, \boldsymbol{r} \pm \boldsymbol{r}')$ in terms of the functions $\{{}_{k}\Psi_{n,\ell}^{m}(\gamma, \boldsymbol{r})\}_{n,\ell,m}$, which are complete and orthonormal in certain Hilbert spaces and which are defined in (2.13). The radial parts of these functions are based on the generalized Laguerre polynomials whose most inportant properties are reviewed in Appendix D.

On the basis of the approach developed in [41–44,46], Guseinov et al. produced an amazing number of articles on addition theorems and related topics [40,45,47–49,51–53,56–74,76–103,107,108,111–119,121–134].

The immediate reason for writing this article is a one-center expansion constructed and applied by Guseinov and Mamedov [122]. They expanded a Slater-type function $\chi_{N,L}^{M}(\beta, \boldsymbol{r})$ with an in general nonintegral principal quantum number $N \in \mathbb{R} \backslash \mathbb{N}$ in terms of Slater-type functions $\{\chi_{n,L}^{M}(\gamma, \boldsymbol{r})\}_{n=L+1}^{\infty}$ with integral principal quantum numbers $n \in \mathbb{N}$ and an in general different common scaling parameter $\gamma \neq \beta > 0$ [122, Eq. (4)]. This expansion was used by Guseinov and Mamedov for the construction of what they called series expansions for overlap integrals of Slater-type functions with nonintegral principal quantum numbers in terms of overlap integrals of Slater-type functions with integral principal quantum numbers.

For Guseinov et al., who had done a lot of work on Slater-type functions with nonintegral principal quantum numbers [45,50,52,54,55,61,68,72,75,77,80,82–84,90,91, 93–96,98,102–106,109–117,119–123,131], such an expansion would be extremely useful: Slater-type functions with nonintegral principal quantum numbers could be replaced by Slater-type functions with integral principal quantum numbers whose multicenter integrals can be evaluated (much) more easily.

It is, however, trivially simple to show that such a one-center expansion, which in my notation can be written as follows,

$$\chi_{N,L}^{M}(\beta, \boldsymbol{r}) = \sum_{n=L+1}^{\infty} \mathbb{X}_n^{(N,L)}(\beta, \gamma)\, \chi_{n,L}^{M}(\gamma, \boldsymbol{r}), \quad N \in \mathbb{R}, \tag{1.2}$$

only exists if the principal quantum number N is a positive integer satisfying $N \geq L+1$. If N is nonintegral or zero, i.e., if $N \in \mathbb{R} \backslash \mathbb{N}$, this expansion does not exist. The nonexistence of this expansion also played a major role in my discussion [207, Sect. 7] of Guseinov's treatment of one-range addition theorems for Slater-type functions. However, my discussion in [207, Sect. 7] was incomplete. Its scope is extended considerably by this article.

From a methodological point of view, we only have to utilize the obvious fact that an expansion of $\chi_{N,L}^{M}(\beta, \boldsymbol{r})$ in terms of Slater-type functions $\{\chi_{n,L}^{M}(\gamma, \boldsymbol{r})\}_{n=L+1}^{\infty}$ with integral principal quantum numbers n and a common scaling parameter $\gamma > 0$ is nothing but a power series expansion of $\exp(\gamma r) \chi_{N,L}^{M}(\beta, \boldsymbol{r})$ about $r = 0$ in disguise. This interpretation of the expansion (1.2) offers some valuable insight. Relatively little is known about the convergence and existence of expansions in terms of Slater-type functions $\{\chi_{n,L}^{M}(\gamma, \boldsymbol{r})\}_n$, but it is normally comparatively easy to decide whether such a corresponding power series expansion about $r = 0$ exists and for which values of r it converges.

We can convert the expansion (1.2) to a more transparent one-dimensional radial problem by canceling the spherical harmonics. Then, the right-hand side of (1.2) can be converted to a power series in γr by multiplying either side of (1.2) by $\exp(\gamma r)$:

$$\mathrm{e}^{(\gamma-\beta)r}\, (\beta r)^{N-1} = \sum_{n=L+1}^{\infty} \mathbb{X}_n^{(N,L)}(\beta, \gamma)\, (\gamma r)^{n-1}. \tag{1.3}$$

Let us now assume that the principal quantum number N is a positive integer satisfying $N \geq L+1$. Then we only have to replace the exponential on the left-hand side of (1.3) by its power series to obtain:

$$(\beta/\gamma)^{N-1} \sum_{\nu=0}^{\infty} \frac{[1-(\beta/\gamma)]^{\nu}}{\nu!} (\gamma r)^{N+\nu-1} = \sum_{n=L+1}^{\infty} \mathbb{X}_n^{(N,L)}(\beta, \gamma) (\gamma r)^{n-1}. \tag{1.4}$$

Comparison of the coefficients of equal powers yields explicit expressions for the coefficients $\mathbb{X}_n^{(N,L)}(\beta, \gamma)$.

But if the principal quantum number N is not a positive integer, the matching of the coefficients of equal powers does not work: On the left-hand side of (1.4) there are either only nonintegral powers or some negative powers, and on the right-hand side there are only integral and nonnegative powers. Accordingly, a power series expansion for $\mathrm{e}^{(\gamma-\beta)r}\,(\beta r)^{N-1}$ can only exist if N is a positive integer satisfying $N \geq L+1$.

Since every power series is also a Taylor series for some function (see for example [155]), the expansion (1.2) can also be derived by doing a Taylor expansion of $\exp\bigl((\gamma-\beta)r\bigr)(\beta r)^{N-1}$ about $r = 0$, yielding the same conclusions. Fractional or nonintegral powers r^{α} with $\alpha \in \mathbb{R}\backslash\mathbb{N}_0$ and thus also $\exp([\gamma-\beta]r)r^{N-1}$ with $N \in \mathbb{R}\backslash\mathbb{N}$ do not have continuous derivatives of arbitrary order at $r = 0$. Thus, $N \in \mathbb{R}\backslash\mathbb{N}$ implies that the leading expansion coefficients $\mathbb{X}_n^{(N,L)}(\beta, \gamma)$ with indices $n \leq \lfloor N \rfloor$ are zero, but all the remaining coefficients with indices $n > \lfloor N \rfloor$ are infinite in magnitude. Here, $\lfloor N \rfloor$ stands for the integral part of N.

The nonexistence problems mentioned above are a direct consequence of the obvious fact that the radial part of a Slater-type function with a nonintegral or negative principal quantum number is not analytic in the sense of complex analysis at $r = 0$. This is so elementary that it is hard to understand why nobody had noticed the nonexistence of the expansion (1.2) for $N \in \mathbb{R}\backslash\mathbb{N}$ before.

In spite of the nonexistence of (1.2) for $N \in \mathbb{R}\backslash\mathbb{N}$, Guseinov and Mamedov [122] had used their version of this one-center expansion for numerical purposes and presented apparently meaningful numerical results for overlap and other, closely related integrals of Slater-type functions with nonintegral principal quantum numbers in [122, Tables 1 and 2].

If these numerical results are genuine—which I assume—then there is only one logically satisfactory conclusion: Contrary to their claim (see the text before Eq. (4) of [122]), Guseinov and Mamedov did not use *expansions* involving an *infinite* number of Slater-type functions with integral principal quantum numbers, which—as discussed above—do not exist for $N \in \mathbb{R}\backslash\mathbb{N}$. Instead, they only employed some *approximations* consisting of a *finite* number of terms and extrapolated—albeit incorrectly—that these finite approximations remain meaningful in the limit of an infinite number of terms.

As is well known from the mathematical literature, truncated expansions, which are approximations consisting of a finite number of terms, may have mathematical properties that are not at all related to those of a complete expansion consisting of an infinite number of terms. In particular, it can happen that a truncated expansion can be mathematically meaningful as well as numerically useful, although its limit as an expansion of infinite length does not exist (see also Appendix E, where the semiconvergence of certain infinite series is reviewed briefly). It is the purpose of this article to investigate this as well as some closely related question.

The one-center expansion used by Guseinov and Mamedov [122, Eq. (4)] was originally derived by Guseinov [46, Eq. (21)] as the one-center limit of a class of addition theorems for Slater-type functions [46, Eq. (15)]. Guseinov's approach is based on one-range addition theorems for Slater-type functions, which are expansions in terms of Guseinov's Laguerre-type functions $\{{}_k\Psi_{n,\ell}^{m}(\gamma, \boldsymbol{r})\}_{n,\ell,m}$. These functions are then replaced by Slater-type functions according to (3.2). Ultimately, this yields addition theorems that are expansions in terms of Slater-type functions with integral principal quantum numbers. Unfortunately, the derivation of these expansions is fairly difficult and involves manipulations whose validity is not at all obvious [204,206,207].

In view of the amazing number of articles on addition theorems and related topics published by Guseinov et al. [40–49,51–53,56–74,76–103,107,108,111–119,121–134], such an investigation should be of some principal interest.

This article sheds some light on certain more subtle differences of orthogonal and nonorthogonal expansions which—although in principle known—are often not sufficiently appreciated and taken into account in the literature on electronic structure calculations.

In Sect. 2, basic features of both one-range and two-range addition theorems are reviewed. Section 3 discusses Guseinov's derivation of expansions in terms of Slater-type functions by rearranging his one-range addition theorems for Slater-type functions with a special emphasis on numerical stability issues. From a mathematical point of view, Guseinov's treatment of addition theorems ultimately boils down to the transformation of a Laguerre series to a power series. The most important properties of this transformation, whose theory had recently been formulated in [207], are reviewed in Sect. 4.

The central results of this manuscript are presented in Sects. 5–7. In Sect. 5 it is shown that the transformation formulas described in Sect. 4 fully explain the nonexistence of Guseinov's rearrangements of one-center expansions in the case of nonintegral principal quantum numbers.

In the case of the simpler one-center expansions, which correspond to the Laguerre series (5.2) for z^ρ with $\rho \in \mathbb{R}\backslash\mathbb{N}_0$, this analysis had already been done in [207, Sect. 3]. But my results for the more complicated one-center expansions, which correspond to the Laguerre series (5.1) for $z^\rho \mathrm{e}^{uz}$ with $\rho \in \mathbb{R}\backslash\mathbb{N}_0$, are new. In [207, Sect. 7] it was only stated on the basis of general analyticity principles that the Laguerre series (5.1) cannot exist if $\rho \in \mathbb{R}\backslash\mathbb{N}_0$, but a detailed analysis of the transformation formulas could not be done. At that time I did not know yet the large index asymptotics of some special Gaussian hypergeometric series ${}_2F_1$ which were derived in Sect. 5. These asymptotic expressions make an asymptotic analysis of the transformation formulas possible.

As discussed in more details in Sect. 2, a one-range addition theorem for a function $f(\boldsymbol{r} \pm \boldsymbol{r}')$ provides for all arguments $\boldsymbol{r}, \boldsymbol{r}' \in \mathbb{R}^3$ a *unique* representation of f in *separated* form that is valid for the whole argument set $\mathbb{R}^3 \times \mathbb{R}^3$. Since the one-center limits of Guseinov's rearranged one-range addition theorems do not exist in the important special case of nonintegral principal quantum numbers, it was argued in [207, Sect. 7] that at least some of Guseinov's rearrangements cannot be one-range addition theorems. However, the exact nature of Guseinov's rearrangements was not yet understood in [207].

Because of technical problems, a straightforward analysis of the transformation formulas described in Sect. 4 is not possible in the case of Guseinov's one-range addition theorems, However, in Sect. 6 it is shown that the rearrangement of Guseinov's one-range addition theorems produces two-range addition theorems. This follows at once from the fact that a Slater-type function $\chi_{N,L}^{M}(\beta, \boldsymbol{r} \pm \boldsymbol{r}')$ or equivalently the function $\mathrm{e}^{\gamma r} \chi_{N,L}^{M}(\beta, \boldsymbol{r} \pm \boldsymbol{r}')$ is singular for $\boldsymbol{r} \pm \boldsymbol{r}' = \boldsymbol{0}$.

Section 7 discusses some numerical implications of the results derived in Sects. 5 and 6. The most important result is that rearrangements of Guseinov's truncated one-center expansions are semiconvergent with respect to a variation of the truncation order if the principal quantum number is nonintegral. This follows from the leading order asymptotic approximation (7.2).

This article is concluded by a summary and an outlook in Sect. 8. Appendices A–E review general aspects of series expansions, the largely complementary features of power series and orthogonal expansions, the for our purposes most important properties of generalized Laguerre polynomials, and semiconvergent expansions.

2 Basic features of addition theorems

Addition theorems are series expansions of a function $f(\boldsymbol{r} \pm \boldsymbol{r}')$ with $\boldsymbol{r}, \boldsymbol{r}' \in \mathbb{R}^3$ in terms of other functions that depend only on either $\boldsymbol{r}$ or $\boldsymbol{r}'$. Because of the completeness and the convenient orthogonality properties of the (surface) spherical harmonics $Y_\ell^m(\theta, \phi)$, it is customary to express the angular parts of addition theorems in terms of spherical harmonics whose arguments correspond to the solid angles $\boldsymbol{r}/r$ and $\boldsymbol{r}'/r'$, respectively.

In atomic and molecular electronic structure theory, we are predominantly interested in addition theorems for functions

$$F_\ell^m(\boldsymbol{r}) = f_\ell(r)\, Y_\ell^m(\boldsymbol{r}/r), \tag{2.1}$$

which can be factored into a radial part $f_\ell(r)$ multiplied by a surface spherical harmonic. In the language of angular momentum theory, such a function $F_\ell^m(\boldsymbol{r})$ is an irreducible spherical tensor with a fixed rank $\ell \in \mathbb{N}_0$.

The best known and probably also the most simple addition theorem of such an irreducible spherical tensor is the Laplace expansion of the Coulomb or Newton potential $1/|\boldsymbol{r} \pm \boldsymbol{r}'|$. As discussed in Hobson's classic book [138, §11 on pp. 16–17], the mathematical tools needed for the construction of this addition theorem were developed by Laplace and Legendre already in the late 18th century. In modern notation, the Laplace expansion can be expressed as follows:

$$\begin{gathered}\frac{1}{|\boldsymbol{r} \pm \boldsymbol{r}'|} = 4\pi \sum_{\lambda=0}^{\infty} \frac{(\mp 1)^\lambda}{2\lambda+1} \frac{r_<^\lambda}{r_>^{\lambda+1}} \sum_{\mu=-\lambda}^{\lambda} \left[Y_\lambda^\mu(\boldsymbol{r}_</r_<)\right]^* Y_\lambda^\mu(\boldsymbol{r}_>/r_>), \\ |\boldsymbol{r}_<| = \min(r, r'), \quad |\boldsymbol{r}_>| = \max(r, r'). \end{gathered}\tag{2.2}$$

The Laplace expansion is the simplest prototype for a large class of addition theorems that possess a characteristic two-range form. Numerous techniques for the derivation of two-range addition theorems are described in the literature. With the possible exception of the so-called Fourier transform method advocated almost simultaneously but independently by Ruedenberg [168] and Silverstone [177], they are all related to power series expansions in one way or the other.

For example, the Laplace expansion (2.2) can be derived easily with the help of the generating function of the Legendre polynomials $P_n(x)$ [154, p. 232]:

$$\left[1 - 2xt + t^2\right]^{-1/2} = \sum_{n=0}^{\infty} P_n(x)\, t^n, \quad -1 < x < 1, \quad |t| < 1. \tag{2.3}$$

Obviously, this generating function is nothing but a power series expansion about $t = 0$. For the derivation of the Laplace expansion (2.2), we only need the so-called spherical harmonic addition theorem (see for example [191, Eq. (1.2-3a)])

$$P_\ell(\cos\theta) = \frac{4\pi}{2\ell+1} \sum_{m=-\ell}^{\ell} \left[Y_\ell^m(\boldsymbol{u}/u)\right]^* Y_\ell^m(\boldsymbol{v}/v), \quad \cos\theta = \frac{\boldsymbol{u}\cdot\boldsymbol{v}}{uv}. \tag{2.4}$$

The two-range form of the Laplace expansion (2.2) is necessary to ensure convergence, because the generating function (2.3) converges only for $|t| < 1$. Thus, the Laplace expansion converges *pointwise* for $r_</r_> < 1$ and diverges for $r_</r_> > 1$.

The use of generating functions of the Gegenbauer polynomials, which generalize the generating function (2.3) of the Legendre polynomials, for the construction of addition theorems of spherically symmetric functions will be discussed briefly in Sect. 6. The two-range forms of these addition theorems follow from the convergence conditions of the corresponding generating functions which are nothing but special power series expansions, usually in the variable r/r' or more precisely in $r_</r_>$.

The most principal approach for the construction of pointwise convergent addition theorems consists in interpreting such an addition theorem as a three-dimensional Taylor expansion (see for example [12, p. 181]):

$$f(\boldsymbol{r} \pm \boldsymbol{r}') = \sum_{n=0}^{\infty} \frac{(\boldsymbol{r}\cdot\nabla')^n}{n!} f(\pm\boldsymbol{r}') = \mathrm{e}^{\boldsymbol{r}\cdot\nabla'} f(\pm\boldsymbol{r}'). \tag{2.5}$$

Thus, the translation operator $\mathrm{e}^{\boldsymbol{r}\cdot\nabla'} = \mathrm{e}^{x\partial/\partial x'}\mathrm{e}^{y\partial/\partial y'}\mathrm{e}^{z\partial/\partial z'}$ generates $f(\boldsymbol{r} \pm \boldsymbol{r}')$ by constructing a three-dimensional Taylor expansion of f about $\pm\boldsymbol{r}'$ with shift vector $\boldsymbol{r}$. Since the variables $\boldsymbol{r}$ and $\boldsymbol{r}'$ are separated, the series expansion (2.5) is indeed an addition theorem.

Of course, the series expansion (2.5) tacitly assumes that $f(\pm\boldsymbol{r}')$ possesses continuous derivatives of arbitrary order with respect to the Cartesian components of its argument $\pm\boldsymbol{r}' = \pm(x', y', z')$. Thus, f has to be *analytic* at $\pm\boldsymbol{r}'$, which guarantees that the series expansion (2.5) converges at least for sufficiently small $|\boldsymbol{r}| > 0$. Eventual singularities of f determine for which values of the shift vector $\boldsymbol{r}$ the three-dimensional Taylor expansion (2.5) converges.

We could also expand f about $\boldsymbol{r}$ and use $\pm\boldsymbol{r}'$ as the shift vector. This would produce an addition theorem for $f(\boldsymbol{r} \pm \boldsymbol{r}')$ in which the roles of $\boldsymbol{r}$ and $\boldsymbol{r}'$ are interchanged. Both approaches are mathematically legitimate and equivalent if f is analytic at $\boldsymbol{r}$, $\boldsymbol{r}'$, and $\boldsymbol{r} \pm \boldsymbol{r}'$ for essentially arbitrary vectors $\boldsymbol{r}, \boldsymbol{r}' \in \mathbb{R}^3$. This is normally not true. Many of the functions, that are of interest in the context of molecular electronic structure calculations, have a singularity at the origin. Obvious examples are the Coulomb potential, which has a pole at the origin, or the commonly used exponentially decaying functions as for example Slater-type functions, which have a branch point singularity at the origin.

Accordingly, for the addition theorem of a function $f(\boldsymbol{r} \pm \boldsymbol{r}')$, which is singular for $\boldsymbol{r} \pm \boldsymbol{r}' = \mathbf{0}$, the natural variables are not $\boldsymbol{r}$ and $\boldsymbol{r}'$, but the vectors $\boldsymbol{r}_<$ and $\boldsymbol{r}_>$ satisfying $|\boldsymbol{r}_<| = \min(r, r')$ and $\boldsymbol{r}_>| = \max(r, r')$. This implies that the expansion formula (2.5) should be rewritten as follows:

$$f(\boldsymbol{r}_< \pm \boldsymbol{r}_>) = \sum_{n=0}^{\infty} \frac{(\boldsymbol{r}_< \cdot \nabla_>)^n}{n!} f(\pm \boldsymbol{r}_>) = \mathrm{e}^{\boldsymbol{r}_< \cdot \nabla_>} f(\pm \boldsymbol{r}_>). \tag{2.6}$$

In this way, the convergence of the three-dimensional Taylor expansion is guaranteed provided that f is analytic everywhere with the possible exception of the origin.

From a practical point of view, the translation operator $\mathrm{e}^{\boldsymbol{r}_< \cdot \nabla_>}$ does not seem to be a particularly useful analytical tool. In electronic structure theory, we are usually interested in addition theorems of irreducible spherical tensors of the type of (2.1), which are defined in terms of the spherical polar coordinates r, θ, and ϕ. Differentiating such an irreducible spherical tensor with respect to the Cartesian components of $\boldsymbol{r}_> = (x_>, y_>, z_>)$ would lead to extremely messy expressions and to difficult technical problems. Thus, it is a seemingly obvious conclusion that the translation operator $\mathrm{e}^{\boldsymbol{r}_< \cdot \nabla_>}$ only provides a formal solution to the problem of separating the variables $\boldsymbol{r}_<$ and $\boldsymbol{r}_>$ of a function $f(\boldsymbol{r}_> \pm \boldsymbol{r}_>)$. Nevertheless, this conclusion is wrong.

The crucial step, which ultimately makes the Taylor expansion method practically useful, is the expansion of the translation operator $\mathrm{e}^{\boldsymbol{r}_< \cdot \nabla_>}$ in terms of differential operators that are irreducible spherical tensors with a fixed rank $\ell \in \mathbb{N}_0$:

$$\mathrm{e}^{\boldsymbol{r}_< \cdot \nabla_>} = 2\pi \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} \left[\mathcal{Y}_\ell^m(\boldsymbol{r}_<)\right]^* \mathcal{Y}_\ell^m(\nabla_>) \sum_{k=0}^{\infty} \frac{r_<^{2k} \nabla_>^{2k}}{2^{\ell+2k} k! (1/2)_{\ell+k+1}}. \tag{2.7}$$

Here, $\mathcal{Y}_\ell^m(\nabla)$ is the so-called spherical tensor gradient operator which is obtained by replacing the Cartesian components of $\boldsymbol{r} = (x, y, z)$ by the Cartesian components of $\nabla = (\partial/\partial x \partial/\partial y, \partial/\partial z)$ in the explicit expression of the solid harmonic $\mathcal{Y}_\ell^m(\boldsymbol{r}) = r^\ell Y_\ell^m(\boldsymbol{r}/r)$ which is a homogeneous polynomial of degree ℓ. More details as well as numerous references can be found in [202, Sect. 2].

It seems that the expansion (2.7) was first published by Santos [173, Eq. (A.6)], who emphasized that this expansion should be useful for the derivation of addition theorems, but he apparently never used it for that purpose.

In [199,201] or in [202, Sect. 7] it was shown that two-range addition theorems of irreducible spherical tensors are nothing but rearranged three-dimensional Taylor expansions about $\pm \boldsymbol{r}_>$ with shift vector $\boldsymbol{r}_<$. Such an expansion converges pointwise and uniformly in the interior of suitable subsets of $\mathbb{R}^3 \times \mathbb{R}^3$ whose boundaries are defined by the singularities of the function which is to be expanded. If the function under consideration has a singularity for $\boldsymbol{r} \pm \boldsymbol{r}' = \mathbf{0}$, the two-range form of its addition theorem is necessary to guarantee pointwise or even uniform convergence in a suitable neighborhood of the expansion point.

There is a different class of addition theorems based on Hilbert space theory. Let us assume that $\{\varphi_{n,\ell}^m(\boldsymbol{r})\}_{n,\ell,m}$ is a *complete* and *orthonormal* function set in the Hilbert space

$$L^2(\mathbb{R}^3) = \left\{ f : \mathbb{R}^3 \to \mathbb{C} \middle| \int |f(\boldsymbol{r})|^2 \, \mathrm{d}^3\boldsymbol{r} < \infty \right\} \tag{2.8}$$

of functions that are square integrable with respect to an integration over the whole $\mathbb{R}^3$. Since any $f \in L^2(\mathbb{R}^3)$ can be expanded in terms of the complete and orthonormal functions $\{\varphi_{n,\ell}^m(\boldsymbol{r})\}_{n,\ell,m}$, a one-range addition theorem for $f(\boldsymbol{r} \pm \boldsymbol{r}')$ can be formulated as follows:

$$f(\boldsymbol{r} \pm \boldsymbol{r}') = \sum_{n\ell m} C_{n,\ell}^m(f; \pm\boldsymbol{r}') \, \varphi_{n,\ell}^m(\boldsymbol{r}), \tag{2.9a}$$

$$C_{n,\ell}^m(f; \pm\boldsymbol{r}') = \int \left[\varphi_{n,\ell}^m(\boldsymbol{r})\right]^* f(\boldsymbol{r} \pm \boldsymbol{r}') \, \mathrm{d}^3\boldsymbol{r}. \tag{2.9b}$$

The expansion (2.9) is a *one-range* addition theorem since the variables $\boldsymbol{r}$ and $\boldsymbol{r}'$ are completely separated in a unique way independent of the lengths of $\boldsymbol{r}$ and $\boldsymbol{r}'$: The dependence on $\boldsymbol{r}$ is contained in the functions $\varphi_{n,\ell}^m(\boldsymbol{r})$, whereas $\boldsymbol{r}'$ occurs only in the expansion coefficients $C_{n,\ell}^m(f; \pm\boldsymbol{r}')$ which are overlap or convolution-type integrals.

Since the functions $\{\varphi_{n,\ell}^m(\boldsymbol{r})\}_{n,\ell,m}$ are by assumption complete and orthonormal in the Hilbert space $L^2(\mathbb{R}^3)$, the existence of the one-range addition theorem (2.9) as well as its convergence in the mean is guaranteed if $f \in L^2(\mathbb{R}^3)$.

The summation limits in (2.9) depend on the exact definition of the function set $\{\varphi_{n,\ell}^m(\boldsymbol{r})\}_{n,\ell,m}$. Unless explicitly specified, this article tacitly uses the convention

$$\sum_{n\ell m} = \sum_{n=1}^{\infty} \sum_{\ell=0}^{n-1} \sum_{m=-\ell}^{\ell}, \tag{2.10}$$

which is in agreement with the usual convention for the bound state hydrogen eigenfunctions.

It is a typical feature of *all* expansions of Hilbert space elements in terms of function sets, which are complete and orthonormal in this Hilbert space, that they do not necessarily converge pointwise but only in the mean with respect to the norm of the corresponding Hilbert space. As is well known from the mathematical literature, convergence in the mean is weaker than pointwise convergence. Accordingly, expansions of that kind are not necessarily suited for a pointwise representation of a function. However, as discussed in more detail in Sect. 6, we must use a weaker form of convergence if we want construct one-range addition theorems for functions that are singular for $\boldsymbol{r} \pm \boldsymbol{r}' = \boldsymbol{0}$. Moreover, we do not really need the stronger pointwise convergence if we only want to evaluate multicenter integrals with the help of addition theorems.

One-range addition theorems of the kind of (2.9) were constructed by Filter and Steinborn [29, Eqs. (5.11) and (5.12)] and later applied by Kranz and Steinborn [149] and by Trivedi and Steinborn [190]. An alternative derivation of these addition theorems based on Fourier transformation combined with weakly convergent expansions of the plane wave $\exp(\pm i \boldsymbol{p} \cdot \boldsymbol{r})$ with $\boldsymbol{p}, \boldsymbol{r} \in \mathbb{R}^3$ was presented in [194, Sect. 7] and in [139]. A similar approach based on the work of Shibuya and Wulfman [176] was pursued by Novosadov [157, Sect. 3].

As discussed in [204, Sect. 3]), it is also possible to formulate one-range addition theorems that converge with respect to the norm of a *weighted* Hilbert space

$$L^2_w(\mathbb{R}^3) = \left\{ f : \mathbb{R}^3 \to \mathbb{C} \,\middle|\, \int w(\boldsymbol{r}) \, |f(\boldsymbol{r})|^2 \, \mathrm{d}^3 \boldsymbol{r} < \infty \right\}, \tag{2.11}$$

where $w(\boldsymbol{r}) \neq 1$ is a suitable positive weight function. If we assume that $f \in L^2_w(\mathbb{R}^3)$ and that the functions $\{\psi^m_{n,\ell}(\boldsymbol{r})\}_{n,\ell,m}$ are complete and orthonormal in $L^2_w(\mathbb{R}^3)$, then we obtain the following one-range addition theorem [204, Eq. (3.6)]:

$$f(\boldsymbol{r} \pm \boldsymbol{r}') = \sum_{n\ell m} \mathbf{C}^m_{n,\ell}(f, w; \pm \boldsymbol{r}') \, \psi^m_{n,\ell}(\boldsymbol{r}), \tag{2.12a}$$

$$\mathbf{C}^m_{n,\ell}(f, w; \pm \boldsymbol{r}') = \int \left[\psi^m_{n,\ell}(\boldsymbol{r}) \right]^* w(\boldsymbol{r}) \, f(\boldsymbol{r} \pm \boldsymbol{r}') \, \mathrm{d}^3 \boldsymbol{r}. \tag{2.12b}$$

A one-range addition theorem of the type of either (2.9) or (2.12) for a function $f : \mathbb{R}^3 \to \mathbb{C}$ is a mapping $\mathbb{R}^3 \times \mathbb{R}^3 \to \mathbb{C}$. Compared to the better known two-range addition theorems like the Laplace expansion (2.2), which depend on $\boldsymbol{r}$ and $\boldsymbol{r}'$ only indirectly via $\boldsymbol{r}_<$ and $\boldsymbol{r}_>$, one-range addition theorems have the highly advantageous feature that they provide unique infinite series representations of functions $f(\boldsymbol{r} \pm \boldsymbol{r}')$ with separated variables $\boldsymbol{r}$ and $\boldsymbol{r}'$ that are valid for the whole argument set $\mathbb{R}^3 \times \mathbb{R}^3$.

In his k-dependent one-range addition theorems for Slater-type functions and related functions, Guseinov used as a complete and orthonormal set the following class of functions [46, Eq. (1)], which—if the mathematical notation (D.2) for the generalized Laguerre polynomials is used—can be expressed as follows [204, Eq. (4.16)]:

$$\begin{aligned} {}_k\Psi^m_{n,\ell}(\gamma, \boldsymbol{r}) &= \left[\frac{(2\gamma)^{k+3} (n-\ell-1)!}{(n+\ell+k+1)!} \right]^{1/2} \mathrm{e}^{-\gamma r} \, L^{(2\ell+k+2)}_{n-\ell-1}(2\gamma r) \, \mathcal{Y}^m_\ell(2\gamma \boldsymbol{r}), \\ & n \in \mathbb{N}, \quad n \geq \ell+1, \quad k = -1, 0, 1, 2, \ldots, \quad \gamma > 0. \end{aligned} \tag{2.13}$$

The restriction to integral values of $k = -1, 0, 1, 2, \ldots$ is unnecessary. The mathematical definition (D.2) of the generalized Laguerre polynomials $U^{(\alpha)}_n(z)$ permits nonintegral superscripts α. Thus, the condition $k = -1, 0, 1, 2, \ldots$ in (2.13) can be replaced by $k \in [-1, \infty)$. If this is done, one only has to replace the factorial $(n+\ell+k+1)!$ in (2.13) by the gamma function $\Gamma(n+\ell+k+2)$.

These functions are orthonormal with respect to the weight function $w(\boldsymbol{r}) = r^k$ (compare also [46, Eq. (4)]):

$$\int \left[{}_k\Psi_{n,\ell}^{m}(\gamma, \boldsymbol{r}) \right]^* r^k \; {}_k\Psi_{n',\ell'}^{m'}(\gamma, \boldsymbol{r}) \, \mathrm{d}^3\boldsymbol{r} = \delta_{nn'} \, \delta_{\ell\ell'} \, \delta_{mm'} . \tag{2.14}$$

Accordingly, these functions are complete and orthonormal in the weighted Hilbert space

$$L_{r^k}^2(\mathbb{R}^3) = \left\{ f : \mathbb{R}^3 \to \mathbb{C} \, \middle| \, \int r^k |f(\boldsymbol{r})|^2 \mathrm{d}^3\boldsymbol{r} < \infty \right\}, \quad k = -1, 0, 1, 2, \ldots . \tag{2.15}$$

As discussed in the text following [204, Eq. (4.20)], the functions ${}_k\Psi_{n,\ell}^{m}(\gamma, \boldsymbol{r})$ can—depending on the value of the free parameter $k = -1, 0, 1, 2, \ldots$—reproduce several other physically relevant complete and orthonormal function sets.

If we set $k = 0$ in (2.15), we retrieve the Hilbert space $L^2(\mathbb{R}^3)$ of square integrable functions defined by (2.8) which because of the Born interpretation of bound state wave functions is the most natural choice for the representation of effective one-particle wave functions in electronic structure calculations.

For $k \neq 0$, there is, however, a problem since we neither have $L^2(\mathbb{R}^3) \subset L_{r^k}^2(\mathbb{R}^3)$ nor $L_{r^k}^2(\mathbb{R}^3) \subset L^2(\mathbb{R}^3)$. Thus, the Hilbert spaces $L^2(\mathbb{R}^3)$ and $L_{r^k}^2(\mathbb{R}^3)$ are for $k \neq 0$ inequivalent. This applies also to approximation processes which (should) converge with respect to the norms of these Hilbert spaces (see for example [206, Appendix E]).

Conceptually, the derivation of a one-range addition is a triviality. This follows from the obvious fact that an arbitrary Hilbert space element can be expanded in terms of a function set that is complete and orthonormal in this Hilbert space.

Unfortunately, this does not imply that the derivation of a one-range addition theorem is necessarily a simple task. The challenging part is the construction of computationally convenient expressions for the overlap integrals (2.9b) or (2.12b), respectively. In realistic applications, we cannot not tacitly assume that the use of one-range addition theorems in multicenter integrals necessarily leads to rapidly convergent expansions (compare for instance the convergence rates reported by Trivedi and Steinborn [190]). Therefore, we must be able to compute the overlap integrals (2.9b) or (2.12b) both efficiently and reliably even for possibly very large indices.

Let me conclude this Section with some short remarks on the relative advantages and disadvantages of some of the various sets of exponentially decaying function sets that are described in the literature.

The best known and most often used exponentially decaying functions are undoubtedly Slater-type functions (1.1) introduced in [178, 179]. Slater himself had argued that sufficiently accurate approximations to numerically determined solutions of effective one-particle Schrödinger equations can be obtained even if the radial nodes of these solutions are completely ignored [178, p. 57]. Slater's prime concern was not accuracy but analytic simplicity [179, p. 42]. In view of the limited computational resources at that time, Slater's pragmatic attitude certainly made sense.

Because of their remarkably simple structure, Slater-type functions are often considered to be the most basic prototypes of all exponentially decaying functions.

However, the simplicity of Slater-type functions in the coordinate representation is deceptive. Slater-type functions have been used with considerable success in the case of atomic electronic structure calculations, where multicenter integrals do not occur.

But there is considerable evidence that in the case of multicenter integrals it is the simplicity of a function in the momentum representation that really matters. As for example discussed in [216], the Fourier transform of a Slater-type function is a comparatively complicated object having the same level of complexity as the Fourier transform of a bound state hydrogen eigenfunction (see for example [194, Sect. 4]). Therefore, it is certainly worth while to look for alternative exponentially decaying function sets with simpler Fourier transforms and also more convenient properties in multicenter problems.

Inspired by previous work of Shavitt [175, Eq. (55) on p. 15], Steinborn and Filter [182, Eqs. (3.1) and (3.2)] introduced the so-called reduced Bessel function

$$\hat{k}_{\nu}(z) = (2/\pi)^{1/2}\, z^{\nu}\, K_{\nu}(z). \tag{2.16}$$

Here, $K_{\nu}(z)$ is a modified Bessel function of the second kind [154, p. 66]. If the order ν is half-integral, $\nu = m + 1/2$ with $m \in \mathbb{N}_0$, the reduced Bessel function is an exponential multiplied by a terminating confluent hypergeometric series ${}_1F_1$ (see for example [217, Eq. (3.7)]):

$$\hat{k}_{m+1/2}(z) = 2^m\, (1/2)_m\, \mathrm{e}^{-z}\, {}_1F_1(-m; -2m; 2z). \tag{2.17}$$

As discussed in more detail in Sect. 6 or in [208, Sect. 4], Steinborn and Filter became interested in reduced Bessel functions because of a known Gegenbauer-type addition theorem which allowed a simple derivation a two-range addition theorem for reduced Bessel functions with half-integral orders (see for example [182, Eq. (3.4)] or, as an improved version [218, Eq. (5.5)]).

In connection with convolution and Coulomb integrals, Filter and Steinborn later introduced the so called B functions as an anisotropic generalization of the reduced Bessel functions with half-integral orders [28, Eq. (2.14)]:

$$B_{n,\ell}^{m}(\beta, \boldsymbol{r}) = \left[2^{n+\ell}(n+\ell)!\right]^{-1} \hat{k}_{n-1/2}(\beta r)\, \mathscr{Y}_{\ell}^{m}(\beta \boldsymbol{r}), \quad n \in \mathbb{Z}. \tag{2.18}$$

B functions are fairly complicated mathematical objects, and (2.18) and (2.17) imply that a B function can be expressed as a linear combination of Slater-type functions with integral principal quantum numbers. Hence, it is not at all clear why the use of the comparatively complicated B functions should offer any advantages over Slater-type functions which possess an exceptionally simple explicit expression in the coordinate representation.

Let us for the moment assume that we form some finite linear combinations of Slater-type functions and that we do some mathematical manipulations with this linear combination. Normally, the complexity of the resulting expression increases, depending on the number of Slater-type functions occurring in the linear combination.

In fortunate cases, however, it may happen that most terms of the resulting expression cancel exactly. Thus, a significant reduction of complexity is also possible if we form appropriate linear combinations.

The Fourier transform of a B function seems to be such a fortunate case since it is of exceptional simplicity among exponentially decaying functions:

$$\begin{aligned} \bar{B}_{n,\ell}^{m}(\alpha, \boldsymbol{p}) &= (2\pi)^{-3/2} \int \mathrm{e}^{-\mathrm{i}\boldsymbol{p}\cdot\boldsymbol{r}}\, B_{n,\ell}^{m}(\alpha, \boldsymbol{r})\, \mathrm{d}^3\boldsymbol{r} \\ &= (2/\pi)^{1/2}\, \frac{\alpha^{2n+\ell-1}}{[\alpha^2 + p^2]^{n+\ell+1}}\, \mathcal{Y}_{\ell}^{m}(-\mathrm{i}\boldsymbol{p}). \end{aligned} \tag{2.19}$$

This is the most consequential and also the most often cited result of my PhD thesis [193, Eq. (7.1-6) on p. 160]. Later, (2.19) was published in [216, Eq. (3.7)]. Independently and almost simultaneously, (2.19) was also derived by Niukkanen [156, Eqs. (57–58)].

The exceptionally simple Fourier transform (2.19) explains why multicenter integrals of B functions are often simpler than the corresponding integrals of other exponentially decaying functions (see for example [170,171,208] and references therein). It also explains why it was comparatively easy to derive two-range [201,218] and one-range [29] addition theorems for B functions.

The exceptionally simple Fourier transform (2.19) also explains why other exponentially decaying functions can be expressed in terms of B functions. For example, a Slater-type function with an integral principal quantum number can be expressed by the following finite sum of B functions [28, Eqs. (3.3) and (3.4)]:

$$\begin{aligned} \chi_{n,\ell}^{m}(\beta, \boldsymbol{r}) = 2^n \sum_{\sigma\ge 0} (-1)^{\sigma}\, & \frac{(-[n-\ell-1]/2)_{\sigma}\, (-[n-\ell]/2)_{\sigma}}{\sigma!} \\ & \times (n-\sigma)!\, B_{n-\ell-\sigma,\ell}^{m}(\beta, \boldsymbol{r}). \end{aligned} \tag{2.20}$$

If $n-\ell$ is *even*, the Pochhammer symbol $(-[n-\ell]/2)_{\sigma}$ causes a termination of the σ summation after a finite number of steps, and if $n-\ell$ is *odd*, this is accomplished by the Pochhammer symbol $(-[n-\ell-1]/2)_{\sigma}$.

It is also possible to express Guseinov's complete and orthonormal functions ${}_{k}\Psi_{n,\ell}^{m}(\gamma, \boldsymbol{r})$ defined by (2.13), which play a central role in Guseinov's work on one-range addition theorems, as a finite sum of B functions. We only have to use [193, Eq. (3.3–35) on p. 45]

$$\mathrm{e}^{-z}\, L_n^{(\alpha)}(2z) = (\alpha + 2n + 1) \sum_{\sigma=0}^{n} \frac{(-2)^{\sigma}\, \Gamma(\alpha+n+\sigma+1)}{(n-\sigma)!\sigma!\, \Gamma(\alpha+2\sigma+2)}\, \hat{k}_{\sigma+1/2}(z) \tag{2.21}$$

to obtain

$$
{}_k\Psi_{n,\ell}^{m}(\gamma, \boldsymbol{r}) = \left\{ \frac{\gamma^{k+3}\,(n+\ell+k+1)!}{2^{k+1}\,(n-\ell-1)!} \right\}^{1/2} \frac{(2n+k+1)\,\Gamma(1/2)\,(\ell+1)!}{\Gamma\bigl(\ell+2+k/2\bigr)\,\Gamma\bigl(\ell+[k+5]/2\bigr)} \times \sum_{\nu=0}^{n-\ell-1} \frac{(-n+\ell+1)_\nu\,(n+\ell+k+2)_\nu\,(\ell+2)_\nu}{\nu!\,\bigl(\ell+2+k/2\bigr)_\nu\,\bigl(\ell+[k+5]/2\bigr)_\nu}\, B_{\nu+1,\ell}^{m}(\gamma, \boldsymbol{r}). \tag{2.22}
$$

Consequently, explicit expressions for multicenter integrals and addition theorems of most exponentially decaying functions—among them Slater-type functions with integral principal numbers and Guseinov's functions—can be derived via the often simpler analogous results for B functions.

3 Guseinov's rearrangements of one-range addition theorems

In [41–44,46], Guseinov derived one-range addition theorems for Slater-type functions $\chi_{N,L}^{M}(\beta, \boldsymbol{r} \pm \boldsymbol{r}')$ with integral or nonintegral principal quantum numbers N by expanding them in terms of his complete and orthonormal functions $\{{}_k\Psi_{n,\ell}^{m}(\gamma, \boldsymbol{r})\}_{n,\ell,m}$ defined by (2.13) with an in general different scaling parameter $\gamma \neq \beta > 0$:

$$
\chi_{N,L}^{M}(\beta, \boldsymbol{r} \pm \boldsymbol{r}') = \sum_{n\ell m} {}_k\mathbf{X}_{n,\ell,m}^{N,L,M}(\gamma, \beta, \pm\boldsymbol{r}')\ {}_k\Psi_{n,\ell}^{m}(\gamma, \boldsymbol{r}), \tag{3.1a}
$$

$$
{}_k\mathbf{X}_{n,\ell,m}^{N,L,M}(\gamma, \beta, \pm\boldsymbol{r}') = \int \left[{}_k\Psi_{n,\ell}^{m}(\gamma, \boldsymbol{r})\right]^{*} r^k\, \chi_{N,L}^{M}(\beta, \boldsymbol{r} \pm \boldsymbol{r}')\, \mathrm{d}^3\boldsymbol{r}. \tag{3.1b}
$$

As long as the principal quantum number N is not too negative, which will be tacitly assumed in the following text, the Slater-type function $\chi_{N,L}^{M}(\beta, \boldsymbol{r} \pm \boldsymbol{r}')$ belongs to the weighted Hilbert spaces $L_{r^k}^2(\mathbb{R}^3)$ defined by (2.15) with $k = -1, 0, 1, 2, \ldots$. Accordingly, the k-dependent one-range addition theorems (3.1), which are special cases of the general addition theorem (2.12), converge in the mean with respect to the norms of their corresponding weighted Hilbert spaces $L_{r^k}^2(\mathbb{R}^3)$.

As already remarked at the end of Sect. 2, the central computational problem occurring in the context of Guseinov's one-range addition theorems (3.1) is the efficient and reliable evaluation of the overlap integrals (3.1b).

Normally, it is much easier to compute overlap integrals of exponentially decaying functions with equal scaling parameters $\beta = \gamma$ than with different parameters $\beta \neq \gamma$. However, Guseinov wanted to have this additional degree of freedom for certain applications. For example, in [66] Guseinov represented the Coulomb potential $1/|\boldsymbol{r} - \boldsymbol{r}'|$ as the limiting case $\beta \to 0$ of the Yukawa potential $\exp(-\beta|\boldsymbol{r} - \boldsymbol{r}'|)/|\boldsymbol{r} - \boldsymbol{r}'|$, which is proportional to the Slater-type function $\chi_{0,0}^{0}(\beta, \boldsymbol{r} - \boldsymbol{r}')$. In this way, Guseinov [66] formally obtained a one-range addition theorem of the Coulomb potential in terms of his functions ${}_k\Psi_{n,\ell}^{m}(\gamma, \boldsymbol{r})$. But this approach leads to other convergence and existence problems [204,206] which will be discussed in more details in [211].

For the evaluation of the overlap integrals (3.1b) occurring in his addition theorems (3.1a), Guseinov uses a simple approach which was first used by Smeyers

[180] in 1966. To the best of my knowledge, this approach was adopted in 1978 by Guseinov [41, Eqs. (6–8)] and consistently used in his later publications. Unfortunately, Smeyers' simple approach is not necessarily good, as already emphasized in 1982 by Trivedi and Steinborn [190, pp. 116–117].

It follows at once from the explicit expression (D.2) of the generalized Laguerre polynomials that Guseinov's functions can be expressed as finite sums of Slater-type functions with integral principal quantum numbers:

$$
{}_k\Psi_{n,\ell}^{m}(\gamma,\boldsymbol{r}) = \sum_{\nu=\ell+1}^{n} {}_k\mathbf{G}_{\nu-\ell-1}^{(n,\ell)}(\gamma)\, \chi_{\nu,\ell}^{m}(\gamma,\boldsymbol{r}), \tag{3.2a}
$$

$$
{}_k\mathbf{G}_{j}^{(n,\ell)}(\gamma) = 2^{\ell}\left[\frac{(2\gamma)^{k+3}(n+\ell+k+1)!}{(n-\ell-1)!}\right]^{1/2} \frac{(-n+\ell+1)_j 2^j}{(2\ell+k+j+2)!j!}. \tag{3.2b}
$$

Accordingly, the overlap integrals (3.1b) can be expressed as finite sums of overlap integrals of Slater-type functions:

$$
{}_k\mathbf{X}_{n,\ell,m}^{N,L,M}(\gamma,\beta,\pm\boldsymbol{r}') = \gamma^{-k} \sum_{\nu=\ell+1}^{n} {}_k\mathbf{G}_{\nu-\ell-1}^{(n,\ell)}(\gamma)\, \mathbf{S}_{\nu+k,\ell,m}^{N,L,M}(\gamma,\beta,\pm\boldsymbol{r}'), \tag{3.3a}
$$

$$
\mathbf{S}_{n,\ell,m}^{N,L,M}(\gamma,\beta,\pm\boldsymbol{r}') = \int \left[\chi_{n,\ell}^{m}(\gamma,\boldsymbol{r})\right]^{*} \chi_{N,L}^{M}(\beta,\boldsymbol{r}\pm\boldsymbol{r}')\, \mathrm{d}^3\boldsymbol{r}. \tag{3.3b}
$$

Inserting this into the addition theorems (3.1) yields (compare [46, Eqs. (15) and (16)]):

$$
\chi_{N,L}^{M}(\beta,\boldsymbol{r}\pm\boldsymbol{r}') = \gamma^{-k} \sum_{n\ell m} {}_k\Psi_{n,\ell}^{m}(\gamma,\boldsymbol{r}) \sum_{\nu=\ell+1}^{n} {}_k\mathbf{G}_{\nu-\ell-1}^{(n,\ell)}(\gamma)\, \mathbf{S}_{\nu+k,\ell,m}^{N,L,M}(\gamma,\beta,\pm\boldsymbol{r}'). \tag{3.4}
$$

Guseinov's approach seems to have the advantage that existing programs for overlap integrals of Slater-type functions can be used for the evaluation of the overlap integrals (3.1b) involving Guseinov's functions. Unfortunately, this seemingly convenient approach can easily lead to stability problems. Numerical instabilities are extremely likely in expressions based on (3.2) if the indices n of the Guseinov functions ${}_k\Psi_{n,\ell}^{m}(\gamma,\boldsymbol{r})$ are large.

In his desire to reduce his whole formalism of one-range addition theorems to Slater-type functions with integral principal quantum numbers, Guseinov even expressed the functions ${}_k\Psi_{n,\ell}^{m}(\gamma,\boldsymbol{r})$ on the right-hand side of (3.4) by Slater-type functions according to (3.2) (compare [46, Eqs. (14–16)]):

$$
\begin{aligned}
\chi_{N,L}^{M}(\beta,\boldsymbol{r}\pm\boldsymbol{r}') = \gamma^{-k} \sum_{n\ell m} \sum_{\nu'=\ell+1}^{n} {}_k\mathbf{G}_{\nu'-\ell-1}^{(n,\ell)}(\gamma)\, \chi_{\nu',\ell}^{m}(\gamma,\boldsymbol{r}) \\
\times \sum_{\nu=\ell+1}^{n} {}_k\mathbf{G}_{\nu-\ell-1}^{(n,\ell)}(\gamma)\, \mathbf{S}_{\nu+k,\ell,m}^{N,L,M}(\gamma,\beta,\pm\boldsymbol{r}').
\end{aligned} \tag{3.5}
$$

In this version of Guseinov's k-dependent addition theorems, the complete and orthogonal functions ${}_k\Psi_{n,\ell}^m(\gamma, \boldsymbol{r})$ do not occur any more and are replaced by Slater-type functions $\chi_{n,\ell}^m(\gamma, \boldsymbol{r})$ with integral principal quantum numbers $n \geq \ell + 1$. Apparently, Guseinov considered this to be a major achievement.

But there is a price to be paid. Firstly, introducing one finite inner sum after the other does not look like a promising computational strategy. Secondly, the numerical stability of Guseinov's transformations is questionable, in particular in the case of (very) large quantum numbers.

Whenever we do calculations of nontrivial complexity with a fixed precision, numerical stability is invariably a very important issue. Let us for example assume that we work with a series expansion whose coefficients are given by complicated expressions such as multiple nested finite sums (this characterization certainly applies to Guseinov's rearranged addition theorems). If alternating signs occur in these nested sums, a loss of significant digits cannot be ruled out, and in the case of (very) large indices, a catastrophic accumulation of rounding errors may even produce completely nonsensical results.

Guseinov's rearranged addition theorems are based on the simple fact that Guseinov's orthogonal functions ${}_k\Psi_{n,\ell}^m(\gamma, \boldsymbol{r})$ can according to (3.2) be expressed as finite sums of Slater-type functions with integral principal quantum numbers. The linear combination (3.2) is nothing but the explicit expression (D.2) of a generalized Laguerre polynomial in disguise. The coefficients in (D.2) and thus also the coefficients in (3.2) have strictly alternating signs.

Sign alternation of the coefficients of the classical orthogonal polynomials is a necessary requirement for an orthogonality relationship of the type of (D.3). But this sign alternation can easily lead to a catastrophic accumulation of rounding errors, if we try to compute an orthogonal polynomial with a large index from its explicit expression. In practice, one usually avoids explicit expressions. It is much better to evaluate orthogonal polynomials via their three-term recursions (see for example [163, Eq. (18.9.1) and Table 18.9.1]). For example, Gautschi, who is generally considered to be one of the leading experts on the stability of linear recurrences, wrote in [33, p. 277]:

> It is our experience, and the experience of many others, that the basic three-term recurrence relation for orthogonal polynomials is generally an excellent means of computing these polynomials, both within the interval of orthogonality and outside of it.

A FORTRAN SUBROUTINE OTHPL, which evaluates classical orthogonal polynomials via their three-term recursions [163, Eq. (18.9.1) and Table 18.9.1], is listed in [220, pp. 23–24]. Another important aspect is that a recursive evaluation is much more efficient, in particular if whole strings of orthogonal polynomials have to be evaluated simultaneously.

As long as the opposite is not explicitly proven, it makes sense to be cautious and to assume that an expression like (3.2), whose coefficients ${}_k\mathbf{G}_j^{(n,\ell)}(\gamma)$ have strictly alternating signs, inherits the stability problems of the explicit expression (D.2) of the generalized Laguerre polynomials from which it was derived. Similarly, the coefficients ${}_k\mathbf{G}_{\nu'-\ell-1}^{(n,\ell)}(\gamma)$ and ${}_k\mathbf{G}_{\nu-\ell-1}^{(n,\ell)}(\gamma)$ in the inner ν' and ν sums in (3.5) have strictly alternating signs.

I am not at all convinced that inner sums based on (D.2), which occur as coefficients in infinite series expansions like the one on the right-hand side of (3.5) or later in (3.7) and (3.8), can be computed in a numerically stable way for large values of the outer summation indices n and ℓ. This has to be investigated (much) more thoroughly.

Another problem is that conventional programs for overlap integrals of Slater-type functions, as they are for instance used in semiempirical calculations, normally cannot be used in the case of (very) large principal and angular momentum quantum numbers. Therefore, one should look for alternative expressions for the overlap integrals (3.1b), which are not based on (3.2) and which permit an efficient and reliable evaluation even for (very) large values of the indices n and ℓ.

Slater-type functions are complete but not orthogonal. But this nonorthogonality can also cause problems. There is a practically very consequential aspect of orthogonal expansions which is often not sufficiently appreciated. Let us assume that f belongs to some Hilbert space $\mathscr{H}$ with inner product $(\cdot|\cdot)$ and that the functions $\{\varphi_n\}_{n=0}^{\infty}$ are complete and orthonormal in $\mathscr{H}$. Then, as discussed in Appendix C, f possesses the orthogonal expansion (C.4) which converges in the mean with respect to the norm $\|\cdot\|$ of $\mathscr{H}$. Moreover, the expansion coefficients $(\varphi_n|f)$ satisfy Parseval's equality (see for example [166, Eq. (II.2) on p. 45])

$$\|f\|^2 = \sum_{n=0}^{\infty} |(\varphi_n|f)|^2. \tag{3.6}$$

Parseval's equality implies that the inner products $(\varphi_n|f)$ are bounded in magnitude and that they vanish as $n \to \infty$. This may well be the main reason why orthogonal expansions tend to be computationally well behaved.

In the case of nonorthogonal expansions of the type of (C.3), quite a few complications can happen. We cannot tacitly assume that the expansion coefficients C_n in (C.3) are necessarily bounded in magnitude. These coefficients can have alternating signs and even increase in magnitude with increasing index n (examples can for instance be found in [144, Table I on p. 166] or [27, Appendix E on pp. 162–164]). Such a behavior of the expansion coefficients can easily lead to a cancellation of significant digits or even to a catastrophic accumulation of rounding errors.

Guseinov approximated the Slater-type function $\chi_{N,L}^{M}(\beta, \boldsymbol{r} \pm \boldsymbol{r}')$ by a truncation of the addition theorem (3.5) including only the first $\mathscr{N}$ terms of the outer n summation and defined the complete addition theorem as the limit $\mathscr{N} \to \infty$ of his $\mathscr{N}$-dependent truncation (compare [46, Eq. (13)]):

$$\begin{aligned} \chi_{N,L}^{M}(\beta, \boldsymbol{r} \pm \boldsymbol{r}') &= \gamma^{-k} \lim_{\mathscr{N}\to\infty} \sum_{n=1}^{\mathscr{N}} \sum_{\ell=0}^{n-1} \sum_{m=-\ell}^{\ell} \\ &\times \sum_{\nu'=\ell+1}^{n} {}_k\mathbf{G}_{\nu'-\ell-1}^{(n,\ell)}(\gamma)\, \chi_{\nu',\ell}^{m}(\gamma, \boldsymbol{r}) \sum_{\nu=\ell+1}^{n} {}_k\mathbf{G}_{\nu-\ell-1}^{(n,\ell)}(\gamma)\, \mathbf{S}_{\nu+k,\ell,m}^{N,L,M}(\gamma, \beta, \pm\boldsymbol{r}'). \end{aligned} \tag{3.7}$$

In the $\mathscr{N}$-dependent part of this expression, Guseinov changed the order of summations and formally expressed this finite sum as a linear combination of Slater-type functions with integral principal quantum numbers [46, Eq. (15)]. In this context, it is in my opinion advantageous to change the order of the finite n and ℓ summations according to $\sum_{n=1}^{\mathscr{N}} \sum_{\ell=0}^{n-1} \to \sum_{\ell=0}^{\mathscr{N}-1} \sum_{n=\ell+1}^{\mathscr{N}}$. Then, we obtain:

$$\chi_{N,L}^{M}(\beta, \boldsymbol{r} \pm \boldsymbol{r}') = \gamma^{-k} \lim_{\mathscr{N}\to\infty} \sum_{\ell=0}^{\mathscr{N}-1} \sum_{m=-\ell}^{\ell} \sum_{t=\ell+1}^{\mathscr{N}} \chi_{t,\ell}^{m}(\gamma, \boldsymbol{r}) \\ \times \sum_{p=t}^{\mathscr{N}} {}_{k}\mathbf{G}_{t-\ell-1}^{(p,\ell)}(\gamma) \sum_{q=\ell+1}^{n} {}_{k}\mathbf{G}_{q-\ell-1}^{(p,\ell)}(\gamma)\, \mathbf{S}_{q+k,\ell,m}^{N,L,M}(\gamma, \beta, \pm\boldsymbol{r}'). \tag{3.8}$$

As long as $\mathscr{N}$ is finite, the transformation of the $\mathscr{N}$-dependent part of (3.7) to the $\mathscr{N}$-dependent part of (3.8) is legitimate. But it is not guaranteed that this transformation is still legitimate in the limit $\mathscr{N} \to \infty$ and that one-range addition theorems can be reformulated as expansions in terms of nonorthogonal Slater-type functions with integral principal quantum numbers. Further details will be given in Sect. 6.

One-range addition theorems for Slater-type functions are fairly complicated mathematical objects, whose series coefficients are essentially overlap integrals. Thus, a detailed analysis of the existence and convergence properties of such an addition theorem is certainly a very demanding task. Consequently, it makes sense to look for simplifications and to pursue an indirect approach. The situation becomes much more transparent if we do not look at addition theorems for Slater-type functions $\chi_{N,L}^{M}(\beta, \boldsymbol{r} \pm \boldsymbol{r}')$, but rather at their angular projections

$$\Xi_{\ell,m}^{N,L,M}(\beta, r, \pm\boldsymbol{r}') = \int\limits_{|\boldsymbol{r}|=1} \left[Y_{\ell}^{m}(\boldsymbol{r}/r)\right]^{*} \chi_{N,L}^{M}(\beta, \boldsymbol{r} \pm \boldsymbol{r}')\, \mathrm{d}^{3}\boldsymbol{r}. \tag{3.9}$$

If we insert the addition theorem (3.1) into this integral and perform the integration over the surface of the unit sphere in $\mathbb{R}^3$, we obtain with the help of the orthonormality of the spherical harmonics an expansion in terms of the radial parts of Guseinov's functions ${}_{k}\Psi_{n,\ell}^{m}(\gamma, \boldsymbol{r})$, which can be reformulated as an expansion in terms of generalized Laguerre polynomials:

$$\mathrm{e}^{\gamma r}\, \Xi_{\ell,m}^{N,L,M}(\beta, r, \pm\boldsymbol{r}') = \sum_{n=\ell+1}^{\infty} {}_{k}\mathbf{X}_{n,\ell,m}^{N,L,M}(\gamma, \beta, \pm\boldsymbol{r}') \\ \times \left[\frac{(2\gamma)^{k+3}(n-\ell-1)!}{(n+\ell+k+1)!}\right]^{1/2} (\gamma r)^{\ell}\, L_{n-\ell-1}^{(2\ell+k+2)}(2\gamma r). \tag{3.10}$$

A further substantial simplifications takes place if we do not consider the fairly complicated one-range addition theorems but rather their much simpler one-center limits $\boldsymbol{r}' = \mathbf{0}$. Then, for fixed $\beta, \gamma > 0$ the overlap integrals ${}_{k}\mathbf{X}_{n,\ell,m}^{N,L,M}(\gamma, \beta, \pm\boldsymbol{r}')$ defined by (3.1b) simplify to become numbers. Moreover, because of the orthonormality of the spherical harmonics only the overlap integrals with $\ell = L$ and $m = M$ can be nonzero.

4 The transformation of Laguerre series to power series

If Guseinov's rearrangements of the one-range addition theorems (3.1) for Slater-type functions $\chi_{N,L}^{M}(\beta, \boldsymbol{r} \pm \boldsymbol{r}')$ are legitimate, we ultimately obtain an expansion of a Slater-type function with an in general nonintegral principal quantum number $N \in \mathbb{R} \backslash \mathbb{N}$ in terms of Slater-type functions $\{\chi_{n,\ell}^{m}(\gamma, \boldsymbol{r})\}_{n\ell m}$ with integral principal quantum numbers n and a common scaling parameter $\gamma > 0$:

$$\chi_{N,L}^{M}(\beta, \boldsymbol{r} \pm \boldsymbol{r}') = \sum_{n\ell m} \mathbb{X}_{n,\ell,m}^{(N,L,M)}(\beta, \gamma, \pm \boldsymbol{r}')\, \chi_{n,\ell}^{m}(\gamma, \boldsymbol{r}). \tag{4.1}$$

If we set $\boldsymbol{r}' = \boldsymbol{0}$, this expansion simplifies and we obtain (1.2).

If the expansion (4.1) exists and converges for the whole argument set $\mathbb{R}^3 \times \mathbb{R}^3$, then it is obviously a one-range addition theorem. Moreover, (4.1) can be reformulated as a power series in γr by shifting the exponential part $\exp(-\gamma r)$ of the Slater-type functions $\chi_{n,\ell}^{m}(\gamma, \boldsymbol{r})$ to the left-hand side:

$$\mathrm{e}^{\gamma r}\, \chi_{N,L}^{M}(\beta, \boldsymbol{r} \pm \boldsymbol{r}') = \sum_{n\ell m} \mathbb{X}_{n,\ell,m}^{(N,L,M)}(\beta, \gamma, \pm \boldsymbol{r}')\, (\gamma r)^{n-1}\, Y_{\ell}^{m}(\boldsymbol{r}/r). \tag{4.2}$$

This expansion can be transformed to an infinite number of ℓ-dependent power series in γr for the angular projections $\Xi_{\ell,m}^{N,L,M}(\beta, r, \pm \boldsymbol{r}')$ defined by (3.9):

$$\mathrm{e}^{\gamma r}\, \Xi_{\ell,m}^{N,L,M}(\beta, r, \pm \boldsymbol{r}') = \sum_{n=\ell+1}^{\infty} \mathbb{X}_{n,\ell,m}^{(N,L,M)}(\beta, \gamma, \pm \boldsymbol{r}')\, (\gamma r)^{n-1}. \tag{4.3}$$

A comparison of (3.10) and (4.3) shows that Guseinov's rearrangements ultimately corresponds to the transformation of a Laguerre series

$$f(z) = \sum_{n=0}^{\infty} \lambda_n^{(\alpha)}\, L_n^{(\alpha)}(z), \tag{4.4a}$$

$$\lambda_n^{(\alpha)} = \frac{n!}{\Gamma(\alpha+n+1)} \int_0^{\infty} z^{\alpha}\, \mathrm{e}^{-z}\, L_n^{(\alpha)}(z)\, f(z)\, \mathrm{d}z, \tag{4.4b}$$

which converges in the mean with respect to the norm of the weighted Hilbert space $L^2_{\mathrm{e}^{-z} z^{\alpha}}\big([0, \infty)\big)$ defined by (D.8), to a power series

$$f(z) = \sum_{n=0}^{\infty} \gamma_n\, z^n, \tag{4.5}$$

which—if it exists—converges pointwise in a suitable subset of the complex plane.

There is, however, the problem that analyticity in the sense of complex analysis and the existence of a Laguerre expansion are completely unrelated concepts. Therefore, we cannot expect that the transformation from (4.4) to (4.5) is necessarily possible in the case of an essentially arbitrary function $f : \mathbb{C} \to \mathbb{C}$.

The convergence and existence problems, which occur in this context, were recently studied in depth in [207]. There, some simple sufficient conditions based on the decay rate and the sign pattern of the Laguerre series coefficients $\lambda_n^{(\alpha)}$ as $n \to \infty$ were formulated. These conditions, which extend previous results by Gottlieb and Orszag [35, p. 42] and by Doha [25, p. 5452], respectively, make it possible to decide whether the transformation of a Laguerre series of the type of (4.4) to a power series produces a mathematically meaningful result or not.

In order to understand better the possible pitfalls and dangers of such a transformation, let us first consider a partial sum of the infinite Laguerre series (4.4):

$$f_M(z) = \sum_{n=0}^{M} \lambda_n^{(\alpha)} L_n^{(\alpha)}(z) \tag{4.6}$$

$$= \sum_{n=0}^{M} \lambda_n^{(\alpha)} \frac{(\alpha+1)_n}{n!} \sum_{\nu=0}^{n} \frac{(-n)_\nu}{(\alpha+1)_\nu} \frac{z^\nu}{\nu!}, \quad M \in \mathbb{N}_0. \tag{4.7}$$

In this partial sum, the power z^p with $0 \le p \le M$ occurs in the Laguerre polynomials $L_p^{(\alpha)}(z),\ L_{p+1}^{(\alpha)}(z), \ldots, L_M^{(\alpha)}(z)$. Thus, we have add up all contributions with $\nu = p$ on the right-hand side of (4.7) to obtain the coefficients of z^p. A short calculation yields [207, Eq. (3.13)]:

$$f_M(z) = \sum_{\nu=0}^{M} \frac{(-z)^\nu}{\nu!} \sum_{\mu=0}^{M-\nu} \frac{(\alpha+\nu+1)_\mu}{\mu!} \lambda_{\mu+\nu}^{(\alpha)}. \tag{4.8}$$

Since the truncated Laguerre series $f_M(z)$ is simply a polynomial of degree M in z, it is always possible to reformulate it by interchanging the order of the nested finite sums. No convergence and/or existence problems can occur.

Unfortunately, this does not mean that the transformation from (4.6) to (4.8) is also possible in the limit $M \to \infty$. In this case, the finite inner sum on the right-hand side of (4.8) becomes an infinite series which can a diverge if the coefficients $\lambda_n^{(\alpha)}$ do not decay sufficiently rapidly as $n \to \infty$. Moreover, the fact that $f_M(z)$ is a mathematically meaningful object does not imply that $f(z)$ possesses a power series expansion of the type of (4.5) which converges in a suitable subset of the complex plane. The expression (4.8) for $f_M(z)$ possesses the following general structure:

$$f_M(z) = \sum_{\mu=0}^{M} \gamma_\mu^{(M)} z^\mu. \tag{4.9}$$

The coefficients $\gamma_n^{(M)}$ depend explicit on the summation limit M, i.e., we have in general $\gamma_n^{(M)} \neq \gamma_n^{(M+1)} \neq \gamma_n^{(M+2)} \neq \ldots$ for all $n \in \mathbb{N}_0$. Thus, we have to show explicitly that the $\gamma_n^{(M)}$ possess for all $n \in \mathbb{N}_0$ well defined limits $\gamma_n = \gamma_n^{(\infty)} = \lim_{M \to \infty} \gamma_n^{(M)}$. Only if all these limits exist, $f(z)$ can possess a convergent power series expansion about $z = 0$. This, however, requires that the Laguerre series coefficients $\lambda_n^{(\alpha)}$ decay sufficiently rapidly as $n \to \infty$.

Let us now consider the transformation of the infinite Laguerre expansion (4.4). The power z^p with $p \geq 0$ occurs in all Laguerre polynomials $L_n^{(\alpha)}(z)$ with $n \geq p$. We obtain the corresponding power series coefficient γ_p, if we add up all contributions with $\nu = p$ in the infinite series

$$f(z) = \sum_{n=0}^{\infty} \lambda_n^{(\alpha)} \frac{(\alpha+1)_n}{n!} \sum_{\nu=0}^{n} \frac{(-n)_\nu}{(\alpha+1)_\nu} \frac{z^\nu}{\nu!}. \tag{4.10}$$

A short calculation yields [207, Eq. (3.14)]:

$$f(z) = \sum_{\nu=0}^{\infty} \frac{(-z)^\nu}{\nu!} \sum_{\mu=0}^{\infty} \frac{(\alpha+\nu+1)_\mu}{\mu!} \lambda_{\mu+\nu}^{(\alpha)}. \tag{4.11}$$

If we compare (4.8) and (4.11), which corresponds to the limit $M \to \infty$ in (4.8), we immediately see that the rearrangement of an infinite Laguerre expansion is not necessarily possible since the power series coefficients γ_n are now given by infinite series. If the inner μ series in (4.11) do not produce finite results, we end up with a formal power series with expansion coefficients that are infinite in magnitude.

Thus, the existence of the power series (4.5) for $f(z)$ depends crucially on the decay rate and the sign pattern of the Laguerre series coefficients $\lambda_n^{(\alpha)}$ as $n \to \infty$. In [207], three different prototypes of large index behavior of the coefficients $\lambda_n^{(\alpha)}$ were discussed:

– algebraic decay with ultimately monotone signs,
– exponential or factorial decay,
– algebraic decay with ultimately strictly alternating signs.

If the coefficients $\lambda_n^{(\alpha)}$ decay algebraically as $n \to \infty$ and ultimately have monotone signs, the inner μ series in (4.11) diverge for sufficiently large outer indices ν [207, Sect. 4]. Thus, a function $f(z)$ represented by a Laguerre expansion with ultimately monotone and algebraically decaying series coefficients $\lambda_n^{(\alpha)}$ cannot be analytic in a neighborhood of the origin $z = 0$.

If the coefficients $\lambda_n^{(\alpha)}$ decay exponentially or even factorially, the inner μ series in (4.11) converge (often quite rapidly), and the function $f(z)$ under consideration is analytic in a suitable neighborhood of the origin $z = 0$ [207, Sect. 5]. This is pretty much the most advantageous situation we can hope for.

These conclusions are in agreement with short remarks by Gottlieb and Orszag [35, p. 42] and by Doha [25, p. 5452], respectively, who had stated without detailed proof that such a Laguerre series converges faster than algebraically if the function under consideration is analytic at the origin. However, both Gottlieb and Orszag [35, p. 42] and Doha [25, p. 5452], respectively, had failed to see that there is a different scenario, which also produces convergent power series expansions about $z = 0$.

Let us assume that the coefficients $\lambda_n^{(\alpha)}$ decay algebraically in magnitude and ultimately have strictly alternating signs. Then, the inner μ series in (4.11) still diverge at least for sufficiently large values of the outer index ν. However, this divergence does not imply that a convergent power series about $z = 0$ does not exist. The strictly alternating signs make it possible to associate something finite to the divergent μ series by employing suitable summation techniques for divergent series. A highly condensed review of summation techniques with a special emphasis on sequence transformations can be found in [207, Appendices A and B], and in [209] there is an admittedly incomplete discussion of the usefulness of sequence transformations beyond the summation of divergent series.

In [207, Sect. 4], several known generating functions of the generalized Laguerre polynomials were recovered by summing divergent inner μ series representing power series coefficients. In these comparatively simple cases, the divergent inner μ series could always be expressed by generalized hypergeometric series with argument -1. However, these generalized hypergeometric series only converge in the interior of the unit circle. Thus, analytic continuation from the interior of the circle of convergence of such a hypergeometric series to its boundary was sufficient to accomplish a summation. In the case of simpler hypergeometric series, this is not too difficult.

A skeptical reader might therefore conclude that a summation is only feasible in the case of comparatively simple problems. This is not true. In [207, Sect. 6] it was shown that it is also possible to sum divergent inner μ series by purely numerical techniques. Particularly good results were obtained by the nonlinear $\mathscr{S}$ transformation which I had introduced in [195, Eq. (8.4-4)] (a highly condensed review of the historical development was given in [210, Sect. 2]). Some authors call this $\mathscr{S}$ transformation the Weniger transformation (see for example [13–15, 22, 152, 188] or [34, Eq. (9.53) on p. 287]). This terminology was also used in the recently published NIST Handbook of Mathematical Functions [163, Chapter 3.9(v) Levin's and Weniger's Transformations] (see also the companion NIST Digital Library of Mathematical Functions under http://dlmf.nist.gov/3.9#v).

The example of divergent but summable inner μ series shows that fairly sophisticated mathematical techniques may be needed to accomplish the transformation of a Laguerre expansion to a power series.

It should be noted that the structure of the formulas, which effect the transformation of a Laguerre series to power series, is of a more general nature, and that very similar transformation formulas occur also in completely different contexts. In [210, Appendix B] it was shown that formulas having analogous structures occur as long as the transformation matrices are triangular and satisfy certain orthogonality conditions. In [210], transformations between factorial series and inverse power series were considered, and the transformation matrices involved Stirling numbers of the first and second kind, respectively.

5 One-center expansions for Slater-type functions

As already mentioned above, the one-center expansion for Slater-type functions with in general nonintegral principal quantum numbers used by Guseinov and Mamedov [122, Eq. (4)] was originally derived by Guseinov [46, Eq. (21)] as the one-center limit of a rearranged addition theorem for Slater-type functions of the type of (3.8) [46, Eq. (15)]. It is, however, both simpler and for our purposes much more instructive to derive first one-center expansions of Slater-type function with both integral and non-integral principal quantum numbers in terms of Guseinov's complete and orthonormal Laguerre-type functions $\{{}_k\Psi_{n,\ell}^{m}(\gamma, \boldsymbol{r})\}_{n\ell m}$ defined by (2.13). In the second step, it is investigated whether and under which conditions these orthogonal expansions can be transformed to expansions in terms of Slater-type functions $\{\chi_{n,\ell}^{m}(\gamma, \boldsymbol{r})\}_{n\ell m}$ with integral principal quantum numbers n.

A convenient starting point for the construction of the one-center expansion of a Slater-type function with an essentially arbitrary principal quantum number in terms of Guseinov's functions is the following Laguerre series [204, Eq. (6.12)]:

$$\begin{aligned} z^{\rho}\,\mathrm{e}^{uz} &= (1-u)^{-\alpha-\rho-1}\,\frac{\Gamma(\alpha+\rho+1)}{\Gamma(\alpha+1)} \\ &\quad\times \sum_{n=0}^{\infty} {}_2F_1\left(-n, \alpha+\rho+1; \alpha+1; \frac{1}{1-u}\right) L_n^{(\alpha)}(z), \\ &\quad \rho \in \mathbb{R}\backslash\mathbb{N}_0, \quad \Re(\alpha+2\rho) > -1, \quad u \in (-\infty, 1/2). \end{aligned} \tag{5.1}$$

The restriction $u \in (-\infty, 1/2)$ is necessary to guarantee the existence of some integrals occurring in the derivation of this expansion. If we assume $\rho = m$ with $m \in \mathbb{N}_0$, no immediately obvious simplification occurs in (5.1). But for $u = 0$, we obtain a terminating Gaussian hypergeometric series ${}_2F_1$ with unit argument that can be expressed in closed form with the help of Gauss' summation theorem [154, p. 40] and we obtain a much simpler expansion [26, Eq. (16) on p. 214]:

$$z^{\rho} = \frac{\Gamma(\rho+\alpha+1)}{\Gamma(\alpha+1)} \sum_{n=0}^{\infty} \frac{(-\rho)_n}{(\alpha+1)_n} L_n^{(\alpha)}(z), \quad \rho \in \mathbb{R}\backslash\mathbb{N}_0, \quad \Re(\alpha+2\rho) > -1. \tag{5.2}$$

If we now set $\rho = m$ with $m \in \mathbb{N}_0$, the infinite series terminates because of the Pochhammer symbol $(-m)_n$ and we obtain instead a finite sum:

$$z^{m} = (\alpha+1)_m \sum_{n=0}^{m} \frac{(-m)_n}{(\alpha+1)_n} L_n^{(\alpha)}(z), \quad m \in \mathbb{N}_0, \quad \Re(\alpha) + 2m > -1. \tag{5.3}$$

The Laguerre expansions listed above can all be transformed to expansions of Slater-type functions in terms of Guseinov's functions. The expansion (5.1) yields the most general case, i.e., we obtain a k-dependent one-center expansion of a Slater-type function $\chi_{N,L}^{M}(\beta, \boldsymbol{r})$ with a nonintegral principal quantum number $N \in \mathbb{R}\backslash\mathbb{N}$ in terms of Guseinov's functions with different scaling parameters $\beta \neq \gamma > 0$ [206, Eq. (5.9)]:

$$\chi_{N,L}^{M}(\beta, \boldsymbol{r}) = \frac{(2\gamma)^{L+(k+3)/2}\, \beta^{N-1}}{[\beta+\gamma]^{N+L+k+2}} \, \frac{\Gamma(N+L+k+2)}{(2L+k+2)!} \times \sum_{\nu=0}^{\infty} \left[\frac{(\nu+2L+k+2)!}{\nu!} \right]^{1/2} {}_k\Psi_{\nu+L+1,L}^{M}(\gamma, \boldsymbol{r}) \times {}_2F_1\left(-\nu, N+L+k+2; 2L+k+3; \frac{2\gamma}{\beta+\gamma}\right). \quad (5.4)$$

This expansion can also be derived by performing the one-center limit $\boldsymbol{r}' = \boldsymbol{0}$ in the addition theorem (3.1).

If we assume in (5.4) that the principal quantum number N of the Slater-type function is a positive integer satisfying $N \geq L+1$, no immediately obvious simplification occurs. But in the case of equal scaling parameters $\beta = \gamma > 0$, which corresponds to $u = 0$ in (5.1), the expansion (5.4) simplifies considerably, yielding [206, Eq. (5.7)]:

$$\chi_{N,L}^{M}(\beta, \boldsymbol{r}) = \frac{(2\gamma)^{-(k+3)/2}}{2^{N-1}} \, \Gamma(N+L+k+2) \times \sum_{\nu=0}^{\infty} \frac{(-N+L+1)_\nu}{\left[(\nu+2L+k+2)!\, \nu!\right]^{1/2}} \, {}_k\Psi_{\nu+L+1,L}^{M}(\beta, \boldsymbol{r}), \quad N \in \mathbb{R}\backslash\mathbb{N}, \quad \beta > 0, \quad k = -1, 0, 1, 2, \ldots. \quad (5.5)$$

If $N \in \mathbb{N}$ and $N \geq L+1$, the infinite series on the right-hand side terminates because of the Pochhammer symbol $(-N+L+1)_\nu$. The resulting finite sum can also be derived directly via (5.3).

With the help of the sufficient conditions formulated in [207] and discussed in Sect. 4, we can analyze whether the Laguerre-type functions ${}_k\Psi_{n,\ell}^{m}(\gamma, \boldsymbol{r})$ in the one-center expansions given above can be replaced by Slater-type functions $\chi_{n,\ell}^{m}(\gamma, \boldsymbol{r})$ with integral principal quantum numbers. But it is simpler and also more transparent to investigate instead whether the equivalent Laguerre expansions (5.1, 5.2), and (5.3) can be transformed to power series.

The most simple situation occurs if we replace in the finite sum (5.3) for the integral power z^m with $m \in \mathbb{N}_0$ the generalized Laguerre polynomials by powers via (D.2) and rearrange the order of the summations [207, Eqs. (3.5) and (3.6)]. Then we arrive at the trivial identity $z^m = z^m$, which proves the correctness of (5.3) but provides no new insight.

In the case of the Laguerre expansion (5.2) for a nonintegral power z^ρ with $\rho \in \mathbb{R}\backslash\mathbb{N}_0$, we face a completely different situation. Firstly, we have no a priori reason to assume that (5.2) converges pointwise. Hilbert space theory only guarantees that this expansion converges in the mean with respect to the norm of the weighted Hilbert space $L^2_{\mathrm{e}^{-z} z^\alpha}\big([0,\infty)\big)$, Moreover, the power function z^ρ is not analytic at $z = 0$ in the case of nonintegral $\rho \in \mathbb{R}\backslash\mathbb{N}_0$. Thus, a mathematically meaningful power series about $z = 0$ cannot exist, and the transformation of the Laguerre expansion (5.2) via (4.11) also must fail.

This is indeed the case. We only need the asymptotic approximation [1, Eq. (6.1.47) on p. 257]

$$\Gamma(z+a)/\Gamma(z+b) = z^{a-b}\left[1+\mathrm{O}(1/z)\right], \quad z\to\infty, \tag{5.6}$$

to obtain the following asymptotic estimate for the coefficients in (5.2):

$$\frac{\Gamma(\rho+\alpha+1)}{\Gamma(\alpha+1)}\,\frac{(-\rho)_n}{(\alpha+1)_n} = \frac{\Gamma(\rho+\alpha+1)}{\Gamma(-\rho)}\,n^{-\alpha-\rho-1}\left[1+\mathrm{O}\big(n^{-1}\big)\right], \quad n\to\infty. \tag{5.7}$$

This asymptotic estimate shows that the coefficients in (5.2) decay algebraically as $n \to \infty$. Moreover, these coefficients ultimately have the same sign. Thus, on the basis of the sufficient conditions formulated in [207] and reviewed in Sect. 4 we can conclude that the inner μ series in (4.11) do not converge for larger values of the outer index ν.

We can also insert the explicit expression (D.2) for the generalized Laguerre polynomials into the infinite series (5.2) and rearrange the order of summations, which yields after some algebra [207, Eq. (3.7)]:

$$z^{\rho} = \frac{\Gamma(\rho+\alpha+1)}{\Gamma(\alpha+1)}\sum_{k=0}^{\infty}(-1)^k\,\frac{(-\rho)_k}{(\alpha+1)_k}\,\frac{z^k}{k!}\,{}_1F_0(k-\rho;1). \tag{5.8}$$

Superficially, it looks as if we succeeded in constructing a power series expansion for the nonintegral power z^{ρ}. However, the generalized hypergeometric series ${}_1F_0$ with unit argument is the limiting case $z \to 1$ of the so-called binomial series [154, p. 38]:

$${}_1F_0(a;z) = \sum_{m=0}^{\infty}\frac{(a)_m}{m!}\,z^m = \sum_{m=0}^{\infty}\binom{-a}{m}(-z)^m = (1-z)^{-a}, \quad |z|<1. \tag{5.9}$$

If we set $a = k - \rho$ with $k \in \mathbb{N}_0$ and $\rho \in \mathbb{R}\backslash\mathbb{N}_0$, we obtain for the ${}_1F_0$ in (5.8):

$${}_1F_0(k-\rho;1) = \lim_{z\to1}(1-z)^{\rho-k} = \begin{cases}\infty, & \rho<0,\\ 0, & k<\rho\ge0,\\ \infty, & k>\rho\ge0.\end{cases} \tag{5.10}$$

Thus, the power series (5.8) for z^{ρ} is purely formal since it contains infinitely many series coefficients that are infinite in magnitude.

The most general case is the Laguerre expansion (5.1) for $z^{\rho}\mathrm{e}^{uz}$ with $\rho \in \mathbb{R}\backslash\mathbb{N}_0$ and $u \in (-\infty, 1/2)$. It is immediately obvious that $z^{\rho}\mathrm{e}^{uz}$ is analytic at $z = 0$ if ρ is integral, i.e., if $\rho = m$ with $m \in \mathbb{N}_0$, and it is nonanalytic if ρ is nonintegral. This implies that the inner μ series in (4.11) diverge if ρ is nonintegral, and it converges if ρ is a nonnegative integer. However, ρ occurs on the right-hand side of (5.1) apart from the prefactor $(1-u)^{-\alpha-\rho-1}\Gamma(\alpha+\rho+1)/\Gamma(\alpha+1)$ only in the terminating hypergeometric series ${}_2F_1(-n, \alpha+\rho+1; \alpha+1; 1/(1-u))$. Since the prefactor does not affect the convergence and existence of the resulting expansions, we have to analyze the asymptotics of the terminating hypergeometric series as $n \to \infty$.

Thus, with the Laguerre series coefficients

$$\lambda_n^{(\alpha)} = (1-u)^{-\alpha-\rho-1} \frac{\Gamma(\alpha+\rho+1)}{\Gamma(\alpha+1)} \times {}_2F_1\left(-n, \alpha+\rho+1; \alpha+1; \frac{1}{1-u}\right), \quad \rho \in \mathbb{R}\backslash\mathbb{N}_0, \tag{5.11}$$

the inner μ series in (4.11) diverge for sufficiently large values of the outer index ν, and with the coefficients

$$\lambda_n^{(\alpha)} = (1-u)^{-\alpha-m-1} (\alpha+1)_m \times {}_2F_1\left(-n, \alpha+m+1; \alpha+1; \frac{1}{1-u}\right), \quad m \in \mathbb{N}_0 \tag{5.12}$$

the inner μ series in (4.11) converge. This is certainly a surprising observation which indicates that the difference between the almost identical terminating hypergeometric series ${}_2F_1$ in (5.11) and (5.12), respectively, is greater than it appears at first sight.

Nevertheless, this puzzle can be resolved by analyzing the large n asymptotics of the terminating hypergeometric series in (5.11) and (5.12), respectively. The study of large parameters of a Gaussian hypergeometric series is an old problem of special function theory with an extensive literature (see for example [159–161,187] and references therein).

Large parameter estimates of that kind turned out be useful in the context of multicenter integrals. In [38, Appendix], we derived and used large parameter estimates for some special Gaussian hypergeometric series to analyze the rate of convergence of certain series expansions for multicenter integrals.

If we apply the linear transformation [154, p. 47]

$${}_2F_1(a, b; c; z) = (1-z)^{-a}\, {}_2F_1\big(a, c-b; c; z/(z-1)\big) \tag{5.13}$$

to the hypergeometric series in (5.12), we obtain:

$${}_2F_1\left(-n, \alpha+m+1; \alpha+1; \frac{1}{1-u}\right) = \left(\frac{u}{u-1}\right)^n {}_2F_1\left(-n, -m; \alpha+1; \frac{1}{u}\right), \quad m, n \in \mathbb{N}_0. \tag{5.14}$$

If n becomes large and m is fixed, the terminating hypergeometric series on the right-hand side can be expressed as follows:

$${}_2F_1\left(-n, -m, \alpha+1; \frac{1}{u}\right) = \sum_{\mu=0}^{m} \frac{(-n)_\mu (-m)_\mu}{(\alpha+1)_\mu} \frac{u^{-\mu}}{\mu!}. \tag{5.15}$$

The asymptotically dominant contribution on the right-hand side is the last term with $\mu = m$. With the help of (5.6) we find $(-n)_m = \mathrm{O}(n^m)$ as $n \to \infty$. Since $u \in (-\infty, 1/2)$ implies $u/(u-1) \in (-1, 1)$, we can conclude that the right-hand side of (5.14) decays exponentially as $n \to \infty$ because of the prefactor $[u/(u-1)]^n$. Thus, the inner μ series in (4.11) converge if the coefficients $\lambda_n^{(\alpha)}$ are chosen according to (5.12).

If we apply the linear transformation (5.13) to the hypergeometric series in (5.11), we do not obtain an expression that would be useful for our purposes. Therefore, we apply instead the analytic continuation formula [154, pp. 47–48]

$$\begin{aligned} {}_2F_1(a, b; c; z) &= \frac{\Gamma(c)\Gamma(c-a-b)}{\Gamma(c-a)\Gamma(c-b)}\, {}_2F_1(a, b; a+b-c+1; 1-z) \\ &\quad + \frac{\Gamma(c)\Gamma(a+b-c)}{\Gamma(a)\Gamma(b)}\, (1-z)^{c-a-b} \\ &\quad \times {}_2F_1(c-a, c-b; c-a-b+1; 1-z), \\ &\qquad |\arg(1-z)| < \pi, \quad c-a-b \neq \pm m, \quad m \in \mathbb{N}_0, \end{aligned} \tag{5.16}$$

to the hypergeometric series in (5.11) and obtain:

$$\begin{aligned} &{}_2F_1\left(-n, \alpha+\rho+1; \alpha+1; \frac{1}{1-u}\right) \\ &\quad = \frac{(-\rho)_n}{(\alpha+1)_n}\, {}_2F_1\left(\alpha+\rho+1, -n; \rho-n+1; \frac{u}{u-1}\right). \end{aligned} \tag{5.17}$$

Application of the linear transformation (5.13) then yields:

$$\begin{aligned} &{}_2F_1\left(-n, \alpha+\rho+1; \alpha+1; \frac{1}{1-u}\right) \\ &\quad = (1-u)^{\alpha+\rho+1}\, \frac{(-\rho)_n}{(\alpha+1)_n}\, {}_2F_1\left(\rho+1, \alpha+\rho+1; \rho-n+1; u\right). \end{aligned} \tag{5.18}$$

If we set $u = 0$ in (5.18), the hypergeometric series on the right-hand side terminates after the first term. Thus, we see once more that (5.1) simplifies for $u = 0$ to yield (5.2).

With the help of (5.6) we find $(\rho - n + 1)_m = \mathrm{O}(n^m)$ as $n \to \infty$. Thus, the hypergeometric series on the right-hand side of (5.18) can for arbitrary $k \in \mathbb{N}_0$ be expressed as follows:

$$\begin{aligned} &{}_2F_1\left(\rho+1, \alpha+\rho+1; \rho-n+1; u\right) \\ &\quad = \sum_{\kappa=0}^{k} \frac{(\rho+1)_\kappa (\alpha+\rho+1)_\kappa}{(\rho-n+1)_\kappa \kappa!}\, u^\kappa + \mathrm{O}\big(n^{-k-1}\big), \quad n \to \infty. \end{aligned} \tag{5.19}$$

For $u \in (-1, 1/2)$, this hypergeometric series converges and we have a convergent asymptotic expansion as $n \to \infty$. For $u \in (-\infty, 1]$, the hypergeometric series diverges, but (5.19) nevertheless holds in the sense of an asymptotic expansion as $n \to \infty$. If we set $k = 0$ in (5.19) and use (5.7), we find that the Laguerre series coefficients in (5.11) satisfy the leading order asymptotics

$$\lambda_n^{(\alpha)} \sim \frac{\Gamma(\rho+\alpha+1)}{\Gamma(\alpha+1)} \frac{(-\rho)_n}{(\alpha+1)_n} \sim \frac{\Gamma(\rho+\alpha+1)}{\Gamma(-\rho)} n^{-\alpha-\rho-1}, \quad n \to \infty. \tag{5.20}$$

This asymptotic estimate, which does not depend on u, shows once more that $z^\rho \mathrm{e}^{uz}$ is not analytic at $z = 0$ if ρ is nonintegral. The inner μ series in (4.11) diverge for sufficiently large values of the outer index ν.

Comparison of (5.20) with (5.7) shows that the Laguerre series coefficients $\lambda_n^{(\alpha)}$ in (5.2), which correspond to $z^\rho \mathrm{e}^{uz}$ with $u \in (-\infty, 1/2)$, and the coefficients in (5.2), which correspond to z^ρ or to $u = 0$ in $z^\rho \mathrm{e}^{uz}$, possess the same leading order asymptotics as $n \to \infty$ that does not depend of u.

6 The transformation of one-range to two-range addition theorems

As discussed in the previous Sections, the legitimacy of Guseinov's rearrangement of a k-dependent one-range addition theorem (3.1), whose series expansions (3.10) for the angular projections (3.9) are essentially Laguerre series of the type of (4.4), can be checked by analyzing the convergence of the transformation formula (4.11). One only has to determine the asymptotic sign pattern and the asymptotic decay rate of the expansion coefficients $\lambda_n^{(\alpha)}$ of the corresponding Laguerre series and employ the sufficient convergence criteria formulated in [207].

As discussed in Sect. 5, this approach works in a very satisfactory way in the case of the Laguerre series (5.1) for $z^\rho \mathrm{e}^{uz}$ or the equivalent one-center expansion (5.4) for the Slater-type function $\chi_{N,L}^M(\beta, \boldsymbol{r})$ with an in general nonintegral principal quantum number $N \in \mathbb{R}\backslash\mathbb{N}$.

The one-center expansions considered in Sect. 5 have the highly advantageous feature that they are comparatively simple. Therefore, we can understand the large index asymptotics of the expansion coefficients via the large index asymptotics of some Gaussian hypergeometric series, whose derivation is not straightforward but nevertheless not too difficult. In this way, we can explain the rate of convergence or divergence of the rearrangements of the Laguerre series (5.1).

Guseinov's k-dependent one-range addition theorems are genuine two-center problems. Therefore, the situation is much more difficult and we are confronted with non-trivial technical problems. The expansion coefficients of such an addition theorem are according to (2.9), (2.12), and (3.1) overlap integrals, which are fairly complicated functions $\mathbb{R}^3 \to \mathbb{C}$ whose asymptotic sign patterns and asymptotic decay rates cannot be determined easily. But even in this troublesome two-center case, we can arrive at some definite conclusions by pursuing an indirect approach based on the analysis of the singularities of the function which is to be expanded.

Our starting point is a k-dependent one-range addition theorem (3.1) for a Slater-type function $\chi_{N,L}^M(\beta, \boldsymbol{r} \pm \boldsymbol{r}')$ with an in general nonintegral principal quantum number

$N \in \mathbb{R} \backslash \mathbb{N}$. We assume that we succeeded in constructing the series expansions (3.10) for the angular projections (3.9) of the one-range addition theorem (3.1).

For the moment, let us also assume that the expansion coefficients of the series expansions (3.10), which are Laguerre series of the type of (4.4), have asymptotic sign patterns and asymptotic decay rates which according to the criteria formulated in [207] guarantee that the transformation formula (4.11) produces functions $\mathbb{C} \to \mathbb{C}$ that are analytic in a neighborhood the origin $z = 0$.

Superficially, it appears that under these circumstances the legitimacy of Guseinov's rearrangement is guaranteed: A k-dependent one-range addition theorem (3.1), which is an expansion in terms of Guseinov's complete and orthonormal functions $\{{}_k\Psi_{n,\ell}^{m}(\gamma, \boldsymbol{r})\}_{n\ell m}$, is transformed to a one-range addition theorem of the type of (4.1), which is an expansions in terms of Slater-type functions $\{\chi_{n,L}^{M}(\gamma, \boldsymbol{r})\}_{n\ell m}$ with integral principal quantum numbers n and a common scaling parameter $\gamma > 0$.

But such a conclusion is premature. The transformed expansion (4.1) in terms of Slater-type functions can only be a one-range addition theorem, i.e., a map $\mathbb{R}^3 \times \mathbb{R}^3 \to \mathbb{C}$, if it converges for *all* $\boldsymbol{r}, \boldsymbol{r}' \in \mathbb{R}^3$. This requires that the power series (4.3) for the angular projections of the expansion (4.2) for $\exp(\gamma r) \chi_{N,L}^{M}(\beta, \boldsymbol{r} \pm \boldsymbol{r}')$ converge for *all* $r, r' \in [0, \infty)$. This is a very demanding requirement, which cannot be satisfied in the case of exponentially decaying functions such as Slater-type functions. In the two-center case, it is irrelevant whether the principal quantum number of the Slater-type function is integral or nonintegral.

A function $f : \mathbb{C} \to \mathbb{C}$ is analytic at the origin $z = 0$ in the sense of complex analysis if it has a power series in z that converges in some neighborhood of $z = 0$. Or to put it differently: Such an f is analytic at $z = 0$ if its power series in z has a circle of convergence with a *nonzero* radius. As is well known, we cannot tacitly assume that the radius of convergence of a power series is necessarily infinite, or equivalently, we cannot assume that f is necessarily an entire function that is analytic for all $z \in \mathbb{C}$.

Therefore, we should look for features of functions analytic at $z = 0$, which rule out an infinite radius of convergence but which do not interfere with the existence of a Laguerre series of the type of (4.4). My subsequent arguments are based on the simple, but nevertheless very consequential fact that power series and Laguerre series differ substantially in the way how they are affected by singularities of the function which is to be expanded.

Power series converge pointwise in their circles of convergence, and in the interior of these circles they not only converge uniformly but they can also be used for the computation of higher derivatives. Since, however, the higher derivatives of a function ultimately become infinite in magnitude at a singularity, the radius of the circle of convergence is determined by the location of that singularity which is closest to the expansion point.

If the function, which is to be expanded, possesses a singularity somewhere in the complex plane $\mathbb{C}$, the radius of convergence of its power series cannot be infinite. This has immediate and undesirable consequence for integrals over the positive real semi-axis $[0, \infty)$ as they typically occur in the theory of Laguerre polynomials or in the radial parts of the three- and six-dimensional integrals in electronic structure theory. If the semi-infinite integration interval is not contained completely in the circle of convergence, the term-wise integration of such a power series either leads to convergence to a wrong result or to divergence.

In that respect, Laguerre series have much more convenient properties precisely because they in general do not converge pointwise. As discussed in more detail in Appendix D, the existence of a Laguerre series of the type of (4.4) for some function $f : \mathbb{C} \to \mathbb{C}$ is guaranteed as long as f belongs to the weighted Hilbert space $L^2_{\mathrm{e}^{-z} z^{\alpha}}\bigl([0,\infty)\bigr)$ defined by (D.8). Of course, f must not have a non-integrable singularity on the integration interval $[0, \infty)$, but singularities away from the positive real semi-axis cause no problems. Loosely speaking, we can say that a Laguerre series simply ignores all singularities which are not located on the integration contour. Power series cannot do that. For them, *all* singularities matter even if they are far away from the integration contour.

These differences between power series and Laguerre series, respectively, can be illustrated by considering the following class of functions:

$$F_{\eta}(z; u, \theta) = \bigl[z^2 + u^2 - 2zu\cos\theta\bigr]^{\eta}, \quad z, u \in \mathbb{C}, \quad \eta, \theta \in \mathbb{R}. \tag{6.1}$$

For $\eta = 1/2$, the function $F_{\eta}(z; u, \theta)$ is nothing but the explicit expression for the difference $|\boldsymbol{x} - \boldsymbol{y}| = [x^2 + y^2 - 2xy\cos\theta]^{1/2}$ of two vectors $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^3$ in spherical polar coordinates in disguise, and for $\eta = -1/2$, it corresponds to the Coulomb or Newton potential $1/|\boldsymbol{x} - \boldsymbol{y}|$.

As long as $F_{\eta}(z; u, \theta)$ does not have a non-integrable singularity on the positive real semi-axis, it belongs to the weighted Hilbert space $L^2_{\mathrm{e}^{-z} z^{\alpha}}\bigl([0,\infty)\bigr)$ defined in (D.8). Therefore, $F_{\eta}(z; u, \theta)$ possesses a Laguerre series of the type of (4.4), although I was not able to find a closed form expression for the coefficients of this expansion.

If η is a nonnegative integer, $\eta = n$ with $n \in \mathbb{N}_0$, $F_{\eta}(z; u, \theta)$ is a polynomial in z and therefore an analytic function for all $z \in \mathbb{C}$. But if $\eta \in \mathbb{R}\backslash\mathbb{N}_0$, $F_{\eta}(z; u, \theta)$ has singularities at

$$z_{1,2} = \Bigl\{\cos\theta \pm \sqrt{[\cos\theta]^2 - 1}\Bigr\}\, u. \tag{6.2}$$

Accordingly, the radius of convergence of its power series about $z = 0$ is equal to $|u|$.

The function $F_{\eta}(z; u, \theta)$ essentially corresponds to the well known generating function

$$\bigl[1 - 2xt + t^2\bigr]^{-\lambda} = \sum_{n=0}^{\infty} C_n^{\lambda}(x)\, t^n, \quad |t| < 1, \quad \lambda \neq 0, \tag{6.3}$$

of the Gegenbauer polynomials [154, p. 222]. Thus, $F_{\eta}(z; u, \theta)$ possesses—depending on the relative magnitudes of $|z|$ and $|u|$—two complementary power series expansions. For $|z/u| < 1$, it possesses a convergent power series in z/u,

$$F_{\eta}(z; u, \theta) = u^{2\eta} \sum_{n=0}^{\infty} C_n^{-\eta}\bigl(\cos\theta\bigr)\, (z/u)^n, \tag{6.4}$$

and for $|z/u| > 1$, it possesses a convergent *inverse* power series in z/u,

$$F_\eta(z; u, \theta) = z^{2\eta} \sum_{n=0}^{\infty} C_n^{-\eta}\big(\cos\theta\big)\,(u/z)^n, \tag{6.5}$$

which can also be interpreted as a convergent power series in u/z.

Let us now assume that the singularities (6.2) of $F_\eta(z; u, \theta)$ with $\eta \in \mathbb{R}\backslash\mathbb{N}$ do not lie on the integration interval $[0, \infty)$ and that we succeeded in constructing its Laguerre series of the type of (4.4), possibly by purely numerical means. Then, the application of the transformation formula (4.11) to this Laguerre series produces—if necessary with the help of nonlinear sequence transformations as described in [207, Sect. 6]—the power series (6.4), which converges for $|z/u| < 1$ and which diverges for $|u/z| < 1$.

The small z series (6.4) accomplishes at least for $|z/u| < 1$ a separation of the variables z and u and therefore resembles a two-range addition theorem. For $|z/u| > 1$, the large z series (6.5) also accomplishes this separation, but I see no obvious way of computing the large z series (6.5) from the Laguerre series for $F_\eta(z; u, \theta)$. Instead, we would have to construct a Laguerre series in u—this is possible since z and u play a symmetrical role in $F_\eta(z; u, \theta)$—from which we can compute the large z series (6.5) which is also a small u series.

These considerations show that if we want to represent $F_\eta(z; u, \theta)$ by power series in z, a two-range scenario cannot be avoided. It does not matter if we start from a Laguerre series which provides a unique representation of $F_\eta(z; u, \theta)$ that is computationally useful in integrals over the whole real semi-axis. The singularities (6.2) of $F_\eta(z; u, \theta)$ with $\eta \in \mathbb{R}\backslash\mathbb{N}$ imply that there can be no power series in z which converges for all $z \in \mathbb{C}$.

In the context of addition theorems, it may be of interest that the generating function (6.3) of the Gegenbauer polynomials can be used for the construction of two-range addition theorems in a relatively straightforward way. If we set $\lambda = -\nu/2$, $t = r_</r_>$, and $x = \cos\theta$ in the generating function (6.3), we obtain the following Gegenbauer expansion for the general power function

$$|\boldsymbol{r}_< \pm \boldsymbol{r}_>|^\nu = r_>^\nu \sum_{n=0}^{\infty} (\mp 1)^n\, C_n^{-\nu/2}(\cos\theta)\,(r_</r_>)^n, \quad \nu \in \mathbb{R}. \tag{6.6}$$

The two-range form of this Gegenbauer expansion is a direct consequence of the convergence condition $|t| < 1$ in (6.3) which translates to the convergence condition $r_</r_> < 1$.

We can easily construct an addition theorem from the Gegenbauer expansion (6.6): We only have to replace the Gegenbauer polynomials by Legendre polynomials. However, the practical realization of this obvious idea had apparently not been so easy. As discussed by Steinborn and Filter [182, pp. 269–270], many authors had quite a few problems with the determination of explicit expressions for the coefficients of the expansion of Gegenbauer polynomials in terms of Legendre polynomials. Also

Steinborn and Filter constructed very messy expressions for these coefficients which are restricted to certain superscripts of the Gegenbauer polynomial [181, Sect. 3].

This is somewhat strange because already at that time a much more convenient expression for these expansion coefficients had been available in the mathematical literature. In Exercise 4 on p. 284 of Rainville's book [165], one finds the following relationship, where $\lfloor m/2 \rfloor$ denotes the integral part of $m/2$ (compare [218, Eq. (5.2)]):

$$C_m^{\mu}(x) = \sum_{s=0}^{\lfloor m/2 \rfloor} \frac{(\mu)_{m-s}\,(\mu-1/2)_s}{(3/2)_{m-s}\,s!}\,(2m-4s+1)\,P_{m-2s}(x). \tag{6.7}$$

This result can be proved via the explicit expression [36, Eq. 7.313.7 on p. 836] for the integral $\int_{-1}^{1}(1-x)^{\alpha}(1+x)^{\nu-1/2}C_m^{\mu}(x)C_n^{\nu}(x)\mathrm{d}x$. One only has to set $\nu = 1/2$ and perform the limit $\alpha \to 0$, which requires, however, some algebraic trickery.

If we now insert (6.7) into (6.6) and rearrange the order of summations, we obtain after some algebra the following expansion in terms of Legendre polynomials:

$$\begin{aligned} |\boldsymbol{r}_< \pm \boldsymbol{r}_>|^{\nu} = r_>^{\nu} \sum_{\ell=0}^{\infty} (\mp 1)^{\ell}\,P_{\ell}(\cos\theta)\,(r_</r_>)^{\ell} \\ \times \frac{(-\nu/2)_{\ell}}{(3/2)_{\ell}}\,{}_2F_1\big(\ell-\nu/2, -[\nu+1]/2; \ell+3/2; [r_</r_>]^2\big). \end{aligned} \tag{6.8}$$

If ν is an even integer, $\nu = 2n$ with $n \in \mathbb{N}_0$, $|\boldsymbol{r}_< \pm \boldsymbol{r}_>|^{\nu}$ is a polynomial in both $r_<$ and $r_<$ and therefore analytic. The infinite ℓ series in (6.8) terminates because of the Pochhammer symbol $(-\nu/2)_{\ell} = (-n)_{\ell}$, implying $\ell \le n$. Similarly, the Gaussian hypergeometric series ${}_2F_1$ in (6.8) terminates since $\ell - \nu/2 = \ell - n$ is either a negative integer or zero.

In (6.8), we only have to replace the Legendre polynomials by spherical harmonics via the so-called spherical harmonic addition theorem (2.4) to obtain an expansion in terms of spherical harmonics, which had originally been derived by Sack [169, Eq. (19)] by solving a partial differential equation and which converges as long as $r_</r_> < 1$ holds:

$$\begin{aligned} |\boldsymbol{r}_< \pm \boldsymbol{r}_>|^{\nu} = 4\pi r_>^{\nu+1} \sum_{\ell=0}^{\infty} (\mp 1)^{\ell} \sum_{m=-\ell}^{\ell} \big[\mathscr{Y}_{\ell}^{m}(\boldsymbol{r}_<)\big]^{*}\,\mathscr{Z}_{\ell}^{m}(\boldsymbol{r}_>) \\ \times \frac{(-\nu/2)_{\ell}}{(3/2)_{\ell}}\,{}_2F_1\big(\ell-\nu/2, -[\nu+1]/2; \ell+3/2; [r_</r_>]^2\big). \end{aligned} \tag{6.9}$$

This two-range addition theorem simplifies considerably and also assumes a one-range form if ν is a positive even integer, $\nu = 2n$ with $n \in \mathbb{N}$ (see above or also [202, pp. 1258–1259]). But for arbitrary $\nu \in \mathbb{R}$, (6.9) is a two-range addition theorem. This is a direct consequence of its derivation via the generating function (6.3) of the Gegenbauer polynomials. which is a power series in t with a nonzero, but finite radius of convergence.

This observation suggests the following interpretation: A two-range addition theorem for a function $f(\boldsymbol{r}_< \pm \boldsymbol{r}_>)$ having its only singularity at $\boldsymbol{r}_< \pm \boldsymbol{r}_> = \boldsymbol{0}$ corresponds to a possibly rearranged power series in $r_<$ with a finite radius of convergence, and this radius is determined by the condition $r_< < r_>$. This interpretation is also confirmed by the differential operator (2.7) which had been the central tool for the derivation of two-range addition theorems in [199,201] or in [202, Sect. 7].

This interpretation also applies to the addition theorem (6.9). For arbitrary $\nu \neq 0, 2, 4, \ldots$, the general power function $|\boldsymbol{r}_< \pm \boldsymbol{r}_>|^\nu$ has a singularity for $\boldsymbol{r}_< \pm \boldsymbol{r}_> = \boldsymbol{0}$, and this singularity determines the radius of convergence of its power series in $r_<$ and enforces a two-range form [199,201,202].

These conclusions about the nature of the addition theorem for the general power function $|\boldsymbol{r}_< \pm \boldsymbol{r}_>|^\nu$ help us to understand some essential features of addition theorems for Slater-type functions that converge pointwise. For the sake of simplicity, let us first consider the so-called $1s$ function

$$\exp\bigl(-\beta|\boldsymbol{r} - \boldsymbol{r}'|\bigr) = \exp\Bigl(-\beta \Bigl[r^2 + r'^2 - 2rr' \cos\theta\Bigr]^{1/2}\Bigr) \tag{6.10}$$

and let us also assume $r' > 0$. If Guseinov's rearrangements are legitimate, then $\exp\bigl(-\beta|\boldsymbol{r} - \boldsymbol{r}'|\bigr)$ must possess an expansion of the type of (4.1) in terms of Slater-type functions $\{\chi_{n,\ell}^m(\gamma, \boldsymbol{r})\}_{n\ell m}$, which converges for the whole argument set $\mathbb{R}^3 \times \mathbb{R}^3$. Obviously, this is equivalent to requiring that $\exp\bigl(\gamma r\bigr) \exp\bigl(-\beta|\boldsymbol{r} - \boldsymbol{r}'|\bigr)$ possesses a power series about $r = 0$, which converges for all $r \in [0, \infty)$. Since, however, $\exp\bigl(\gamma r\bigr)$ is an entire function, whose power series in r converges in the whole complex plane $\mathbb{C}$, we can ignore it for the moment. It is sufficient to analyze whether the $1s$ function (6.10) possesses a convergent power series in r and for which values of r and r' this series converges.

If we expand the exponential on the right-hand side of (6.10), we obtain:

$$\exp\bigl(-\beta|\boldsymbol{r} - \boldsymbol{r}'|\bigr) = \sum_{\kappa=0}^{\infty} \frac{(-\beta)^\kappa}{\kappa!} [r^2 + r'^2 - 2rr' \cos\theta]^{\kappa/2}. \tag{6.11}$$

If the index κ is even, $\kappa = 2k$ with $k \in \mathbb{N}_0$, then $[r^2 + r'^2 - 2rr' \cos\theta]^k$ is a polynomial in r which is obviously analytic for all $r \in [0, \infty)$. But if κ is odd, $\kappa = 2k + 1$ with $k \in \mathbb{N}_0$, we are in trouble. We can use the generating function (6.3) of the Gegenbauer polynomials to obtain a power series expansion in r/r'

$$\begin{aligned} [r^2 + r'^2 - 2rr' \cos\theta]^{k+1/2} &= r'^{2k+1} \bigl[1 + (r/r')^2 - 2(r/r') \cos\theta\bigr]^{k+1/2} \\ &= r'^{2k+1} \sum_{j=0}^{\infty} C_j^{-k-1/2}\bigl(\cos\theta\bigr)\, (r/r')^j. \end{aligned} \tag{6.12}$$

Unfortunately, the Gegenbauer expansion (6.12) converges only if $r/r' < 1$ holds. Therefore, the expansion obtained in this way corresponds to the case $|\boldsymbol{r}| < |\boldsymbol{r}'|$ of the two-range addition theorem for $|\boldsymbol{r} \pm \boldsymbol{r}'|^{k+1/2}$ which is a special case of (6.9).

This has some far-reaching consequences for the analyticity of the 1s function $\exp\bigl(-\beta|\boldsymbol{r}-\boldsymbol{r}'|\bigr)$ at $r = 0$. The odd powers in the power series expansion (6.11) are singular for $\boldsymbol{r}-\boldsymbol{r}' = \boldsymbol{0}$. This fact makes it impossible to construct for either $\exp\bigl(-\beta|\boldsymbol{r}-\boldsymbol{r}'|\bigr)$ or $\exp(\gamma r)\exp\bigl(-\beta|\boldsymbol{r}-\boldsymbol{r}'|\bigr)$ with $r' > 0$ a power series in r that converges for all $r \in [0,\infty)$. This is only possible in the one-center case $\boldsymbol{r}' = \boldsymbol{0}$. Consequently, a one-range addition theorem of the type of (4.1), which converges pointwise for all $\boldsymbol{r} \in \mathbb{R}^3$ or equivalently for all $r \in [0,\infty)$, cannot exist for the 1s function if $\boldsymbol{r}' \neq \boldsymbol{0}$.

An explicit expression for two-range addition theorem for the 1s function (6.10) can be derived easily via the following Gegenbauer-type addition theorem for the modified Bessel function $w^{-\nu}K_\nu(\gamma w)$ with $w = \bigl[\rho^2 + r^2 - 2r\rho\cos\theta\bigr]^{1/2}$, $0 < \rho < r$, and $\nu \in \mathbb{C}\backslash\mathbb{N}_0$ [154, pp. 106–107]:

$$w^{-\nu}K_\nu(\gamma w) = 2^\nu\,\gamma^{-\nu}\,\Gamma(\nu)\,(r\rho)^{-\nu}\sum_{n=0}^{\infty} C_n^\nu(\cos\theta)\,I_{\nu+n}(\gamma\rho)\,K_{\nu+n}(\gamma r). \tag{6.13}$$

Here, $I_{\nu+n}(\gamma\rho)$ and $K_{\nu+n}(\gamma r)$ are modified Bessel function of the first and second kind, respectively [154, p. 66].

The modified Bessel function $w^{-\nu}K_\nu(\gamma w)$ in (6.13) is essentially a reduced Bessel function $\hat{k}_\nu(\gamma w)$ defined by (2.16). On the basis of (2.4, 6.7), and (6.13), the following two-range addition theorem for reduced Bessel functions with half-integral orders can be derived in a fairly straightforward way ([182, Eq. (3.4)] or, as an improved version [218, Eq. (5.5)]):

$$\begin{aligned}
\hat{k}_{n-1/2}\bigl(\beta|\boldsymbol{r}_< \pm \boldsymbol{r}_>|\bigr) &= \frac{(-1)^n 8\pi}{(2n-1)!!}\,(\beta r_<)^{n-1/2}(\beta r_>)^{n-1/2} \\
&\times \sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell} (\mp 1)^\ell \bigl[Y_\ell^m(\boldsymbol{r}_</r_<)\bigr]^* Y_\ell^m(\boldsymbol{r}_>/r_>) \\
&\times \sum_{\nu=0}^{n} \frac{(-n)_\nu (1/2-n)_{\ell+\nu}}{\nu!(3/2)_{\ell+\nu}}\,(\ell+2\nu-n+1/2) \\
&\times I_{\ell+2\nu-n+1/2}(\beta r_<)K_{\ell+2\nu-n+1/2}(\beta r_>).
\end{aligned} \tag{6.14}$$

This addition theorem was quite consequential for my later scientific interests. In my diploma thesis [192], which was published in condensed form in [183], I used this addition theorem for the evaluation of simple multicenter integrals of reduced Bessel functions.

If we set $m = 0$ in (2.17), we obtain $\hat{k}_{1/2}(z) = \mathrm{e}^{-z}$. Thus, we only have to set $n = 1$ in (6.14) to obtain a two-range addition theorem for the 1s function. At first sight, neither the addition theorem (6.14) nor its special case with $n = 1$ looks like a power series expansion in $r_<$. However, the modified Bessel functions $I_{\ell+2\nu-n+1/2}(\beta r_<)$ is defined by a power series in $\beta r_<$ [154, p. 66], which shows that the addition theorem (6.14) is nothing but an infinite multitude of ℓ-dependent rearranged power series expansions in $r_<$.

The same conclusions hold for the following two-range addition theorem of a B function [201, Eq. (5.11)] which can be viewed to be an anisotropic generalization of the addition theorem (6.14) for a reduced Bessel function:

$$
\begin{aligned}
B_{n,\ell}^{m}(\beta, \mathbf{r}_< \pm \mathbf{r}_>) = {} & \frac{(2\pi)^{3/2}}{(-2)^{n+\ell}} \sum_{\ell_1=0}^{\infty} \sum_{m=-\ell_1}^{\ell_1} (\mp 1)^{\ell_1} \left[\mathscr{Y}_{\ell_1}^{m_1}(\mathbf{r}_<) \right]^* \\
& \times \sum_{q=0}^{n+\ell} \frac{(-2)^q}{(n+\ell-q)!} (\beta r_<)^{n+\ell-\ell_1-q-1/2} I_{n+\ell+\ell_1-q+1/2}(\beta r_<) \\
& \times \sum_{\ell_2=\ell_2^{\min}}^{\ell_2=\ell_2^{\max}} {}^{(2)} \langle \ell_2 m + m_1 | \ell_1 m_1 | \ell m \rangle \\
& \times \sum_{s=0}^{\min(q,\Delta\ell_2)} (-1)^s \binom{\Delta\ell_2}{s} B_{q-\ell_2-s,\ell_2}^{m+m_1}(\beta, \mathbf{r}_>).
\end{aligned}
\tag{6.15}
$$

Other two-range addition theorems of B functions are discussed in [218, Sects. 4 and 5].

In (6.15), $\langle \ell_2 m + m_1 | \ell_1 m_1 | \ell m \rangle$ is a so-called Gaunt coefficient [31] which corresponds to the integral of the product of three spherical harmonics over the surface of the unit sphere in $\mathbb{R}^3$. The selection rules of this Gaunt coefficient (see for example [215, Sect. 3] or [202, Appendix C]) imply that $\Delta\ell_2 = (\ell + \ell_1 - \ell_2)/2$ in (6.15) is always either zero or a positive integer. The symbol $\sum^{(2)}$ in (6.15) indicates that the summation proceeds in steps of two.

Since a Slater-type function with an integral principal quantum number can according to (2.20) be expressed as a finite sum of B functions, we can conclude that the two-range addition theorem of a Slater-type function obtained by forming linear combinations of (6.15) is nothing but an infinite multitude of rearranged power series expansions in $r_<$.

These considerations apply also to Slater-type functions $\chi_{N,L}^{M}(\beta, \boldsymbol{r}_< \pm \boldsymbol{r}_>)$ with nonintegral principal quantum numbers N or to $\exp(\gamma r)\chi_{N,L}^{M}(\beta, \boldsymbol{r}_< \pm \boldsymbol{r}_>)$. These functions are obviously singular for $\boldsymbol{r}_< \pm \boldsymbol{r}_> = \boldsymbol{0}$, which implies that their power series expansions about $r_< = 0$ can only converge for $r_< < r_>$. Consequently, an expansion of the type of (4.1) in terms of Slater-type functions $\{\chi_{n,\ell}^{m}(\gamma, \boldsymbol{r})\}_{n,\ell,m}$ with integral principal quantum numbers n and a common scaling parameter $\gamma > 0$, that converges *pointwise* for *all* $\boldsymbol{r}, \boldsymbol{r}' \in \mathbb{R}^3$, cannot exist.

These considerations can be generalized further: Let us assume that $f(\boldsymbol{r} \pm \boldsymbol{r}')$ with $r' > 0$ is singular for $\boldsymbol{r} \pm \boldsymbol{r}' = \boldsymbol{0}$ but analytic elsewhere. Accordingly, a power series expansion for either $f(\boldsymbol{r} \pm \boldsymbol{r}')$ or for $\mathrm{e}^{\gamma r} f(\boldsymbol{r} \pm \boldsymbol{r}')$ about $r = 0$ can only converge for $r < r'$. This rules out the existence of an expansion of $f(\boldsymbol{r} \pm \boldsymbol{r}')$ in terms of Slater-type functions $\chi_{n,\ell}^{m}(\gamma, \boldsymbol{r})\}$ with integral principal quantum numbers n and a common scaling parameter $\gamma > 0$, that converges pointwise for all $\boldsymbol{r}, \boldsymbol{r}' \in \mathbb{R}^3$.

As shown in [199,201] or in [202, Sect. 7], pointwise convergent addition theorems are nothing but rearranged Taylor expansions. Thus, the assumed singularity of such an $f(\boldsymbol{r} \pm \boldsymbol{r}')$ for $\boldsymbol{r} \pm \boldsymbol{r}' = \boldsymbol{0}$ implies that a pointwise convergent addition theorem must have a two-range form.

Slater-type functions as well as all the other commonly used exponentially decaying basis functions have a singularity at the origin. Consequently, their pointwise convergent addition theorems must have a two-range form. In contrast, the Gaussian function $\exp(-\beta|\boldsymbol{r} \pm \boldsymbol{r}'|^2)$ is analytic for all $\boldsymbol{r}, \boldsymbol{r}' \in \mathbb{R}^3$. Consequently, it possesses a one-range addition theorem that converges pointwise [142, Eq. (8)].

It makes no difference if we start from a Laguerre series for a given function. If we apply the transformation formula (4.11) to the series expansions (3.10) for the angular projections (3.9) of Guseinov's one-range addition theorem (3.1) for $\chi_{N,L}^{M}(\beta, \boldsymbol{r} \pm \boldsymbol{r}')$, we obtain power series expansions in r for the angular projections which converge or diverge, depending on the relative magnitude of $\boldsymbol{r}$ and $\boldsymbol{r}'$.

Let us now assume that $f(\boldsymbol{r} \pm \boldsymbol{r}')$ is a function which is singular for $\boldsymbol{r} \pm \boldsymbol{r}' = \boldsymbol{0}$ and that we know its two-range addition theorem. If we accept the premise that its two-range addition theorem is nothing but a multitude of rearranged power series expansions in r that converge for $r/r' < 1$, then the uniqueness of a power series in the interior of its circle of convergence implies that Guseinov's rearrangements of one-range addition theorems cannot produce anything new. We obtain a two-range addition theorem for $\exp(\gamma r) f(\boldsymbol{r} \pm \boldsymbol{r}')$ by forming the Cauchy product of the power series for $\exp(\gamma r)$ with the possibly rearranged ℓ-dependent power series in r that occur in the two-range addition theorem for $f(\boldsymbol{r} \pm \boldsymbol{r}')$. In the final step, we only have to multiply the resulting addition theorem for $\exp(\gamma r) f(\boldsymbol{r} \pm \boldsymbol{r}')$ by $\exp(-\gamma r)$ or its power series to arrive at the possibly rearranged addition theorem for $f(\boldsymbol{r} \pm \boldsymbol{r}')$ from which we started.

The discussion of this Section may create the false impression that singularities of basis functions for electronic structure calculations are something very negative. This is certainly true in the case of analytical manipulations since virtually all manipulations becomes more difficult in the presence of singularities. However, Kato [141] had shown that the singularities of an atomic or molecular Hamiltonian translate to corresponding singularities of the eigenfunctions, commonly called cusps. But a cusp is just another word for a singularity. Thus, the ability of basis functions to reproduce the singularities of exact wave functions is of considerable importance for the rate of convergence of an electronic structure calculation.

Gaussian functions do not have singularities like exponentially decaying functions. In my opinion, this is the main reason why their multicenter integrals can be evaluated much more easily than the corresponding integrals of exponentially decaying functions. At the same time, the absence of singularities is also a major drawback of Gaussian functions. Many Gaussian functions are needed to approximate functions possessing singularities with sufficient accuracy.

7 Numerical implications of truncated expansions

The analysis of Sects. 1 and 5 shows that the one-center expansion (1.2) of a Slater-type function $\chi_{N,L}^{M}(\beta, \boldsymbol{r})$ in terms of Slater-type functions $\{\chi_{n,L}^{M}(\gamma, \boldsymbol{r})\}_{n=L+1}^{\infty}$ with integral principal quantum numbers $n \in \mathbb{N}$ and a common scaling parameter $\gamma > 0$ does not exist if the principal quantum number N is nonintegral. The leading coefficients of (1.2) are zero, and the higher coefficients are infinite in magnitude.

The nonexistance of (1.2) is a direct consequence of the fact that the radial part of $\chi_{N,L}^{M}(\beta, \boldsymbol{r})$ with $N \in \mathbb{R}\backslash\mathbb{N}$ is not analytic at $r = 0$. As shown in Sect. 5, this nonexistance can also be shown by applying the transformation formula (4.11) to the radial part of a k-dependent one-center expansion (5.4) for $\chi_{N,L}^{M}(\beta, \boldsymbol{r})$. In the case of nonintegral quantum numbers, the transformation formula (4.11) produces power series coefficients that are either zero or infinite in magnitude.

In Sect. 6 it was shown that the rearrangement of a k-dependent one-range addition theorem (3.1), which is a much more complicated expansion than its one-center limit (5.4), also does not produce the desired result. Both $\chi_{N,L}^{M}(\beta, \boldsymbol{r} \pm \boldsymbol{r}')$ and $\exp(\gamma r)\chi_{N,L}^{M}(\beta, \boldsymbol{r} \pm \boldsymbol{r}')$ with $r' > 0$ are analytic at $r = 0$. Consequently, the application of the transformation formula (4.11) to the series expansions of the angular projections of $\exp(\gamma r)\chi_{N,L}^{M}(\beta, \boldsymbol{r} \pm \boldsymbol{r}')$ produces mathematically meaningful power series expansions in r. Unfortunately, these power series expansions have a finite radius of convergence and they converge only for $r < r'$. This follows at once from the fact that both $\chi_{N,L}^{M}(\beta, \boldsymbol{r} \pm \boldsymbol{r}')$ and $\exp(\gamma r)\chi_{N,L}^{M}(\beta, \boldsymbol{r} \pm \boldsymbol{r}')$ are singular for $\boldsymbol{r} \pm \boldsymbol{r}' = \boldsymbol{0}$. Accordingly, Guseinov's rearrangements transform a *one-range addition theorem* for $\chi_{N,L}^{M}(\beta, \boldsymbol{r} \pm \boldsymbol{r}')$ to a *two-range addition theorem*. This is certainly not what Guseinov had tried to achieve.

But these observations do not tell the whole truth, and in particular they do not imply that Guseinov's approach is necessarily doomed. There is overwhelming evidence that Guseinov never transformed a *complete* one-range addition theorem of the type of (3.1) containing an infinite number of terms. Instead, Guseinov only transformed truncations of either addition theorems or their one-center limits, which all contain a finite number of terms only. Thus, Guseinov exclusively did his rearrangements with an analog of (4.8), which transforms a truncated Laguerre series of the type of (4.6) to a polynomial of the type of (4.9). To the best of my knowledge, Guseinov never used the complete transformation formula (4.11) and only claimed—probably on the basis of an insufficient amount of numerical evidence—that his transformed truncations remain meaningful in the limit of infinite expansion lengths, but he never provided convincing evidence supporting his claim.

The radial parts of the angular projections of Guseinov's truncations are apart from a common exponential $\exp(-\gamma r)$ finite linear combinations of generalized Laguerre polynomials in $2\gamma r$. Thus, for finite truncation orders $\mathscr{N}$, Guseinov's rearrangements are legitimate and produce polynomials in r.

In actual calculations, we always have to truncate infinite series expansions after a finite number of terms unless we are fortunate enough to find a way of expressing a series in closed form. Therefore, a skeptical reader might argue that Guseinov's approach is completely satisfactory from a practical point of view, and that my insistence on the convergence and existence of infinite series expansions, which in actual calculations have to be truncated and thus do not really occur in practice, is nothing but a mathematical over-sophistication.

However, Guseinov's rearranged addition theorems do not only suffer from the fact that in the limit of infinite expansions lengths they either do not exist or that they lose their one-range nature. These rearrangements cause also other problems which become particularly evident if one tries to achieve a (very) high accuracy by including a large number of terms in Guseinov's truncations.

One serious problem was already discussed in Sect. 3. As explained there, I have grave doubts that a Guseinov function ${}_k\Psi_{n,\ell}^{m}(\gamma, \boldsymbol{r})$ can be expressed in a numerically stable way as a finite sum of Slater-type functions $\{\chi_{n',\ell}^{m}(\gamma, \boldsymbol{r})\}_{n'=\ell+1}^{n}$ via (3.2) if the index n is large. This applies also to the substitution of overlap integrals involving Guseinov functions by finite sums of overlap integrals involving Slater-type functions via (3.3). Both (3.2) and (3.3) are based on the explicit expression (D.2) of the generalized Laguerre polynomial $L_n^{(\alpha)}(z)$, which tends to become numerically unstable if its index n becomes large. The reason is that the coefficients of orthogonal polynomials have strictly alternating signs.

The substitution of a function set, which is complete and orthonormal in a given Hilbert space, by a function set, which is only complete, but not orthogonal, also causes some nontrivial problems. In Sect. 3 it was emphasized that orthogonal expansions tend to be computationally well behaved because Parseval's equality (3.6) guarantees that their series coefficients are bounded in magnitude and vanish for large indices. In contrast, the series coefficients of nonorthogonal expansions are not necessarily bounded in magnitude and do not necessarily vanish with increasing index.

These complications with unbounded coefficients can be demonstrated convincingly by considering a truncation of the comparatively simple one-center expansion (5.4). This ansatz corresponds to the following approximation of a Slater-type function $\chi_{N,L}^{M}(\beta, \boldsymbol{r})$ with an in general nonintegral principal quantum number $N \in \mathbb{R}\backslash\mathbb{N}$ by a finite sum of Guseinov functions:

$$\begin{aligned}\chi_{N,L}^{M}(\beta, \boldsymbol{r}) \approx {} & \frac{(2\gamma)^{L+(k+3)/2}\,\beta^{N-1}}{[\beta+\gamma]^{N+L+k+2}} \frac{\Gamma(N+L+k+2)}{(2L+k+2)!} \\ & \times \sum_{\nu=0}^{\mathscr{N}} \left[\frac{(\nu+2L+k+2)!}{\nu!}\right]^{1/2} {}_k\Psi_{\nu+L+1,L}^{M}(\gamma, \boldsymbol{r}) \\ & \times {}_2F_1\left(-\nu, N+L+k+2; 2L+k+3; \frac{2\gamma}{\beta+\gamma}\right). \end{aligned} \tag{7.1}$$

If $\chi_{N,L}^{M}(\beta, \boldsymbol{r})$ belongs to the weighted Hilbert space $L_{r^k}^{2}(\mathbb{R}^3)$ defined by (2.15), this $\mathscr{N}$-dependent approximation is mathematically meaningful, and we can be sure that it converges in the mean with respect to the norm of $L_{r^k}^{2}(\mathbb{R}^3)$ as $\mathscr{N} \to \infty$.

We only have to cancel the spherical harmonics and remove the exponential on the right-hand side of (7.1) to see that the finite sum on the right-hand side corresponds to a truncated Laguerre series of the type of (4.6). If we now apply the transformation formula (4.8) to this truncated Laguerre series, we ultimately obtain an approximation of the Slater-type function $\chi_{N,L}^{M}(\beta, \boldsymbol{r})$ with $N \in \mathbb{R}\backslash\mathbb{N}$ as a finite linear combination of Slater-type functions $\chi_{n,L}^{M}(\gamma, \boldsymbol{r})$ with integral principal quantum numbers n.

For finite values of the truncation order $\mathscr{N}$, all coefficients of this approximation to $\chi_{N,L}^{M}(\beta, \boldsymbol{r})$ are well defined and finite. Unfortunately, this does not imply that this expression remains well behaved in the limit $\mathscr{N} \to \infty$. For large values of $\mathscr{N}$, the leading coefficients of the resulting expression approach zero and the higher coefficients diverge in magnitude.

This can also be demonstrated by inserting the expansion coefficients of the Laguerre series (5.2) for $z^{\rho} \mathrm{e}^{uz}$ with nonintegral $\rho \in \mathbb{R} \backslash \mathbb{N}_0$ into the μ series in (4.11). If we replace the exact expressions for the Laguerre series coefficients of the later terms of the μ series with indices $\mu \geq M$ by their leading order asymptotic approximations (5.20), we obtain the following leading order asymptotic approximation:

$$\sum_{\mu=M}^{\infty} \frac{(\alpha+\nu+1)_{\mu}}{\mu!} \lambda_{\mu+\nu}^{(\alpha)} \sim \frac{\Gamma(\rho+\alpha+1)}{\Gamma(-\rho)\Gamma(\alpha+\nu+1)} \sum_{\mu=M}^{\infty} \mu^{\nu-\rho-1}, \quad M \to \infty. \tag{7.2}$$

The infinite series on the right-hand side is nothing but the tail of the Dirichlet series $\zeta(s) = \sum_{n=0}^{\infty} (n+1)^{-s}$ for the Riemann zeta function with $s = \rho - \nu + 1$ (see for example [154, p. 21]). As is well known, the Dirichlet series for $\zeta(s)$ converges for $\Re(s) > 1$ and diverges for $\Re(s) \leq 1$. Thus, the series (7.2) converges for $\nu < \rho$, and it diverges for $\nu > \rho$.

If $\Re(s)$ is only slightly larger than 1, the convergence of the Dirichlet series $\sum_{n=0}^{\infty} (n+1)^{-s}$ can become prohibitively slow (the horrifying example of the Dirichlet series with $s = 1.01$ is discussed in [214, p. 194]). The slowest convergence on the right-hand side of (7.2) occurs for the largest value of ν satisfying $\nu < \rho$, i.e., for $\nu = \lfloor \rho \rfloor$, where $\lfloor \rho \rfloor$ is the integral part of ρ. In this case, convergence can become so slow that it is practically impossible to evaluate the series on the right-hand of (7.2) with sufficient accuracy by adding up its terms successively. Instead, one has to employ suitable convergence acceleration techniques as for example the Euler-Maclaurin formula (see for example [214, Sect. 2] and references therein). In this context, it may be of interest that the Euler-Maclaurin formula for the Riemann zeta function and other asymptotic approximations to truncation errors of series representations for special functions can also be derived by solving systems of linear equations [203].

A skeptical reader might argue that my digression on the convergence properties of the Dirichlet series for the Riemann zeta is of no interest in the context of molecular electronic structure. However, I personally became interested in the Riemann zeta function because of certain infinite series expansions occurring in expressions for molecular integrals of exponentially decaying functions involving the Coulomb potential. The convergence properties of these expansions closely resemble that of the Dirichlet series for $\zeta(s)$ with $\Re(s)$ not much larger than 1 (see for example [38, Tables I, II, V, VI, and VII] or [184, Table 1]).

The slow convergence of the series on the right-side of (7.2) for ν only slightly smaller than ρ makes it (very) hard or even practically impossible to observe by purely numerical means that the leading terms of the formal power series for $z^{\rho} \mathrm{e}^{uz}$ with nonintegral $\rho \in \mathbb{R} \backslash \mathbb{N}_0$ vanish.

Moreover, the series on the right-hand side of (7.2) diverges for $\nu > \rho$, but it diverges quite slowly if ν is only slightly larger than ρ. Quite a few terms are needed to observe the divergence of such an infinite series in the case of small or moderately large values of ν. There is also the additional complication that it is by no means easy to establish unambiguously the divergence of a series of the type of (7.2) if only a finite number of terms are available [158].

A further complication occurs if we do not rearrange an infinite Laguerre series of the type of (4.4) via the complete transformation formula (4.11), which uses *all* Laguerre series coefficients $\lambda_n^{(\alpha)}$ with $n \in \mathbb{N}_0$, but via (4.8) which transforms the partial sum $f_M(z)$ of the Laguerre series (4.4) to a polynomial of degree M in z. Since the transformation formula (4.8) only uses the coefficients $\lambda_0^{(\alpha)}, \lambda_1^{(\alpha)}, \ldots, \lambda_M^{(\alpha)}$ and since M is in practice only moderately large, neither the vanishing of power series coefficients with $\nu < \rho$ nor the divergence of the coefficients with $\nu > \rho$ can be observed easily (everything remains finite). Consequently, I would not be surprised if Guseinov and Mamedov, who certainly had done test calculations, simply overlooked the nonexistence of their one-center expansion [122, Eq. (4)] in the limit $\mathscr{N} \to \infty$.

It would have been interesting if Guseinov and Mamedov had applied sequence transformations, because this could have helped them to see the vanishing or the divergence of their coefficients more clearly. My suggestion may sound paradoxical because sequence transformations are normally used to accelerate convergence or to associate a finite value to a divergent sequence or series. It was, however, shown in recent articles by Beckermann, Kalyagin, Matos, and Wielonsky [8], Beckermann, Matos, and Wielonsky [9], Brezinski [16], Brezinski and Redivo Zaglia [17], and Guilpin, Gacougnolle, and Simon [39] that sequence transformations can also be used to determine the location of discontinuities of functions more precisely or to show them more clearly. By a slight abuse of language, such an application of sequence transformations could be called *acceleration of divergence*.

Guseinov's and Mamedov's inability of observing any problems with their rearranged one-center expansions highlights once more the dangers of relying entirely on numerical test calculations without trying to understand the subtleties of the underlying mathematics.

One should also take into account that the apparent convergence of the sum of the leading terms of an infinite series to the correct limit does not prove the existence of this series, let alone its converges to the correct limit. As discussed in Appendix E, the phenomenon of *semiconvergence*—initial apparent convergence of the leading terms of an infinite series followed by divergence if more terms are included—is well established in the literature.

The examples in Appendix E on semiconvergence and related phenomena should suffice to convince even a skeptic that misinterpretations of seemingly convincing numerical evidence can happen easily. It also happened to me. In [196] I misinterpreted my summation results obtained by applying Wynn's epsilon algorithm [219], the d variant [195, Eq. (7.3-9)] of Levin's transformation [151], and the d variant of the so-called $\mathscr{S}$ transformation [195, Eq. (8.4-4)] to the partial sum of the first 22 perturbation series coefficients of the factorially divergent Rayleigh-Schrödinger perturbation series for the ground state energy of the quartic anharmonic oscillator. All calculations were done in FORTRAN 77 on a Cyber 180-995 E with a precision of approximately 29 decimal digits (for more details, see [205, pp. 7–8]).

Unfortunately, my conclusion in [196] that Levin's transformation produces a convergent result—although perfectly plausible at that time—was premature and based on the incomplete evidence provided by the first 22 perturbation series coefficients. In [213], we repeated my previous calculations using now 200 perturbation series coefficients calculated exactly with the help of Maple's rational arithmetic, and we did the summation calculations in Maple with a precision of up to 1000 decimal digits and transformation orders as high as $k = 199$. These calculations showed unambiguously that Levin's transformation failed to produce convergent results in the case of higher transformation orders, and that this failure could not be attributed to numerical instabilities. The divergence of Levin's transformation was also confirmed in [197, Table 2]. A similar divergence of Levin's transformation was later observed by Čížek, Zamastil, and Skála [19, p. 965] in the case of the hydrogen atom in an external magnetic field.

Of course, my misinterpretation in [196] or similar problems of other authors do not rule out the possibility that carefully conducted purely numerical investigations can provide valuable theoretical insight. In [10] we formulated with the help of some numerical techniques developed in [200] the conjecture that the factorially divergent perturbation expansion of a certain non-Hermitian $\mathscr{P}\mathscr{T}$-symmetric anharmonic oscillator is a Stieltjes series. Recently, our conjecture, whose correctness implies the Padé summability of this perturbation expansion, was proved rigorously by Grecchi, Maioli, and Martinez [37].

Let us now assume that we rearrange a truncation (7.1) of the one-center expansion (5.4) for $\chi_{N,L}^{M}(\beta, \boldsymbol{r})$ with nonintegral principal quantum number $N \in \mathbb{R}\backslash\mathbb{N}$. If the truncation order $\mathscr{N}$ in (7.1) is small, its increase will certainly improve the accuracy of the rearranged truncation. However, for sufficiently large values of $\mathscr{N}$, the behavior of the rearranged truncations changes. The leading order asymptotic approximation (7.2) implies that the accuracy ultimately deteriorates with increasing $\mathscr{N}$, and for $\mathscr{N} \to \infty$, the rearranged truncations ultimately become mathematically meaningless. Thus, rearranged truncations of the one-center expansion (5.4) are semiconvergent with respect to a variation of $\mathscr{N}$ for nonintegral principal quantum numbers $N \in \mathbb{R}\backslash\mathbb{N}$.

The semiconvergence of the rearranged truncations implies that they can be used for computational purposes at least for sufficiently small truncation orders $\mathscr{N}$. But obviously, one should be careful. It is necessary to investigate for which values of $\mathscr{N}$ the intrinsic pathologies of the rearranged expansions become intolerable. The leading order asymptotic approximation (7.2) indicates that even fairly large values of $\mathscr{N}$ should produce acceptable results, but additional and in particular more detailed numerical investigations, which also try to estimate the detrimental effect of possible numerical instabilities, would certainly be desirable.

One can look at the rearrangements of truncations (7.1) also from a different perspective. As discussed in Appendix C, *finite* approximations to a function $f \in \mathscr{H}$ of the type of (C.1) in terms of a function set, that is complete but nonorthogonal in some Hilbert space $\mathscr{H}$, can be constructed by minimizing the mean square deviation (C.2), although we cannot tacitly assume that these finite approximations can be extended to infinite expansions of the type of (C.3).

Thus, is certainly legitimate to *approximate* a Slater-type function $\chi_{N,L}^{M}(\beta, \boldsymbol{r})$ with a nonintegral principal quantum number $N \in \mathbb{R}\backslash\mathbb{N}$ by a finite linear combination of

Slater-type functions $\chi_{n,L}^{M}(\gamma, \boldsymbol{r})$ with integral principal quantum numbers n. However, a determination of the coefficients of these approximations via a purely numerical minimization of the mean square deviation does not look like a promising computational strategy in the context of addition theorems or multicenter integrals. In such a case, Guseinov's approach is most likely the better alternative.

The truncations (7.1) of the one-center expansion (5.4) are simple enough to permit a detailed mathematical analysis of Guseinov's rearrangements. But we would of course be much more interested in understanding the subtleties of the rearrangements of the truncations

$$\chi_{N,L}^{M}(\beta, \boldsymbol{r} \pm \boldsymbol{r}') \approx \sum_{n=1}^{\mathcal{N}} \sum_{\ell=0}^{n-1} \sum_{m=-\ell}^{\ell} {}_{k}\mathbf{X}_{n,\ell,m}^{N,L,M}(\gamma, \beta, \pm\boldsymbol{r}') \, {}_{k}\Psi_{n,\ell}^{m}(\gamma, \boldsymbol{r}) \qquad (7.3)$$

of a k-dependent addition theorem (3.1). The overlap integral ${}_{k}\mathbf{X}_{n,\ell,m}^{N,L,M}(\gamma, \beta, \pm\boldsymbol{r}')$ in (7.3) is defined by by (3.1b).

Since the k-dependent addition theorems (3.1) are genuine two-center problems, it is not at all easy to do a rigorous analysis of the mathematical properties of rearrangements of the truncations (7.3). Let me emphasize once more that there is a fundamental difference between the one-center case analyzed in Sect. 5 and the two-center case analyzed in Sect. 6. In the limit of infinite truncation orders $\mathcal{N}$, Guseinov's rearrangements of one-center expansions for Slater-type functions with nonintegral principal quantum numbers produce mathematically meaningless expansions, and for finite values of $\mathcal{N}$ these rearrangements are semiconvergent.

In the two-center case, Guseinov's rearrangements of one-range addition theorems produce mathematically meaningful expansions, but they only converge for $r < r'$. Consequently, these expansions correspond to the small r parts of two-range addition theorems. This is certainly not what Guseinov had tried to achieve.

Apart from being an undesirable result, the two-center nature of rearrangements of the truncations (7.3) in the limit of infinite truncation orders $\mathcal{N}$ is also a possible source of problems. For finite values of $\mathcal{N}$, the truncations (7.3) are obviously one-range addition theorems: The vector $\boldsymbol{r}$ occurs exclusively in the Guseinov functions ${}_{k}\Psi_{n,\ell}^{m}(\gamma, \boldsymbol{r})$, and $\boldsymbol{r}'$ occurs exclusively in the overlap integral ${}_{k}\mathbf{X}_{n,\ell,m}^{N,L,M}(\gamma, \beta, \pm\boldsymbol{r}')$. This applies also to their rearrangements. The vectors $\boldsymbol{r}$ and $\boldsymbol{r}'$ are still separated even if the Guseinov functions are replaced by Slater-type functions with integral principle quantum numbers via (3.2) and the overlap integrals involving Guseinov functions by overlap integrals of Slater-type functions via (3.3).

But in the limit of infinite truncation orders $\mathcal{N}$, a change resembling a phase transition takes place: The resulting rearranged expansions lose their advantageous one-range nature and converge to two-range addition theorems. As is well known, the decay rate of the coefficients γ_n of a power series $f(z) = \sum_{n=0}^{\infty} \gamma_n z^n$ as $n \to \infty$ determines the convergence type of this series: If γ_n decays factorially as $n \to \infty$, $f(z)$ is entire, and if γ_n decays only exponentially, the radius of convergence of its power series is finite. Thus, the expansion coefficients of the Slater-type functions $\chi_{n,\ell}^{m}(\gamma, \boldsymbol{r})$ in Guseinov's rearranged addition theorems apparently decay at most exponentially since these expansions only converge for $r < r'$.

Otherwise, very little can be said about the $\mathcal{N}$-dependence of Guseinov's rearrangements of the truncations (7.3). The problem is that in Sect. 6 the mathematical properties of Guseinov's rearranged addition theorems were analyzed via the singularity of a Slater-type function $\chi_{N,L}^{M}(\beta, \boldsymbol{r} \pm \boldsymbol{r}')$ for $\boldsymbol{r} \pm \boldsymbol{r}' = \mathbf{0}$, but not via the transformation formula (4.11). We would need the large index asymptotics of the overlap integrals ${}_{k}\mathbf{X}_{n,\ell,m}^{N,L,M}(\gamma, \beta, \pm \boldsymbol{r}')$ in (3.1). On the basis of our current level of understanding, such an asymptotic analysis seems to be out of reach. We do not have anything resembling a two-center analog of the leading order asymptotic approximation (7.2) which turned out to be so very useful in the one-center case.

Guseinov's rearrangements of one-range addition theorems can be used to construct *approximations* to a Slater-type function $\chi_{N,L}^{M}(\beta, \boldsymbol{r} \pm \boldsymbol{r}')$ with both integral and nonintegral principal quantum numbers in terms of a *finite* number of Slater-type functions $\chi_{n,\ell}^{m}(\gamma, \boldsymbol{r})$ with integral principal quantum numbers n. As in the one-center case, such a finite approximation of the type of (C.1) can—at least in principle—be constructed by minimizing the mean square deviation (C.2), although such a numerical determination of the expansion coefficients is most likely not a very good idea in the context of multicenter integrals.

But there remains a principal problem. If we use a two-range addition theorem in a multicenter integral and do not take into account its two-range nature by splitting up the integration interval of the resulting radial integration, we may well end up either with convergence to the wrong limit or even with a divergent series expansion for the multicenter integral.

For finite truncation orders $\mathcal{N}$, Guseinov's rearrangements of the truncations (7.3) are one-range addition theorems since the vectors $\boldsymbol{r}$ and $\boldsymbol{r}'$ are completely separated. Thus, these rearranged truncations can safely be used in multicenter integrals, and it is not necessary to split up the integration contour. But in the limit $\mathcal{N} \to \infty$, these rearrangements lose their convenient one-range property. Consequently, their careless use in a multicenter integral without splitting up the integration contour may produce either a wrong or a divergent result.

It makes sense to assume that the ultimate two-range nature of the rearrangements of the truncations (7.3) becomes noticeable already for sufficiently large, but finite values of $\mathcal{N}$. It is therefore conceivable that multicenter integrals, whose integrands contain a rearrangement of a truncations (7.3), are semiconvergent with respect to a variation of $\mathcal{N}$. Obviously, the exact behavior of these integrals as $\mathcal{N} \to \infty$ certainly does not only depend on the approximation to the addition theorem, but also on the remaining integrand. This certainly makes a detailed analysis even more difficult.

These considerations are for the moment essentially speculation. A sufficiently rigorous analysis of this possible semiconvergence cannot be done yet. We lack some necessary mathematical tools such as a two-center analog of the leading order asymptotic expansion (7.2) which was so very useful in the one-center case.

8 Summary and outlook

Infinite dimensional function spaces and in particular Hilbert spaces are of considerable importance not only in quantum theory, but also in approximation theory and in functional analysis. Accordingly, there is an extensive literature discussing these function spaces, both from a purely mathematical point of view and also from the perspective of quantum physics.

It is an obvious idea to try to understand the properties of these admittedly complicated function spaces by emphasizing the analogies to the simpler n-dimensional real and complex vector spaces $\mathbb{R}^n$ and $\mathbb{C}^n$, respectively. Often, this approach provides valuable insight. Nevertheless, there are dangers. Infinite dimensional function spaces possess certain peculiarities which do not exist in the case of n-dimensional vector spaces. Naive generalizations and overly optimistic analogies can therefore be badly misleading.

For example, in the n-dimensional vector spaces $\mathbb{R}^n$ or $\mathbb{C}^n$ any set of n linearly independent vectors can be used as a basis, which means that every vector belonging to either $\mathbb{R}^n$ or $\mathbb{C}^n$ can be expressed as a linear combination of n linearly independent vectors. There is also no principal problem if we want to replace one basis by another: All linearly independent sets of n vectors are in that respect equivalent. Orthogonality of the basis vectors in n-dimensional vector spaces is convenient since it greatly simplifies certain operations, but it is not really essential.

In infinite dimensional function spaces, the situation is much more complicated. Firstly, a basis now consists of an infinite number of elements which always raises the question of convergence. Moreover, there are different convergence types, which are in general incompatible. Secondly, a basis in a function space has to be complete, i.e., the span of this basis has to be dense in the function space.

As discussed in Appendix C, the completeness of a basis suffices to guarantee that finite expansion of the type of (C.1) exist. In addition, completeness implies that the corresponding mean square deviation (C.2) can be made as small as we like by increasing the length of the finite expansion. Therefore, it is a seemingly obvious conclusion that the completeness of a basis implies the existence of infinite expansions of the type of (C.3) in terms of this basis. Unfortunately, this conclusion is wrong. The existence of an infinite expansion is only guaranteed if the basis is not only complete, but also orthogonal. These facts are well known, but nevertheless often ignored. They are also the basis of this article.

In [41–44,46], Guseinov derived one-range addition theorems for Slater-type functions $\chi_{N,L}^{M}(\beta, \boldsymbol{r} \pm \boldsymbol{r}')$ with integral and nonintegral principal quantum numbers N by expanding them in terms of his Laguerre-type functions $\{{}_k\Psi_{n,\ell}^{m}(\gamma, \boldsymbol{r})\}_{n,\ell,m}$. For a given $k = -1, 0, 1, 2, \ldots$, these functions defined by (2.13) are complete and orthonormal in the corresponding weighted Hilbert space $L_{r^k}^2(\mathbb{R}^3)$ defined by (2.15). Guseinov's approach is mathematically sound as long as the Slater-type function $\chi_{N,L}^{M}(\beta, \boldsymbol{r} \pm \boldsymbol{r}')$ belongs to $L_{r^k}^2(\mathbb{R}^3)$. Such a one-range addition theorem converges in the mean with respect to the norm of the Hilbert space $L_{r^k}^2(\mathbb{R}^3)$, but not necessarily pointwise.

However, Guseinov considered it to be advantageous to replace in his k-dependent addition theorems the complete and orthonormal functions $\{{}_k\Psi_{n,\ell}^{m}(\gamma, \boldsymbol{r})\}_{n,\ell,m}$, whose radial parts are according to (2.13) essentially generalized Laguerre polynomials, by complete, but nonorthogonal Slater-type functions $\{\chi_{n,\ell}^{m}(\gamma, \boldsymbol{r})\}_{n,\ell,m}$ with integral principal quantum numbers via (3.2). Ultimately, Guseinov's approach corresponds to the replacement of a Laguerre series of the type of (4.4) by a power series of the type of

(4.5). Unfortunately, this approach is not necessarily legitimate and can easily lead to nontrivial convergence and existence problems, which had already been discussed in [207], albeit in a less detailed way.

Because of these principal problems, Guseinov cannot tacitly assume that the transformation of his one-range addition theorems, which are expansions in terms of his complete and orthonormal Laguerre-type functions, to expansions of the type of (4.1) in terms of the complete, but nonorthogonal Slater-type functions are necessarily legitimate. This has to be demonstrated explicitly, but Guseinov had only done this in a very superficial way. There is considerable evidence that Guseinov et al. had only done some purely numerical tests.

The deficiencies of Guseinov's approach become particularly evident in the case of the one-center expansion (1.2) for a Slater-type function $\chi_{N,L}^{M}(\beta, \boldsymbol{r})$ with an in general nonintegral principal quantum number N in terms of Slater-type functions $\{\chi_{n,L}^{M}(\gamma, \boldsymbol{r})\}_{n=L+1}^{\infty}$ with integral principal quantum numbers n and an in general different common scaling parameter $\gamma \neq \beta > 0$. Guseinov [46, Eq. (21)] had constructed this expansion by performing the one-center limit of a rearranged truncated addition theorem for Slater-type functions [46, Eq. (15)]. This one-center limit was later used by Guseinov and Mamedov [122] for the construction of series expansions for overlap integrals of Slater-type functions with nonintegral principal quantum numbers.

It is, however, trivially simple to show that Guseinov's one-center expansion (1.2) does not exist if the principal quantum number N is nonintegral. As discussed in Sect. 1, this follows at once from the simple and yet consequential fact that expansions in terms of Slater-type functions with integral principal quantum numbers and a common scaling parameter are nothing but power series expansions about $r = 0$ in disguise. Moreover, every power series is also a Taylor series for some function (see for example [155]).

This fact is extremely helpful because the factors, which govern the analyticity of a function, are fairly well understood. It is trivially simple to show that the radial part of $\exp(\gamma r)\chi_{N,L}^{M}(\beta, \boldsymbol{r})$ is not analytic in the sense of complex analysis at $r = 0$ if the principal quantum number N is not a positive integer satisfying $N \geq L + 1$. Thus, a power series in r for $\exp(\gamma r)\chi_{N,L}^{M}(\beta, \boldsymbol{r})$ with $N \in \mathbb{R}\backslash\mathbb{N}$ cannot exist, which implies that the one-center expansion (1.2) for $\chi_{N,L}^{M}(\beta, \boldsymbol{r})$ does not exist if $N \in \mathbb{R}\backslash\mathbb{N}$.

We arrive at the same conclusion if we apply the transformation formula (4.11) to the k-dependent expansions (5.4) for $\chi_{N,L}^{M}(\beta, \boldsymbol{r})$ in terms of Guseinov's complete and orthonormal functions or to the equivalent Laguerre series (5.1) for $z^{\rho}\mathrm{e}^{uz}$, from which (5.4) was derived. As discussed in Sect. 5, the large index asymptotics of the coefficients in the Laguerre series (5.1) clearly shows that the expansion (1.2) for $\chi_{N,L}^{M}(\beta, \boldsymbol{r})$ in terms of Slater-type functions does not exist if N is nonintegral.

In principle, the same strategy could also be pursued if one-range addition theorems for $\chi_{N,L}^{M}(\beta, \boldsymbol{r} \pm \boldsymbol{r}')$, which are k-dependent two-center expansions in terms of Guseinov's complete and orthonormal function $\{{}_{k}\Psi_{n,\ell}^{m}(\gamma, \boldsymbol{r})\}_{n,\ell,m}$, are rearranged. The expansion coefficients of these addition theorems are overlap integrals. On the basis of our current level of mathematical understanding, it is, however, very difficult or even practically impossible to determine the large index asymptotics of these complicated integrals. Fortunately, by means of an indirect approach it is nevertheless possible to arrive at some useful conclusions about the validity of Guseinov's rearrangements of his one-range addition theorems.

My key argument in Sect. 6 is again analyticity in the sense of complex analysis. If a function $f : \mathbb{C} \to \mathbb{C}$ has a singularity somewhere in the complex plane, its power series about the origin cannot have an infinite radius of convergence. In contrast, singularities affect Laguerre expansions only if they are nonintegrable and located on the integration contour $[0, \infty)$.

Both $\exp(-\beta|\boldsymbol{r} \pm \boldsymbol{r}'|)$ as well as $\exp(\gamma r) \exp(-\beta|\boldsymbol{r} \pm \boldsymbol{r}'|)$ are for $r' > 0$ analytic at $r = 0$. Accordingly, these functions possess power series expansions in r which converge in a vicinity of the expansion point $r = 0$. However, $\exp(-\beta|\boldsymbol{r} \pm \boldsymbol{r}'|)$ is singular for $\boldsymbol{r} \pm \boldsymbol{r}' = \boldsymbol{0}$. Thus, the power series expansions for both $\exp(-\beta|\boldsymbol{r} \pm \boldsymbol{r}'|)$ and $\exp(\gamma r) \exp(-\beta|\boldsymbol{r} \pm \boldsymbol{r}'|)$ converge only for $r < r'$. This implies that a one-range addition theorem for the $1s$ function $\exp(-\beta|\boldsymbol{r} \pm \boldsymbol{r}'|)$, which converges pointwise for all $\boldsymbol{r}, \boldsymbol{r}' \in \mathbb{R}^3$ or equivalently for all $r, r' \in [0, \infty)$, cannot exist.

These considerations apply also to other Slater-type functions $\chi_{N,L}^{M}(\beta, \boldsymbol{r} \pm \boldsymbol{r}')$ with integral or nonintegral principal quantum numbers N. If $r' > 0$, these functions as well as the related functions $\exp(\gamma r)\chi_{N,L}^{M}(\beta, \boldsymbol{r} \pm \boldsymbol{r}')$ are analytic at $r = 0$, but they also have a singularity at $\boldsymbol{r} \pm \boldsymbol{r}' = \boldsymbol{0}$. Therefore, an expansion of the type of (4.1) in terms of Slater-type functions with integral principal quantum numbers and a common scaling parameter, that converges pointwise for all $\boldsymbol{r}, \boldsymbol{r}' \in \mathbb{R}^3$, cannot exist. Instead, we obtain the small r part of a two-range addition theorem, either by doing a Taylor expansion of $\chi_{N,L}^{M}(\beta, \boldsymbol{r} \pm \boldsymbol{r}')$ about $r = 0$ or by applying the transformation formula (4.11) to the angular projections (3.10).

The results of Sects. 5 and 6 can be summarized as follows: The one-center expansion (1.2) for $\chi_{N,L}^{M}(\beta, \boldsymbol{r})$ does not exist if N is nonintegral, and the expansion (4.1) for $\chi_{N,L}^{M}(\beta, \boldsymbol{r} \pm \boldsymbol{r}')$, which looks like a one-range addition theorem, has a two-range form since it converges only for $|\boldsymbol{r}| < |\boldsymbol{r}'|$. Therefore, one might be tempted to dismiss Guseinov's rearrangements of expansions in terms of generalized Laguerre polynomials as being both useless and dangerous.

However, the situation is more complicated than it may look at first sight. As discussed in Sect. 7, Guseinov apparently never rearranged infinite one-center expansions of the type of (5.4) or infinite one-range addition theorems of the type of (3.4), although this can be done in a systematic way with the help of the transformation formula (4.11).

Instead, Guseinov exclusively rearranged *finite* truncations of his infinite expansions such as the truncation (7.3) of the addition theorem (3.7) or the truncation (7.1) of its one-center limit (5.4), all with a finite truncation order $\mathscr{N}$. This is highly consequential. If we replace in a truncated Laguerre series of the type of (4.6) the generalized Laguerre polynomials by powers, for example via (4.8), there can be no convergence or existence problems because the resulting expression is simply a polynomial.

Accordingly, Guseinov's rearrangements of truncated one-center and two-center expansions produce approximations to $\chi_{N,L}^{M}(\beta, \boldsymbol{r})$ and $\chi_{N,L}^{M}(\beta, \boldsymbol{r} \pm \boldsymbol{r}')$, respectively, that consist of a *finite* number of Slater-type functions $\chi_{n,\ell}^{m}(\gamma, \boldsymbol{r})$ with integral principal quantum numbers and a common scaling parameter. Since only a finite number of terms is transformed in these rearrangements, there can be no existence problems. Nevertheless, Guseinov's approach is affected bu some serious problems beyond the possible numerical stability problems discussed in Sect. 3.

In Sect. 7 it is shown that rearrangements of the truncations (7.1) of the one-center expansion (5.4) are *semiconvergent* with respect to the truncation order $\mathscr{N}$ if the principal quantum number N of the Slater-type function is nonintegral. It follows from the leading order asymptotic approximation (7.2) that the accuracy of these approximations first increases with increasing truncation order $\mathscr{N}$, but for larger values of $\mathscr{N}$ the accuracy decreases again, and in the limit of infinite truncation orders, everything goes to pieces.

The situation is not nearly so well understood in the case of rearrangements of truncations (7.3) of the k-dependent addition theorem (3.7). For finite truncation orders $\mathscr{N}$, these rearrangements are one-range addition theorems, but as $\mathscr{N} \to \infty$ they converge to two-range addition theorems.

It makes sense to assume that the ultimate two-range nature of these rearrangements becomes noticeable in integrals already for sufficiently large, but finite values of $\mathscr{N}$. Thus, it is conceivable that at least certain multicenter integrals containing such rearranged truncations might turn out to be semiconvergent with respect to $\mathscr{N}$. For the moment, these considerations are essentially speculations, since substantial mathematical knowledge is still lacking.

As is well known from the literature, the use of semiconvergent expansions can offer computational benefits under favorable circumstances. In the case of Guseinov's rearranged truncations of one-center and two-center expansions this may also be the case. However, the use of semiconvergent expansions or of other approximations, whose limit of infinite truncation order either does not exist or has undesirable features, clearly involves some risks. So, before using such an approximation in an actual calculation, we firstly must try to understand the inherent risks, and secondly, we must convince ourselves that we will be able to handle these risks. It would be extremely negligent to ignore these risks and treat a semiconvergent expansion like a convergent expansion.

The examples mentioned above or the ones given in Appendix E should suffice to convince even a skeptic reader that the apparent convergence of the leading terms of an infinite series *alone* does not prove anything. We also need some additional mathematical insight indicating convergence.

Numerical demonstrations have obvious limitations. It is always desirable to augment them by sufficiently rigorous mathematical investigations. Unfortunately, rigorous proofs are extremely difficult in a research topic as complex and computer oriented as electronic structure theory. In the vast majority of all problems in electronic structure theory, a rigorous mathematical analysis is out of reach and we have to be content with numerical demonstrations, in spite of their obvious limitations and their capacity of misleading us. However, the construction of addition theorems and their application in multicenter integrals is a mathematical problem, and—as shown in this article—quite a few things can be understood on the basis of mathematical considerations. Guseinov's strategy of relying entirely on numerical demonstrations without trying to understand the underlying mathematics is not acceptable from a methodological point of view.

A General aspects of series expansions

For the sake of simplicity, let us consider functions $F\colon \mathbb{C} \to \mathbb{C}$. A *series expansion* $\sum_{n=0}^{\infty} u_n \mathscr{U}_n(z)$ for such a function $F(z)$ requires a sequence $\{u_n\}_{n=0}^{\infty}$ of fixed coefficient and a sequence $\{\mathscr{U}_n(z)\}_{n=0}^{\infty}$ of known functions $\mathscr{U}_n\colon \mathbb{C} \to \mathbb{C}$.

To make the expansion $\sum_{n=0}^{\infty} u_n \mathscr{U}_n(z)$ useful, it has to represent $F(z)$ in some sense. Thus, we assume that $\sum_{n=0}^{\infty} u_n \mathscr{U}_n(z)$ converges to $F(z)$ according to some specified convergence type and we write:

$$F(z) = \sum_{n=0}^{\infty} u_n \, \mathscr{U}_n(z). \tag{A.1}$$

Numerous different convergence types occur in practice. Important examples are pointwise convergence, which is typical of classical complex analysis or also of two-range addition theorems, convergence in the mean with respect to the norm of some Hilbert space, which is typical of most one-range addition theorems, or even distributional or weak convergence in the sense of Schwartz [174].

Therefore, the indiscriminate use of the "=" sign for all convergence types is potentially misleading since it suggests a uniqueness which does not exist. Depending on the convergence type, an "=" sign can have a completely different meaning, or to put it differently, series expansions of the type of (A.1) can have very different mathematical properties. Moreover, different convergence types are in general incompatible, i.e., the convergence of a series expansion for a given convergence type does not imply that this series converges also with respect to another convergence type.

It is, however, overly restrictive to insist that a series expansion of the type of (A.1) must converge in some sense to be practically useful. Divergent, but summable series expansions are simply to useful to be discarded, not only in mathematics, but in particular in quantum physics (see for example [150] and references therein). In numerous scientific applications, there is no alternative to the summation of divergent series. A condensed review of divergent series and their summation can be found in [207, Appendices A and B].

Let us now assume that we have a sequence of approximate expressions of the following kind:

$$F_N(z) = \sum_{n=0}^{N} u_n^{(N)} \, \mathscr{U}_n(z), \quad N \in \mathbb{N}_0. \tag{A.2}$$

The superscript N in $u_n^{(N)}$ indicates that the coefficients may depend explicitly on the summation limit N, i.e., we in general have $u_n^{(N)} \neq u_n^{(N+1)} \neq u_n^{(N+2)} \neq \ldots$ for fixed $n, N \in \mathbb{N}_0$.

Let us now also assume that the approximants $F_N(z)$ converge to $F(z)$ as $N \to \infty$ in some sense. This raises the question whether the resulting expression $F(z) = \lim_{N\to\infty} F_N(z)$ constitutes an expansion of $F(z)$ in terms of the functions $\{\mathscr{U}_n(z)\}_{n=0}^{\infty}$.

The answer is that this is in general not true. The convergence of the approximants $F_N(z)$ to $F(z)$ as $N \to \infty$ only means that we can make the difference between $F_N(z)$ and $F(z)$, whose exact meaning depends on the convergence type, as small as we like by increasing N as much as necessary. This does not guarantee that the coefficients $u_n^{(N)}$ in (A.2) have for all $n \in \mathbb{N}_0$ unique limits $u_n = u_n^{(\infty)} = \lim_{N\to\infty} u_n^{(N)}$. Thus, the existence of a convergent sequence of approximants of the type of (A.2) does not imply the existence of a series expansion of the type of (A.1).

B Glory and misery of power series

It is probably justified to claim that power series

$$f(z) = \sum_{\nu=0}^{\infty} \frac{f^{(\nu)}(z_0)}{\nu!} (z - z_0)^{\nu} = \sum_{\nu=0}^{\infty} c_{\nu} (z - z_0)^{\nu} \tag{B.1}$$

are the most important *analytical* tools not only in mathematical analysis, but also in the mathematical treatment of scientific and engineering problems.

As is well known, power series can be differentiated *term-by-term* under relatively mild conditions. Accordingly, it is an obvious idea to try to solve differential equations in terms of power series. A large part of special function theory consists of the construction and analysis of power series solutions to the ordinary differential equations that are of relevance in mathematical physics. Since power series can also be integrated *term-by-term* under very mild conditions, they are also indispensable for the construction of explicit expressions for integrals involving functions that possess power series representations.

While the usefulness of power series in analytical manipulations cannot be overemphasized, it is nevertheless also true that a power series representation for a given function is at best a mixed blessing from a purely numerical point of view. The problem is that power series expansions converge in circles about the expansion point. As is well known, the radius of such a circle of convergence is determined by the location the closest singularity of the function under consideration. Thus, the radius of convergence of a power series expansion can be zero, finite and infinite.

In general, a power series in $z - z_0$ is numerically useful only if z and z_0 differ slightly, i.e., in the immediate vicinity of the expansion point z_0. Then, a few terms of the series normally suffice to produce excellent approximations. But close to the boundary of its circle of convergence, the rate of convergence of such a power series expansion can become prohibitively slow. In my opinion, the current popularity of Padé approximants, which normally converge much more rapidly than the partials sums from which they are constructed (see for example the monograph of Baker and Graves-Morris [5] and references therein), is largely due to the combined effect of the undeniable analytical usefulness of power series and their (very) limited usefulness as computational tools.

A nonzero, but finite radius of convergence of a power series can also cause serious problems in integrals. As is well known, a series expansion for the integrand can be integrated termwise if it converges uniformly for the whole integration interval.

Otherwise, we have to be prepared that termwise integration either generates a wrong result or even a divergent series expansion for the integral. Thus, if we want to replace a part of an integrand by its power series expansion, we are on the safe side only if the integration interval is completely contained in the circle of convergence. In particular in the case of infinite or semi-infinite integration intervals, this is normally not the case.

C Orthogonal expansions

The analyticity of a function $f: \mathbb{C} \to \mathbb{C}$ in the sense of complex analysis is undeniably a highly desirable feature. In the interior of suitable subsets of $\mathbb{C}$, f can be represented by power series expansions which converge pointwise and uniformly, and it is also comparatively easy to compute derivatives of f in this way. Nevertheless, it is often advantageous to use instead of power series alternative expansions that converge in a weaker sense.

Let $\mathscr{V}$ be an infinite dimensional vector space with inner product $(\cdot|\cdot): \mathscr{V} \times \mathscr{V} \to \mathbb{C}$ and its corresponding norm $\|\cdot\|: \mathscr{V} \to \mathbb{R}_+$ defined by $\|f\| = (f|f)^{1/2}$ with $f \in \mathscr{V}$. If every Cauchy sequence in $\mathscr{V}$ converges with respect to the norm $\|\cdot\|$ to an element of $\mathscr{V}$, then $\mathscr{V}$ is called a *Hilbert space*.

Let us now assume that f is an element of some Hilbert space $\mathscr{H}$ and that the functions $\{\varphi_m\}_{m=0}^{\infty}$ are linearly independent and complete in $\mathscr{H}$. Then, we can construct approximations

$$f_M = \sum_{m=0}^{M} C_m^{(M)} \varphi_m \tag{C.1}$$

to f, where M is a *finite* integer. The expansion coefficients $C_m^{(M)}$, which in general depend on the summation limit M, are chosen in such a way that the mean square deviation

$$\|f - f_M\|^2 = (f - f_M | f - f_M) \tag{C.2}$$

becomes minimal.

The finite approximation (C.1) converges to f as $M \to \infty$ if (C.2) can be made as small as we like by increasing M. It therefore looks natural to assume that f possesses an *infinite expansion*

$$f = \sum_{m=0}^{\infty} C_m \varphi_m \tag{C.3}$$

in terms of the linearly independent and complete functions $\{\varphi_m\}_{m=0}^{\infty}$ with well defined expansion coefficients $C_m = \lim_{M\to\infty} C_m^{(M)}$.

As discussed in Appendix A, this naturally looking assumption is not necessarily true. In general, the coefficients $C_m^{(M)}$ in (C.1) do not only depend on m, f, and

$\{\varphi_m\}_{m=0}^{\infty}$, but also on the summation limit M. It is not a priori clear whether the coefficients $C_m^{(M)}$ in (C.1) possess well defined limits $C_m = \lim_{M\to\infty} C_m^{(M)}$, or whether an infinite expansion of the type of (C.3) exists. In fact, expansions of that kind may or may not exist.

It is one of the central results of approximation theory that for arbitrary $f \in \mathscr{H}$ the mean square deviation $\| f - f_M \|^2$ becomes minimal if the functions $\{\varphi_m\}_{m=0}^{\infty}$ are not only linearly independent and complete, but also orthonormal satisfying $(\varphi_m|\varphi_{m'}) = \delta_{mm'}$ for all $m, m' \in \mathbb{N}_0$, and if the coefficients are chosen according to $C_m^{(M)} = (\varphi_m|f)$ (see for example [24, Theorem 9 on p. 51]).

If the functions $\{\varphi_m\}_{m=0}^{\infty}$ are complete and orthonormal in the Hilbert space $\mathscr{H}$ and if the expansion coefficients in (C.1) are chosen according to $C_m^{(M)} = (\varphi_m|f)$, then the expansion coefficients do not depend on M. Thus, the limit $M \to \infty$ is possible, and $f \in \mathscr{H}$ possesses an *infinite* series expansion

$$f = \sum_{m=0}^{\infty} (\varphi_m|f)\, \varphi_m \tag{C.4}$$

and this expansion converges in the mean with respect to the norm $\| \cdot \|$ of $\mathscr{H}$.

The fact, that the completeness of a function set $\{\varphi_m\}_{m=0}^{\infty}$ in an infinite dimensional Hilbert space $\mathscr{H}$ alone does not suffice to guarantee the existence of expansions of the type of (C.3), is highly consequential. Nevertheless, it is occasionally overlooked, although this insufficiency is well documented both in the mathematical literature (see for example [24, Theorem 10 on p. 54] or [137, Section 1.4]) as well as in the literature on electronic structure calculations [143–148]). Horrifying examples of nonorthogonal expansions with pathological properties can be found in [144, Section III.I].

If the Hilbert space $\mathscr{H}$ is an infinite dimensional vector space consisting of function $f, g\colon \mathbb{C} \to \mathbb{C}$, the inner product $(f|g)$ of $\mathscr{H}$ is usually identified with an integral $\int_a^b w(z)[f(z)]^* g(z) \mathrm{d}z$, where $w(z)$ is an appropriate positive weight function. Moreover, the complete orthonormal functions $\{\varphi_m\}_{m=0}^{\infty}$ in $\mathscr{H}$ are normally related to a suitable subclass $\{\mathscr{P}_m(z)\}_{m=0}^{\infty}$ of the classical orthogonal polynomials of mathematical physics, as specified by the integration limits a and b and the weight function $w(z)$. In this case, the general orthogonal expansion (C.4) boils down to the expansion of a function $f(z)$ in terms of orthogonal polynomials:

$$f(z) = \sum_{m=0}^{\infty} \mathscr{C}_m\, \mathscr{P}_m(z). \tag{C.5}$$

It is generally accepted that orthogonal expansions are extremely useful mathematical tools and that they have many highly advantageous features. This is, however, not the whole truth, in particular if we want to approximate functions. Hilbert space theory only guarantees that an orthogonal expansion converges in the mean with respect to the corresponding norm $\| \cdot \|$, but not necessarily pointwise or even uniformly. Thus, convergence in the mean is a comparatively weak form of convergence, and orthogonal expansions are not necessarily a good choice if we are predominantly interested in the local properties of a function. However, convergence in the mean is usually completely satisfactory for the evaluation of integrals.

D Generalized Laguerre polynomials

The surface spherical harmonics $Y_\ell^m(\theta, \phi)$ are complete and orthonormal with respect to an integration over the surface of the unit sphere in $\mathbb{R}^3$ (an explicit proof can for instance be found in [164, Section III.7.6]). Since more complex Hilbert spaces can be constructed by forming tensor products of simpler Hilbert spaces (see for example [164, Section II.6.5]), we only have to find suitable radial functions that are complete and orthogonal with respect to an integration from 0 to ∞ (see also [147, Lemma 6 on p. 31]). Thus, we more or less automatically arrive at function sets based on the generalized Laguerre polynomials.

The *generalized Laguerre polynomials* $L_n^{(\alpha)}(z)$ with $\Re(\alpha) > -1$ and $n \in \mathbb{N}_0$ are orthogonal with respect to an integration over the positive real semiaxis $[0, \infty)$ with weight function $w(z) = z^\alpha \exp(-z)$. In the mathematical literature, they are defined either via the *Rodrigues relationship*

$$L_n^{(\alpha)}(z) = z^{-\alpha} \frac{\mathrm{e}^z}{n!} \frac{\mathrm{d}^n}{\mathrm{d}z^n} \left[\mathrm{e}^{-z} z^{n+\alpha}\right] \tag{D.1}$$

or as a terminating confluent hypergeometric series ${}_1F_1$:

$$L_n^{(\alpha)}(z) = \frac{(\alpha+1)_n}{n!} \, {}_1F_1(-n; \alpha+1; z) = \frac{(\alpha+1)_n}{n!} \sum_{\nu=0}^{n} \frac{(-n)_\nu}{(\alpha+1)_\nu} \frac{z^\nu}{\nu!}. \tag{D.2}$$

The generalized Laguerre polynomials satisfy for $\Re(\alpha) > -1$ and $m, n \in \mathbb{N}_0$ the orthogonality relationship

$$\int_0^\infty z^\alpha \, \mathrm{e}^{-z} \, L_m^{(\alpha)}(z) \, L_n^{(\alpha)}(z) \, \mathrm{d}z = \frac{\Gamma(\alpha+n+1)}{n!} \, \delta_{mn}. \tag{D.3}$$

Accordingly, the polynomials

$$\mathscr{L}_n^{(\alpha)}(z) = \left[\frac{n!}{\Gamma(\alpha+n+1)}\right]^{1/2} L_n^{(\alpha)}(z), \quad n \in \mathbb{N}_0, \quad \alpha > -1, \tag{D.4}$$

are for $\Re(\alpha) > -1$ *orthonormal* with respect to an integration over the interval $[0, \infty)$ involving the weight function $z^\alpha \exp(-z)$:

$$\int_0^\infty \mathrm{e}^{-z} \, z^\alpha \, \mathscr{L}_m^{(\alpha)}(z) \, \mathscr{L}_n^{(\alpha)}(z) \, \mathrm{d}z = \delta_{mn}. \tag{D.5}$$

Alternatively, we can also use the functions

$$\Phi_n^{(\alpha)}(z) = \left[\frac{n!}{\Gamma(\alpha+n+1)} \right]^{1/2} \mathrm{e}^{-z/2} \, z^{\alpha/2} \, L_n^{(\alpha)}(z), \quad n \in \mathbb{N}_0, \tag{D.6}$$

which are for $\Re(\alpha) > -1$ *orthonormal* with respect to an integration over the interval $[0, \infty)$:

$$\int_0^\infty \Phi_m^{(\alpha)}(z) \, \Phi_n^{(\alpha)}(z) \, \mathrm{d}z = \delta_{mn}. \tag{D.7}$$

The completeness of the generalized Laguerre polynomials in the weighted Hilbert space

$$L^2_{\mathrm{e}^{-z} z^\alpha}\big([0, \infty)\big) = \left\{ f \colon [0, \infty) \to \mathbb{C} \,\middle|\, \int_0^\infty \mathrm{e}^{-z} \, z^\alpha \, |f(z)|^2 \, \mathrm{d}z < \infty \right\} \tag{D.8}$$

is a classic result of mathematical analysis (see for example [137, p. 33], [172, pp. 349–351], or [189, pp. 235–238]).

In general, Laguerre expansions converge only in the mean, but not necessarily pointwise (see for example [4]). Additional conditions, which a function has to satisfy in order to guarantee that its Laguerre expansion converges pointwise, were discussed by Szegö [186, Theorem 9.1.5 on p. 246] (see also [29, Appendix]).

In this article, exclusively the mathematical notation is used. A different convention for Laguerre polynomials is frequently used in the quantum mechanical literature. For example, Bethe and Salpeter [11, Eq. (3.5)] define *associated Laguerre functions* $\big[L_n^m(z)\big]_{\mathrm{BS}}$ with $n, m \in \mathbb{N}_0$ via the Rodrigues-type relationships

$$\big[L_n^m(z)\big]_{\mathrm{BS}} = \frac{\mathrm{d}^m}{\mathrm{d}z^m} \big[L_n(z)\big]_{\mathrm{BS}}, \tag{D.9a}$$

$$\big[L_n(z)\big]_{\mathrm{BS}} = \mathrm{e}^z \, \frac{\mathrm{d}^n}{\mathrm{d}z^n} \big[\mathrm{e}^{-z} z^n\big]. \tag{D.9b}$$

Comparison of (D.1) and (D.9b) implies:

$$L_n^{(m)}(z) = \frac{(-1)^m}{(n+m)!} \big[L_{n+m}^m(z)\big]_{\mathrm{BS}}. \tag{D.10}$$

The convention of Bethe and Salpeter [11] is also used in the books by Condon and Shortley [21, Eqs. (6) and (9) on p. 115] and by Condon and Odabaşi [20, Eq. (2) on p. 189] as well as in the numerous articles by Guseinov et al.

In my opinion, the use of associated Laguerre functions defined by (D.9) is not recommendable. It follows from (D.10) that these functions cannot express generalized Laguerre polynomials $L_n^{(\alpha)}$ with nonintegral superscripts α. This is both artificial and unnecessary. For example, the eigenfunctions $\Omega_{n,\ell}^{m}(\beta, \boldsymbol{r})$ of the Hamiltonian $\beta^{-2}\nabla^2 - \beta^2 r^2$ of the three-dimensional isotropic harmonic oscillator contain generalized Laguerre polynomials in r^2 with half-integral superscripts (see for example [194, Eq. (5.4)] and references therein).

E Semiconvergence

If the sum of the leading terms of an infinite series seems to approach the correct limit, it looks natural to conclude that increasing the number of terms will improve the accuracy of the approximation, and that ultimately the partial sums will converge to the correct limit. Unfortunately, this assumption is overly optimistic and in spite of its apparent plausibility not necessarily true.

Many series are known whose partial sums initially seem to converge. If however, further terms are included, the accuracy decreases, and ultimately the sequence of partial sums diverges. In the literature, this phenomenon is well established and usually called *semiconvergence* (see for example [162, p. 2, Footnote†]). To the best of my knowledge, this terminology was introduced by Stieltjes [185] already in 1886.

Semiconvergence is best known in connection with factorially divergent asymptotic inverse power series for special functions. In Arfken's book [3, Chapter 5.10], one can find a comprehensive discussion of the semiconvergence of the divergent asymptotic series of the incomplete gamma function $\Gamma(a, z)$ [163, Eq. (8.11.2)] and its special case, the asymptotic series for the exponential integral $E_1(z)$ [163, Eq. (6.12.1)]. In my opinion, Arfken's treatment is well suited as a first introduction to this topic. Other examples of semiconvergent series are the factorially divergent asymptotic series for the complementary error function $\mathrm{erfc}(z)$ [163, Eq. (7.12.1)], and the modified Bessel and Whittaker functions of the second kind $K_\nu(z)$ and $W_{\kappa,\mu}(z)$, respectively [163, Eqs. (10.40.4) and (13.19.3)].

If the argument of such a divergent asymptotic inverse power series is sufficiently large, then the truncation of such a divergent series in the vicinity of the minimal term can lead to excellent approximations to the function it represents. Nevertheless, these partial sums diverge if further terms beyond the minimal term are included (see for example [34, Figure 2.2 on p. 35]).

Accordingly, the accuracy, which can be obtained by truncating a semiconvergent inverse power series in the vicinity of the minimal term, depends crucially on the magnitude of the argument. If the argument is large, excellent approximations can often be obtained. The situation is not so good if the argument is small, because then the truncation of a semiconvergent series can only provide relatively crude approximations. But even for small arguments, it is often possible to obtain very accurate approximations by using the partial sums of a semiconvergent series as input data in nonlinear sequence transformations [198,212].

Semiconvergent series occur also quite abundantly in quantum mechanical perturbation expansions. For example, Ahlrichs [2] showed that the total energy of interacting molecular systems A and B can be expressed by a semiconvergent series, the so called $1/R$-expansion.

Other phenomena closely resembling semiconvergence are also known. Baumel, Crocker, and Nuttall [7] showed that in the case of scattering calculations with complex basis functions low order approximations can produce good results although the whole scheme ultimately diverges, and Gautschi [32] observed initial apparent convergence to the wrong limit in the case of continued fractions for Kummer functions.

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