Bessel−Zernike Discrete Variable Representation Basis†

Charles Cerjan

Lawrence Livermore National Laboratory, Livermore California 94550

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The connection between the Bessel discrete variable basis expansion and a specific form of an orthogonal set of Jacobi polynomials is demonstrated. These so-called Zernike polynomials provide alternative series expansions of suitable functions over the unit interval. Expressing a Bessel function in a Zernike expansion provides a straightforward method of generating series identities. Furthermore, the Zernike polynomials may also be used to efficiently evaluate the Hankel transform for rapidly decaying functions or functions with finite support.

1. Introduction

The discrete variable representation (DVR) technique, introduced and developed by Light and co-workers,[1] has proven to be a useful procedure in many applications.[2] This approach emphasizes the duality between function spaces and their discrete analogues which, as a practical matter, leads to numerical efficiency based upon physical intuition. For example, one of the first, and most powerful, analytical techniques typically taught in quantum mechanics is the expansion of a wave function in terms of some suitable basis set composed of functions selected for their physical suitability, or perhaps, their ease of integration, such as Gaussian forms. Such expansion sets are generically known as Galerkin bases[3] and in the most favorable circumstances possess exponential convergence. The outstanding difficulty with this powerful approach, though, is the difficulty arising from the evaluation of the potential matrix elements. For complicated, many-body potential functions it is difficult to obtain a suitable Galerkin-type basis. Thus, the remarkable utility of a suitable DVR resides in its ability to greatly facilitate the evaluation of these difficult potential energy matrix elements since physically extraneous points may be easily recognized and discarded. After the initial successful applications to spectroscopic line identification in large molecules, extensive generalization of the method led to diverse applications.[2]

A particularly useful DVR basis set on the radial half-line is based upon the Fourier−Bessel, or more generally the Dini, representation of a function.[4] The Fourier−Bessel expansion attempts to expand a suitable function in terms of the positive zeros of a chosen order Bessel function. The zeros scale the argument of the Bessel function to ensure orthogonality on the unit interval.[5] A more general choice of argument scaling, rather than the zeros of the Bessel function, is due to Dini, and it has the technical advantage of ensuring convergence of the series at the interval endpoints.

Solutions to the radial Schrodinger equation and the closely related Hankel transform may be effectively expressed in terms of this representation. More specifically, if a radial cutoff is introduced with subsequent scaling of the radial half-line to the unit interval, two classes of DVR basis sets may be realized. The first class is constructed by diagonalizing the position coordinate in any suitable orthogonal set which essentially produces a Gaussian quadrature.[6] The second, generalized procedure also produces a radially bounded version of the Fourier−Bessel series designed for both cylindrical and spherical Bessel transforms.[7] Both DVR classes are closely related to the development below which is also intrinsically based upon the bounded radial interval. In the context of a DVR based upon radially unbounded functions, though, it has been conjectured that a relationship to an orthogonal (finite) polynomial set should exist for this particular DVR basis set.[8] Motivated by this suggestion, an explicit connection between the Bessel series and a form of the Jacobi polynomials may in fact be demonstrated for the radially bounded representation.

In the following, a brief summary of the properties of the Zernike polynomials will be presented; their relationship to the Bessel series is then established with some interesting resulting identities. The next section emphasizes the specialized use of the two representations in the evaluation of Hankel transforms with application to a simple radial function. A discussion of the limitations of this approach concludes the manuscript.

2. Bessel−Zernike Expansion

The Zernike, or circle polynomials, are well-known in optical physics to be very convenient for expressing the various diffractive aberrations in a lens.[9] This basis set is specifically contructed to be orthogonal on the unit interval with radial weighting

$$\int_0^1 R_n^l(\rho) R_{n'}^l(\rho)\rho \, d\rho = \frac{1}{2(n+1)}\delta_{nn'} \tag{1}$$

where $R_n^l(\rho)$ signifies a Zernike polynomial of integer order n and integer degree l as a function of the radial variable ρ. The Zernike polynomials are a special case of the Jacobi polynomials[9,10]

$$P_{n'}^{(\alpha,\beta)}(x) = (-1)^{n'}\frac{R_n^l(\rho)}{\rho^\alpha} \tag{2}$$

where $P_{n'}^{(\alpha,\beta)}(x)$ are the standard Jacobi polynomials[11] with $x = 1 - 2\rho^2$, $\beta = 0$, $\alpha = l$, and $n' = (n - l)/2$. Consequently, these polynomials possess several three-term recurrence relationships for both degree and order; they satisfy the hypergeometric

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differential equation; and, additionally, the functions have definite parity for even and odd order. As a standard orthogonal polynomial set, the Jacobi polynomials are intimately related to other, better known, orthogonal sets. Specifically, when $\beta = 0$ and $\alpha = 0$, the Legendre polynomials of order n' are obtained; when $\beta = \alpha = \lambda - 1/2$, the Gegenbauer, or ultraspherical, polynomials of order n' and degree λ arise; and the Chebyshev polynomials of order n' are recovered when $\lambda = 0$.[4]

By completeness on the unit interval, a suitable function, $f(\rho)$, may be expanded in a Zernike basis set

$$f(\rho) = \sum_{n=l}^{\infty} b_n R_n^l(\rho) \tag{3}$$

where the overlap coefficients are

$$b_n = \int_0^1 f(\rho) R_n^l(\rho)\rho \, d\rho \tag{4}$$

In particular, monomial powers of ρ could be so expressed so that a function with a convergent Taylor's series expansion could be rewritten in terms of the Zernike basis set. (This approach is not suitable for numerical applications because the resulting matrix inversion would be unstable for large orders.) In applications of the DVR using the Zernike expansion, the quadrature points and weights are readily obtained from standard computational techniques that generate the Gauss–Jacobi quadrature values for the special choices of α and β above.

Although the Zernike polynomials are most simply expressed as finite sums of integral powers of ρ, these polynomials may be equivalently defined by a Rodrigues' differentiation formula that is most convenient for integration on the unit interval. Using the differentiation formula, the integral of the product of an integral order Bessel function and a Zernike polynomial with matching degree may be shown to be another Bessel function[9]

$$\int_0^1 R_n^l(\rho) J_l(k\rho)\rho \, d\rho = (-1)^{(n-l)/2} \frac{J_{n+1}(k)}{k} \tag{5}$$

An immediate consequence of this simple overlap integral is a direct connection between Bessel function and Zernike polynomial expansions on the unit interval.

The Fourier–Bessel series expansion expresses some suitable function, $f(\rho)$, on the unit interval in terms of a Bessel function of fixed order, $J_l(\rho)$, whose argument is scaled by the zeros of that Bessel function, α_{lm}

$$f(\rho) = \sum_{m=1}^{\infty} \frac{2c_m}{J_{l+1}^{\;2}(\alpha_{lm})} J_l(\alpha_{lm}\rho) \tag{6}$$

where the coefficients, c_m,are determined by the overlap integrals

$$c_m = \int_0^1 f(\rho) J_l(\alpha_{lm}\rho)\rho \, d\rho \tag{7}$$

Applying the Fourier-Bessel expansion to a fixed degree Zernike polynomial produces

$$R_n^l(\rho) = 2(-1)^{(n-l)/2} \sum_{m=1}^{\infty} \frac{J_{n+1}(\alpha_{lm})}{\alpha_{lm} J_{l+1}^{\;2}(\alpha_{lm})} J_l(\alpha_{lm}\rho) \tag{8}$$

and, using eqs 3 and 4, a fixed order Bessel function may be expanded as

$$J_l(\alpha_{lm}\rho) = \sum_{n=l}^{\infty} (-1)^{(n-l)/2} \frac{J_{n+1}(\alpha_{lm})}{\alpha_{lm}} R_n^l(\rho) \tag{9}$$

displaying the expected duality between the two basis set choices. These expressions thus relate the Fourier–Bessel series to a series of orthogonal polynomials on the unit interval.

3. Special Cases

The complementary series representations above lead to some interesting special cases. For example, when $n = l \neq 0$, the Zernike polynomial reduces to $R_n^n(\rho) = \rho^n$. Thus, eq 8 implies that

$$\rho^n = 2\sum_{m=1}^{\infty} \frac{J_n(\alpha_{nm}\rho)}{\alpha_{nm} J_{n+1}(\alpha_{nm})} \tag{10}$$

which is a well-known result.[4] The series expansion in eq 8 clearly generalizes this expression when $n \neq l$. There is a subtlety that should be noted when handling the Fourier–Bessel series, though. In general, the series expression for suitable functions will not converge at $\rho = 1$.[5] Indeed, inserting this value into eq 10 leads to a contradiction. To obtain a convergent expansion over the entire unit interval, the Dini expansion must be used in place of the Fourier–Bessel expansion.[5] This form replaces the coefficients in eq 7 with the integral

$$d_m = 2\gamma_{lm}^{\;2}\{\gamma_{lm}^{\;2}[J_l'(\gamma_{lm})]^2 + (\gamma_{lm}^{\;2} - l^2)[J_l(\gamma_{lm})]^2\}^{-1} \int_0^1 f(\rho) J_l(\gamma_{lm}\rho)\rho \, d\rho \tag{11}$$

where the γ_{lm} are now the zeros of the equation $zJ_l'(z) + aJ_l(z) = 0$. The value of a determines whether the expansion must include additional terms in the series expansion, providing absolute convergence over the unit interval.[5] That is, when $l + a > 0$, no additional terms are required. If $l + a = 0$ or $l + a < 0$, then an additional term appears in the series expansion. It should be noted that the use of the Dini expansion is not significantly more complicated than the simpler Fourier–Bessel choice since the roots appearing in the expansion must be determined numerically in any event. The choice $a = 0$ when $l > 0$, for example, would be useful for numerical evaluations.[12]

The above expressions also lead to some simple summation formulas. Using eqs 1 and 8, it is straightforward to derive the equality

$$\frac{1}{2(n+1)} = 2\sum_{m=1}^{\infty} \frac{J_{n+1}^{\;2}(\alpha_{lm})}{\alpha_{lm}^{\;2}\, J_{l+1}^{\;2}(\alpha_{lm})} \tag{12}$$

which produces, in the special case of $n = l$

$$\frac{1}{4(n+1)} = \sum_{m=1}^{\infty} \frac{1}{\alpha_{nm}^2} \tag{13}$$

Similarly, by using the orthogonality of the scaled Bessel functions on the unit interval, eq 9 leads to a discrete form of the orthogonality relationship

$$\frac{J_{l+1}^{\;2}(\alpha_{lm})}{2} = \sum_{n=l}^{\infty} \frac{J_{n+1}^{\;2}(\alpha_{lm})}{\alpha_{lm}^{\;2}} \tag{14}$$

4. Hankel Transform Application

The application of the Fourier–Bessel series to the numerical evaluation of the lth order Hankel transform has been indepen-

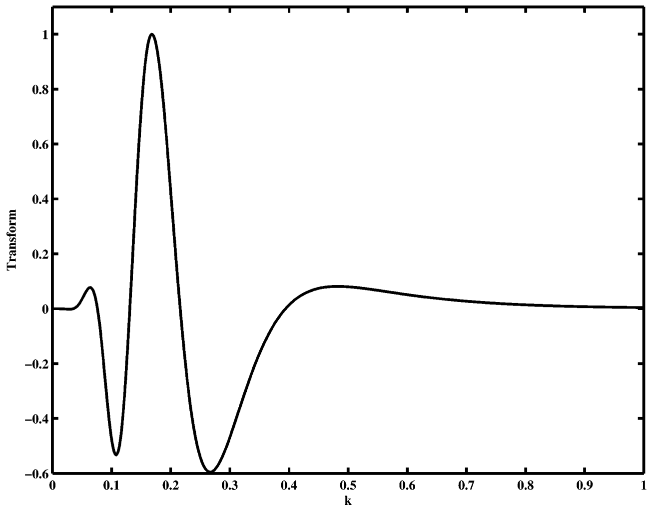

Figure 1. Approximate fourth order Hankel transform of a Laguerre function obtained from the Zernike expansion.

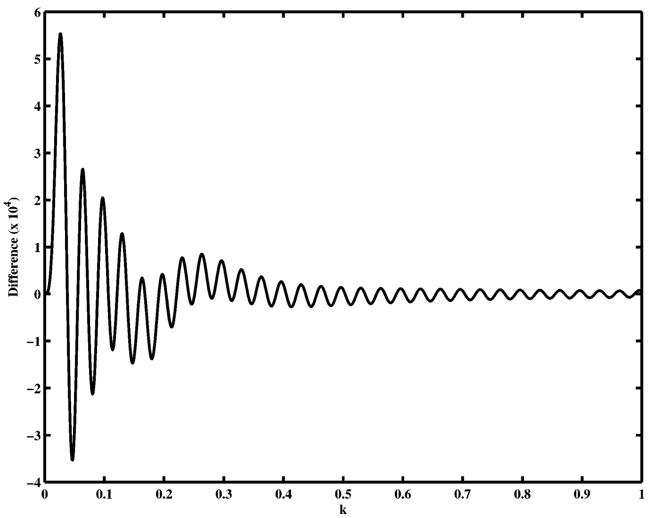

Figure 2. Difference between the analytical and approximate fourth order Hankel transform of the selected Laguerre function.

dently discovered several times in chemical and optical physics.[13] The complementary relationship of the Zernike expansion to the Fourier−Bessel discretization of the Hankel transform suggests another route to the evaluation of the transform. Recall that the lth order Hankel transform and its inverse are integrations over the infinite radial interval with a Bessel function kernel

$$\hat{f}(k) = 2\pi \int_0^{\infty} f(\rho) J_l(2\pi k\rho)\rho \, d\rho \tag{15}$$

and

$$f(\rho) = 2\pi \int_0^{\infty} \hat{f}(k) J_l(2\pi k\rho) k \, dk \tag{16}$$

Since the Zernike overlap integral in eq 5 separates the product in the argument of a Bessel function, a Zernike basis expansion of the transform kernel offers another approach to the evaluation of the Bessel integration. These integrals are manifestly over an infinite range. To use the orthogonality of either the Fourier-Bessel or Zernike functions over the unit interval, it is first necessary to choose a cutoff and scale the integral to the unit interval. (If the function vanishes identically beyond some finite value only a scaling is required of course.) Thus, the original

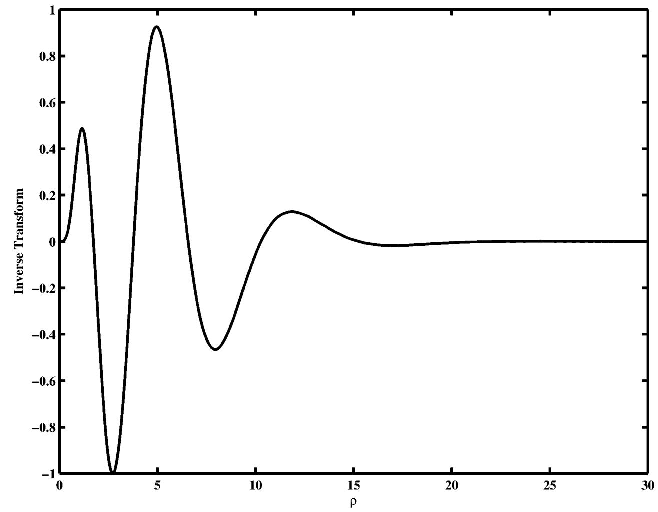

Figure 3. Inverse Hankel transform of the chosen Laguerre function by Fourier-Bessel series evaluation using the Zernike representation of the direct transform.

transform integral is approximated by

$$\hat{f}(k) \approx 2\pi R^2 \int_0^1 f(R\rho) J_l(2\pi kR\rho)\rho \, d\rho \tag{17}$$

for a finite cutoff value, R. Re-expressing the Bessel integration by a sum over Zernike polynomials yields

$$\hat{f}(k) \approx 2\pi R^2 \sum_{n=l}^{\infty} (-1)^{(n-l)/2} \frac{J_{n+1}(2\pi Rk)}{2\pi Rk} \int_0^1 f(R\rho) R_n^{\,l}(\rho)\rho \, d\rho \tag{18}$$

Several unusual aspects of this expression should be noted. If the function, $f(\rho)$, has a finite Taylor's series expansion and vanishes identically beyond some finite value, the Zernike series will truncate and the overlap integrals are straightforwardly obtained. Also, even when $f(\rho)$ extends over the entire half-line, the evaluation of the overlap integral may be performed at arbitrary points, that is, by any suitable integration scheme. Since the k dependence has been separated from the overlap integration, the high accuracy of the Bessel function evaluation is not compromised by any approximations incurred in the evaluation of these integrals. Thus, with suitable series convergence, it might be possible to obtain derivatives or perform other operations upon the transformed function. In one sense, the Zernike expansion fits the transformed function to a series of Bessel functions. As another practical point, the various terms in the expansion are independent of one another so that, if the series is first calculated for N terms, the extension to, say, $2N$ terms only requires another N evaluations. Finally, the value of the selected Zernike polynomials may be stored at the integration points for continued evaluation.

As a simple example of this approach, the fourth order Hankel transform of the associated Laguerre function, $L_6^{\,4}(\rho) \exp(-\rho)$, was evaluated with a cutoff at 30 and including 100 terms in the expansion. The Zernike overlap integrals were calculated by Simpson's rule quadrature with a spacing of 0.001 on the unit interval. No attempt was made to optimize any of these quantities. The resulting approximate transform, scaled to its largest value, is plotted in Figure 1. Since this particular Hankel transform also has an analytical expression, a comparison to the exact result is possible. The difference between the approximate and exact transform is shown in Figure 2. For this range of transform variable, k, the maximum deviation is about

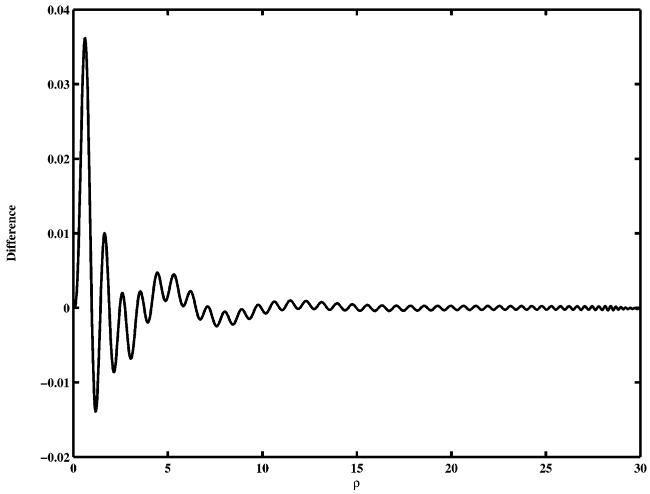

Figure 4. Difference between the analytical inverse Hankel transform and the Fourier−Bessel representation.

0.0006. The largest deviations are found near the origin due to the use of a cutoff.

The inverse transform was also evaluated using the Fourier−Bessel series expansion[13] for the approximation to the direct transform using the Zernike expansion and for the exact direct transform using the analytical expression. The cutoff was chosen to be the same as that for the direct transform, 30, and 256 zeros were selected as the quadrature points. The approximate inverse transform, scaled to its largest absolute value, calculated in this way is plotted in Figure 3 as a function of radial distance. The difference between the exact and approximate inverse transforms is displayed in Figure 4. Again, the largest deviations from the exact values are found near the origin and are relatively larger than those deviations for the direct transform.

5. Conclusions

A simple connection between the Fourier−Bessel and Zernike polynomial expansions on the unit interval has been demonstrated which provides an alternative understanding of the complementarity between the Fourier−Bessel series and a particular orthogonal polynomial basis set. This complementarity has the practical consequence of offering a choice of basis set: rapidly decreasing functions might be approximated more efficiently by simple polynomials than by the superposition of many Bessel functions. Indeed, some classes of strictly truncated functions are much more suited to a Zernike basis set than the Fourier−Bessel basis set.

As described above, the Zernike expansion might also be useful for evaluating certain classes of Hankel transforms. For functions that are nonzero for the entire infinite interval, though, it is necessary to introduce a cutoff parameter. This strategy is often problematic since the long range contributions to the integral are lost resulting in errors near the origin of the transformed function. Another difficulty with the Zernike expansion is the calculation of high order Zernike polynomials which might be required for a large number of summation terms. These polynomials are themselves rapidly oscillating and their evaluation can be unstable. Large order approximations exist for the Jacobi polynomials which avoid the recurrence relations and are suitable everywhere except near the endpoints.[4] These approximations might be useful for some classes of functions but are probably not suitable for general applications. Overall, the general numerical efficacy of the Zernike expansion is currently unresolved, but it is clear that the complementarity to the Fourier−Bessel expansion provides another approach to the approximation of functions on the unit interval.

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