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A band factorization technique for transition matrix element asymptotics

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Abstract

A new method of evaluating transition matrix elements between wave functions associated with orthogonal polynomials is proposed. The technique relies on purely algebraic manipulation of the associated recurrence coefficients. The form of the matrix elements is perfectly suited to very large quantum number calculations by using asymptotic series expansions. In practice, this allows the accurate and fast numerical treatment of transition matrix elements in the quasi-classical limit. Examples include the matrix elements of x^p in the harmonic oscillator basis, and connections with the Wigner $3j$ symbols.

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1. Introduction

In this paper we offer a new approach to the numerical evaluation of transition matrix elements of the form

$$\int \Psi_n(Q) f(Q) \Psi_m(Q)\,\mathrm{d}Q, \tag{1}$$

where Q denotes the set of coordinates of a quantum system, and $\mathrm{d}Q$ the product of the differentials of these coordinates. Eigenfunctions Ψ_n and Ψ_m belong to the discrete spectrum of the Hamiltonian operator and f is a given physical quantity. The numerical treatment of (1) has been the topic of numerous papers in the field of quantum chemistry and physics and a complete survey would merit a separate paper. In the quasi-classical limit, the wavelengths of particles are small in comparison with the characteristic dimensions of the system and the wavefunctions Ψ_n of the quasi-classical state (i.e. with large quantum number $n \gg 1$) oscillate strongly [1]. This considerably complicates a direct numerical evaluation of the transition matrix elements, even using modern computers. To alleviate this problem, several numerical techniques have been devised, see, for instance, [2–4]. Alternatively, asymptotic approximations have been proposed using the WKJB approximation [1] or other methods [5].

In this work asymptotic series expansions to *any* order with respect to the small parameter $\epsilon = \mathcal{O}(1/n)$ are established for several specific cases. These results have potential application to a wide range of quantum problems. The proposed method relies on the well known connection between the wave functions and the classical orthogonal polynomials such as those ascribed to Hermite, Legendre and Laguerre, which can serve as a Hermitian basis for the space of square-integrable functions [2,6–8]. By construction, these polynomials satisfy either a two-term or a three-term recurrence relation [9]. This property allows an analytical treatment of integrals of the type (1) when the function f is expanded in its Taylor series. Furthermore, these new integration formulas are perfectly suited for very large quantum number calculations by using asymptotic series expansions. In the following, for brevity, we restrict attention to the class of orthogonal polynomials satisfying a two-term recurrence relation. The generalization to three-term recurrence relations will be the subject of future work.

2. Band factorization for two-term recurrence relations

In this section we consider maps of $l(\mathbb{Z})$ (the space of real-valued sequences) onto itself. In particular, we turn our atten-

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tion to the two-term recurrence operator

$$\mathsf{T}: l(\mathbb{Z}) \to l(\mathbb{Z}), \tag{2}$$

satisfying the recurrence relation

$$\mathsf{T}\mathsf{e}_n = b_{n-1}\mathsf{e}_{n-1} + a_n \mathsf{e}_{n+1}, \tag{3}$$

where $\{\mathsf{e}_n, n \in \mathbb{Z})$ is the standard canonical basis of $l(\mathbb{Z})$, i.e.

$$\mathsf{e}_n = (\ldots, \delta_{-1,n}, \delta_{0,n}, \delta_{1,n}, \delta_{2,n}, \ldots)^{\mathrm{T}}, \tag{4}$$

in which δ denotes the usual Kronecker symbol and T the vector transpose. Given a positive integer p, we wish to establish the exact form for the pth iteration operator $(\mathsf{T})^p$. It is convenient for the analysis to write T in the form of the *infinite* dimensional bidiagonal matrix

$$\mathsf{T} = \mathsf{A} + \mathsf{B} = \begin{pmatrix} \ddots & \ddots & \ddots & & & & \\ & a_{-2} & 0 & b_{-1} & & & \\ & & a_{-1} & 0 & b_0 & & \\ & & & a_0 & 0 & b_1 & \\ & & & & a_1 & 0 & b_2 \\ & & & & & \ddots & \ddots & \ddots \end{pmatrix}, \tag{5}$$

where A and B are, respectively, the lower and the upper part of T, i.e. A contains the a_n elements and B the b_n elements. Here A is an infinite matrix with only the sub-diagonal entries, which henceforth is referred to as a 1-band structure matrix. Similarly, B has a 1-band structure but only with the super-diagonal non-zero. We now call d_n the series of coefficients

$$d_n = a_n b_n, \quad \forall n \in \mathbb{Z}, \tag{6}$$

and define the family of shifted diagonal operators D_k as

$$\mathsf{D}_k \mathsf{e}_n = d_{n+k}\mathsf{e}_n, \quad \forall (n,k) \in \mathbb{Z}^2. \tag{7}$$

Now, assuming for the moment that $a_n \neq 0$ for all n, then we can define the pseudo inverse operator $\mathsf{A}^{[-1]}$ as

$$\mathsf{A}^{[-1]}\mathsf{e}_n = \frac{1}{a_{n-1}}\mathsf{e}_{n-1}. \tag{8}$$

This can be generalized to any integer power $q \in \mathbb{Z}$ as follows

$$\mathsf{A}^{[q]} = \left\{ \begin{array}{ll} (\mathsf{A})^q, & q \geqslant 1 \\ \mathsf{I}, & q = 0 \\ (\mathsf{A}^{[-1]})^{|q|}, & q \leqslant -1 \end{array} \right\}, \tag{9}$$

where I is the identity. With this definition, the following properties hold

$$\mathsf{A}\mathsf{A}^{[q]} = \mathsf{A}^{[q+1]} \quad \text{and} \quad \mathsf{A}^{[-1]}\mathsf{A}^{[q]} = \mathsf{A}^{[q-1]}. \tag{10}$$

Because of the 1-band structure of A, it is straightforward to show that

$$\mathsf{A}^{[q]}\mathsf{e}_n = \prod_{l=0}^{q-1} a_{n+l}\mathsf{e}_{n+q} \quad \text{and}$$
$$\mathsf{A}^{[-q]}\mathsf{e}_n = \frac{1}{\prod_{l=1}^{|q|} a_{n-l}}\mathsf{e}_{n-q}, \tag{11}$$

for any positive integer q. This means that raising A to the power q shifts the non-zero diagonal band q places 'down' the matrix. The property (11), and the definition of the operator D (7) yields

$$\mathsf{D}_k \mathsf{A}^{[q]}\mathsf{e}_n = \prod_{l=0}^{q-1} a_{n+l} d_{n+q+k}\mathsf{e}_{n+q} = \mathsf{A}^{[q]}\mathsf{D}_{k+q}\mathsf{e}_n,$$
$$\forall q \geqslant 1. \tag{12}$$

A similar formula holds for negative powers. To summarize, the diagonal operators commute with $\mathsf{A}^{[q]}$ as follows

$$\mathsf{D}_k \mathsf{A}^{[q]} = \mathsf{A}^{[q]}\mathsf{D}_{k+q}, \quad \forall q \in \mathbb{Z}. \tag{13}$$

We can now establish the key result of this paper:

Proposition 1. *Given a positive integer p, then $(\mathsf{T})^p$ admits the band factorization*

$$(\mathsf{T})^p = \sum_{q=0}^{p} \mathsf{A}^{[p-2q]}\mathsf{S}_q^p, \tag{14}$$

where S_q^p is the diagonal operator

$$\mathsf{S}_q^p = \sum_{\{i_t\} \in \mathcal{I}_q^p} \prod_{l=1}^{q} \mathsf{D}_{i_l - l}, \quad p \geqslant q \geqslant 1 \quad \text{and} \quad \mathsf{S}_0^p = \mathsf{I}, \tag{15}$$

and the set of indices $\mathcal{I}_q^p$ is associated with the nested sum

$$\sum_{\{i_t\} \in \mathcal{I}_q^p} = \sum_{i_q=0}^{p-q} \sum_{i_{q-1}=0}^{i_q} \cdots \sum_{i_2=0}^{i_3} \sum_{i_1=0}^{i_2}. \tag{16}$$

Proof. We shall prove (14) by induction. The factorization obviously holds for $p = 1$ since $\mathsf{B}\mathsf{A} = \mathsf{D}_0$. Therefore,

$$\mathsf{T} = \mathsf{A} + \mathsf{B} = \mathsf{A} + \mathsf{D}_0\mathsf{A}^{[-1]} = \mathsf{A} + \mathsf{A}^{[-1]}\mathsf{D}_{-1}$$
$$= \mathsf{A}\mathsf{S}_0^1 + \mathsf{A}^{[-1]}\mathsf{S}_1^1. \tag{17}$$

Assuming (14) holds for a given p, then

$$\begin{aligned}(\mathsf{T})^{p+1} &= \big(\mathsf{A} + \mathsf{D}_0\mathsf{A}^{[-1]}\big)(\mathsf{T})^p \\ &= \sum_{q=0}^{p} \mathsf{A}^{[p+1-2q]}\mathsf{S}_q^p + \sum_{q=0}^{p} \mathsf{A}^{[p-1-2q]}\mathsf{D}_{p-1-2q}\mathsf{S}_q^p \\ &= \mathsf{A}^{[p+1]}\mathsf{S}_0^p + \sum_{q=1}^{p} \mathsf{A}^{[p+1-2q]}\big(\mathsf{S}_q^p + \mathsf{D}_{p+1-2q}\mathsf{S}_{q-1}^p\big) \\ &\quad + \mathsf{A}^{[-p-1]}\mathsf{D}_{-p-1}\mathsf{S}_p^p \end{aligned} \tag{18}$$

and by definition,

$$\begin{aligned}\mathsf{S}_q^{p+1} &= \sum_{i_q=0}^{p+1-q} \sum_{i_{q-1}=0}^{i_q} \cdots \sum_{i_1=0}^{i_2} \prod_{l=1}^{q} \mathsf{D}_{i_l - l} \\ &= \mathsf{S}_q^p + \mathsf{D}_{p+1-2q} \sum_{i_{q-1}=0}^{p-(q-1)} \cdots \sum_{i_1=0}^{i_2} \prod_{l=1}^{q-1} \mathsf{D}_{i_l - l} \\ &= \mathsf{S}_q^p + \mathsf{D}_{p+1-2q}\mathsf{S}_{q-1}^p, \quad 1 \leqslant q \leqslant p. \end{aligned} \tag{19}$$

Thus, given the fact that $\mathsf{S}_0^{p+1} = \mathsf{S}_0^p = \mathsf{I}$ and $\mathsf{S}_{p+1}^{p+1} = \mathsf{D}_{-p-1}\mathsf{S}_p^p$, we end up with the result

$$(\mathsf{T})^{p+1} = \sum_{q=0}^{p+1} \mathsf{A}^{[p+1-2q]}\mathsf{S}_q^{p+1}, \tag{20}$$

which completes the proof. □

We now have $(\mathsf{T})^p$ in a very useful closed form, consisting of a sum of 1-band matrices each occupying the $(p-2q)$th diagonal position, ranging from p to $-p$ in steps of two. In practice, negative powers in (14) are less convenient to manipulate but a similar factorization holds by defining the series of 1-band operators $\mathsf{B}^{[q]}$; this gives the alternative form

$$(\mathsf{T})^p = \sum_{q=0}^{p} \mathsf{S}_q^p \mathsf{B}^{[p-2q]}, \tag{21}$$

which from (14) gives the relationship

$$\mathsf{A}^{[p-2q]}\mathsf{S}_q^p = \mathsf{S}_{p-q}^p \mathsf{B}^{[2q-p]}. \tag{22}$$

Among other things, this identity reveals that the band factorization holds for any series of coefficients and the restriction made earlier that $a_n \neq 0$ can be lifted. For the sake of clarity, we consider separately the odd and even powers. After some algebra we can derive the final form

$$(\mathsf{T})^{2p}\mathsf{e}_n = \sum_{q=0}^{p-1} \mathsf{e}_n \cdot \mathsf{S}_q^{2p}\mathsf{e}_n \left(\prod_{l=0}^{2p-2q-1} a_{n+l}\mathsf{e}_{n+2p-2q} + \prod_{l=1}^{2p-2q} b_{n-l}\mathsf{e}_{n-2p+2q} \right) + \mathsf{S}_p^{2p}\mathsf{e}_n, \tag{23}$$

and

$$(\mathsf{T})^{2p+1}\mathsf{e}_n = \sum_{q=0}^{p} \mathsf{e}_n \cdot \mathsf{S}_q^{2p+1}\mathsf{e}_n \left(\prod_{l=0}^{2p-2q} a_{n+l}\mathsf{e}_{n+2p+1-2q} + \prod_{l=1}^{2p+1-2q} b_{n-l}\mathsf{e}_{n-2p-1+2q} \right), \tag{24}$$

where the dot symbol stands for the usual scalar product and we have explicitly

$$\mathsf{e}_n \cdot \mathsf{S}_q^p \mathsf{e}_n = \sum_{\{i_l\}\in\mathcal{I}_q^p} \prod_{l=1}^{q} a_{n+i_l-l} b_{n+i_l-l}, \quad 1 \leqslant q \leqslant p, \tag{25}$$

and $\mathsf{e}_n \cdot \mathsf{S}_0^p \mathsf{e}_n = 1$.

We end this section by noting that the band factorization technique can easily be extended to the three-term recurrence operator $\mathsf{T}'\mathsf{e}_n = b_{n-1}\mathsf{e}_{n-1} + \mathsf{e}_n + a_n\mathsf{e}_{n+1}$. In this case, the diagonal is simply the identity. Applying the Leibniz rule yields the following band factorization

$$(\mathsf{T}')^p = (\mathsf{A} + \mathsf{I} + \mathsf{B})^p = \sum_{r=0}^{p}\sum_{q=0}^{r} \mathcal{C}_r^p \mathsf{A}^{[r-2q]}\mathsf{S}_q^r, \tag{26}$$

where $\mathcal{C}_r^p$ stands for the usual binomial coefficient. The band factorization for a general three-term recurrence relation would be an interesting and useful direction for future work.

3. Application to transition matrix element evaluation

We consider a system of polynomials $f_n(x)$, $n = 0, 1, 2 \ldots$, orthogonal on the interval $x \in I$ with respect to a weight function $w(x)$. More specifically we are interested in the class of orthogonal polynomials satisfying the following recurrence relation:[1]

$$\bar{a}_{1n} f_{n+1}(x) = \bar{a}_{3n} x f_n(x) - \bar{a}_{4n} f_{n-1}(x). \tag{27}$$

For instance, Hermite, Legendre, Chebyshev and Gegenbauer polynomials all fall into this class. These polynomials are orthogonal with respect to $w(x)$ as

$$\int_I w(x) f_n(x) f_m(x)\,\mathrm{d}x = h_n \delta_{n,m}. \tag{28}$$

It is convenient to introduce the normalized function

$$\psi_n(x) = \sqrt{\frac{w(x)}{h_n}} f_n(x), \tag{29}$$

so that the previous recurrence relation reads simply

$$x\psi_n(x) = a_{n-1}\psi_{n-1}(x) + b_n\psi_{n+1}(x), \tag{30}$$

in which

$$a_{n-1} = \sqrt{\frac{h_{n-1}}{h_n}} \frac{\bar{a}_{4n}}{\bar{a}_{3n}} \quad \text{and} \quad b_n = \sqrt{\frac{h_{n+1}}{h_n}} \frac{\bar{a}_{1n}}{\bar{a}_{3n}}. \tag{31}$$

At this point, it should be remarked that the two series a_n and b_n are necessarily equivalent since, by using orthogonality properties, we find that

$$a_{n-1} = \int_I x\psi_n(x)\psi_{n-1}(x)\,\mathrm{d}x \quad \text{and} \quad b_n = \int_I x\psi_n(x)\psi_{n+1}(x)\,\mathrm{d}x; \tag{32}$$

hence $a_n = b_n$ and T is a symmetric matrix in this context. Now, let us define the vector function $\Psi(x)$ as

$$\Psi(x) = \sum_{m\in\mathbb{N}} \psi_m(x)\mathsf{e}_m, \tag{33}$$

then the recurrence relation can be written in the matrix form

$$x\Psi(x) = \mathsf{T}\Psi(x) = \sum_{m\in\mathbb{N}} \psi_m(x)\,\mathsf{T}\mathsf{e}_m, \tag{34}$$

where T is the two-term recurrence operator introduced in the previous section. Since polynomials are only defined for positive integers, we must put by convention the decoupling condition

$$a_{-1} = b_{-1} = 0, \tag{35}$$

so that coefficients with negative indices a_n, b_n for $n < -1$ can be chosen arbitrarily since they are decoupled from their positive counterpart.

[1] We strictly take the same notation as in [9], p. 782, and the bar symbol is introduced to avoid any confusion with coefficients a_n from Eq. (3).

Now, from (34), it is clear that, given any positive integer p, we have

$$x^p \Psi(x) = (\mathsf{T})^p \Psi(x) = \sum_{m\in\mathbb{N}} \psi_m(x)(\mathsf{T})^p \mathsf{e}_m, \tag{36}$$

which, by using orthogonality properties, yields

$$I_{n,m}^p = \int_I x^p \psi_n(x)\psi_m(x)\,\mathrm{d}x = \mathsf{e}_m \cdot (\mathsf{T})^p \mathsf{e}_n = \mathsf{e}_n \cdot (\mathsf{T})^p \mathsf{e}_m. \tag{37}$$

Eq. (37) with the explicit form (23) and (24) are the main result of this paper. Since T is symmetric, we only consider situations where $m \geqslant n$ and introduce the separation index s as the positive integer $s = m - n$. We call σ the quantity

$$\sigma = \frac{p-s}{2}, \tag{38}$$

and then (37) can be rewritten as the following explicit integration formula

$$I_{n,n+s}^p = \int_I x^p \psi_n(x)\psi_{n+s}(x)\,\mathrm{d}x = \begin{cases} F(s,n)G(\sigma,p,n) & \text{if } \sigma \in \mathbb{N}, \\ 0 & \text{otherwise,} \end{cases} \tag{39}$$

where

$$F(s,n) = \prod_{l=0}^{s-1} a_{n+l} \quad \text{if } s \neq 0, \quad \text{and} \quad F(0,n) = 1, \tag{40}$$

$$G(\sigma,p,n) = \sum_{\{i_t\}\in\mathcal{I}_\sigma^p} \prod_{l=1}^{\sigma} a_{n+i_l-l}^2 \quad \text{if } \sigma \neq 0, \quad \text{and} \quad G(0,p,n) = 1, \tag{41}$$

and the nested sum over $\mathcal{I}_\sigma^p$ is defined in (16). Table 1 displays the explicit form for the normalized functions and their recurrence relation coefficients a_n for classical orthogonal polynomials (superscripts H, L, G and C, relating to Hermite, Legendre, etc., are added to avoid any confusion). Notations are strictly identical with Table 22.2, p. 774 in [9]. All functions are defined over the interval $I = [-1, 1]$ except the Hermite polynomials for which $I = (-\infty, \infty)$. Note that recurrence coefficients associated with Hermite, Legendre and Gegenbauer polynomials have the remarkable properties of automatically satisfying the decoupling condition (35). This fact is exploited in [12].

At first sight, formula (41) appears to be rather inefficient from a computational point of view since it contains $\sigma \mathrm{Card}(\mathcal{I}_\sigma^p) = \sigma \mathcal{C}_\sigma^p$ products. However, from (19), it can be seen that coefficients $G(\sigma, p, n)$ can be efficiently computed via the recursion relation

$$G(\sigma,p,n) = G(\sigma,p-1,n) + a_{n+p-2\sigma}^2 G(\sigma-1,p-1,n), \tag{42}$$

with the convention that $G(\sigma, p, n) = 0$ whenever $\sigma > p/2$ or $\sigma < 0$. So, $G(\sigma, p, n)$ can be numerically recovered with as little as $\mathcal{O}(p^2/2)$ products. The recursion relation (42) is not surprising since the expression (41) is nothing else but the analytical result of an iteration process. At this point, the reader may wonder about the usefulness of the integration formula (39) since the integral could be directly computed via the recursion

$$I_{n,m}^p = a_{m-1} I_{n,m-1}^{p-1} + a_m I_{n,m+1}^{p-1}, \tag{43}$$

at a similar computational cost, see for instance [7,10]. However, the expression (39) has the great advantage of revealing the analytical form of $I_{n,m}^p$ which is extremely useful when evaluating the integral for large mode numbers.

4. Asymptotic series expansion

In this section we exploit the explicit integration formula (39). For large order n, a quick examination of Table 1 reveals that all recurrence coefficients a_n behave asymptotically as

$$a_{n+l} = \omega_n\big(1 + \epsilon\alpha_l + \epsilon^2\beta_l + \cdots\big), \tag{44}$$

where we introduce the small parameter $\epsilon = \mathcal{O}(1/n)$ (its precise form is established in each particular example). Substituting the asymptotic form in (40) yields

$$F(s,n) = (\omega_n)^s\big(1 + \epsilon f_1(s) + \epsilon^2 f_2(s) + \mathcal{O}(\epsilon^3)\big), \tag{45}$$

where

$$f_1(s) = \sum_{l=0}^{s-1} \alpha_l \quad \text{and} \quad f_2(s) = \frac{1}{2}\sum_{l=0}^{s-1}\sum_{k=0}^{s-1} \alpha_l\alpha_k(1-\delta_{l,k}) + \sum_{l=0}^{s-1}\beta_l. \tag{46}$$

Similarly,

$$G(\sigma,p,n) = (\omega_n)^{2\sigma}\mathcal{C}_\sigma^p\big(1 + \epsilon g_1(\sigma,p) + \epsilon^2 g_2(\sigma,p) + \mathcal{O}(\epsilon^3)\big) \tag{47}$$

Table 1
Normalized function ψ_n and its two-term recurrence coefficients a_n for the classical orthogonal polynomials. For the sake of clarity we put $v(x) = \sqrt{2}(1-x^2)^{1/4}$ in the normalized Gegenbauer and Chebyshev polynomials

Polynomial	Normalized function	a_n
Hermite, H_n	$\psi_n^H = \frac{1}{\sqrt{\pi^{1/2}2^n n!}} H_n(x) e^{-x^2/2}$	$\sqrt{\frac{n+1}{2}}$
Legendre, P_n	$\psi_n^L = (\frac{2n+1}{2})^{1/2} P_n(x)$	$\frac{1}{2}(\frac{(n+1)^2}{(n+1)^2-1/4})^{1/2}$
Gegenbauer, $C_n^{(\alpha)}$ ($\alpha > -\frac{1}{2}$)	$\psi_n^G = (\frac{n!(n+\alpha)\Gamma^2(\alpha)}{\pi\Gamma(n+2\alpha)})^{1/2} v(x)^{2\alpha-1} C_n^{(\alpha)}(x)$	$\frac{1}{2}(\frac{(n+2\alpha)(n+1)}{(n+\alpha)(n+1+\alpha)})^{1/2}$
Chebyshev, U_n	$\psi_n^C = \frac{1}{\sqrt{\pi}} v(x) U_n(x)$	$\frac{1}{2}$

with

$$g_1(\sigma, p) = 2\left(\mathcal{C}_\sigma^p\right)^{-1} \sum_{\{i_l\}\in\mathcal{I}_\sigma^p} \sum_{l=1}^{\sigma} \alpha_{i_l-l} \tag{48}$$

and

$$g_2(\sigma, p) = \left(\mathcal{C}_\sigma^p\right)^{-1} \sum_{\{i_l\}\in\mathcal{I}_\sigma^p} \left(2\sum_{l=1}^{\sigma} \beta_{i_l-l} + \sum_{l=1}^{\sigma}\sum_{k=1}^{\sigma} \alpha_{i_l-l}\alpha_{i_k-k}(2-\delta_{l,k})\right), \tag{49}$$

where, as already mentioned, $\mathcal{C}_\sigma^p$ is the binomial coefficient. In all these summations, it is understood that $f_1(0) = f_2(0) = g_1(0, p) = g_2(0, p) = 0$. To summarize, the non-zero transition matrix elements yield the following asymptotic expansion

$$\int_I x^p \psi_n(x)\psi_m(x)\,\mathrm{d}x = (\omega_n)^p \mathcal{C}_\sigma^p\left(1 + \epsilon A_1(\sigma, p) + \epsilon^2 A_2(\sigma, p) + \mathcal{O}(\epsilon^3)\right), \tag{50}$$

where by convention, $m \geqslant n$ and the quantity $\sigma = (p - (m - n))/2$ is a positive integer. The corrective terms are explicitly given by

$$A_1(\sigma, p) = f_1(p - 2\sigma) + g_1(\sigma, p) \tag{51}$$

and

$$A_2(\sigma, p) = f_2(p - 2\sigma) + g_2(\sigma, p) + f_1(p - 2\sigma)g_1(\sigma, p). \tag{52}$$

These asymptotic results are now exploited for three specific examples.

4.1. Hermite polynomials

We shall firstly apply the asymptotic form for the Hermite polynomials, which have the normalized functional form

$$\psi_n^H(x) = \frac{1}{\sqrt{\pi^{1/2}2^n n!}} H_n(x)\,\mathrm{e}^{-x^2/2}, \tag{53}$$

where $H_n(x)$ can be found explicitly in [9] for example. The associated recurrence coefficients for $\psi_n^H(x)$ have the asymptotic form

$$a_{n+l} = \left(\frac{n+1}{2}\right)^{1/2}\left(1 + \epsilon\frac{l}{2} - \epsilon^2\frac{l^2}{8} + \cdots\right) \quad \text{with } \epsilon = \frac{1}{n+1}. \tag{54}$$

Note this choice of ϵ; another form, such as $\epsilon = 1/n$, would lead to a more complicated (and slightly more slowly convergent) expansion. Thus, in (44) we have $\alpha_l = l/2$ and $\beta_l = -l^2/8$. This yields

$$\int_{-\infty}^{\infty} x^p \psi_n^H(x)\psi_m^H(x)\,\mathrm{d}x = \left(\frac{n+1}{2}\right)^{p/2} \mathcal{C}_\sigma^p\left(1 + \epsilon A_1(\sigma, p) + \epsilon^2 A_2(\sigma, p) + \mathcal{O}(\epsilon^3)\right). \tag{55}$$

There is no simple expression for the corrective terms $A_1(\sigma, p)$ and $A_2(\sigma, p)$ for general σ and p. We list in Tables 2 and 3 the value of these respective coefficients for the first few values of σ and p.

We shall compare these asymptotic expressions with the exact formula for the non-zero matrix element given in [11], that is,

$$\int_{-\infty}^{\infty} x^p \psi_n^H(x)\psi_m^H(x)\,\mathrm{d}x = 2^{\mu-\frac{p}{2}}\left(\frac{m!}{n!}\right)^{1/2} p! \sum_{l=\mu}^{\min(n,m)} \frac{\mathcal{C}_l^n}{2^l(m-l)!(l-\mu)!}, \tag{56}$$

where $\mu = (n + m - p)/2$ is an integer.

Eq. (56) clearly indicates the difficulties encountered in evaluating these coefficients with such formulae when using standard double-precision floating point arithmetic as n increases. Since the value of the factorial of n goes beyond the accuracy level of 32 bit machines even for moderately small n, computed values of (56) are expected to be corrupted by round-off errors. In Tables 4 and 5 the computed values of the transition matrix elements are shown for the two specific cases: $p = s = 3$ and $p = 5$, $s = 3$. All calculations are carried out with double precision arithmetic. The last column shows the round-off errors caused by a large quantum number and the computed values

Table 2
Values of the corrective terms $A_1(\sigma, p)$ associated with the Hermite polynomial

	$p=1$	$p=2$	$p=3$	$p=4$	$p=5$
$\sigma=0$	0	1/2	3/2	3	5
$\sigma=1$	.	−1/2	0	1	5/2
$\sigma=2$	.	.	.	−1	0

Table 3
Values of the corrective terms $A_2(\sigma, p)$ associated with the Hermite polynomial

	$p=1$	$p=2$	$p=3$	$p=4$	$p=5$
$\sigma=0$	0	−1/8	−1/8	1	5
$\sigma=1$	.	0	0	1/8	11/8
$\sigma=2$	.	.	.	1/2	1/2

Table 4
Comparison between the asymptotic expressions and the analytical formula, $p=3$, $s=3$, $\sigma=0$

	$n=8$	$n=1024$	$n=262144$
Leading order	9.5459	11602.21220	47453404.3413
First order	11.136	11619.19105	47453675.8709
Second order	11.122	11619.18967	47453675.8708
Analytical	11.124	11619.18967	47453675.8356

Table 5
Comparison between the asymptotic expressions and the analytical formula, $p = 5, s = 3, \sigma = 1$

	$n = 8$	$n = 1024$	$n = 262144$
Leading order	214.78	29730668.783	31099181702683.
First order	274.44	29803182.609	31099478286460.
Second order	278.09	29803221.519	31099478287082.
Analytical	278.10	29803221.521	31099478265649.

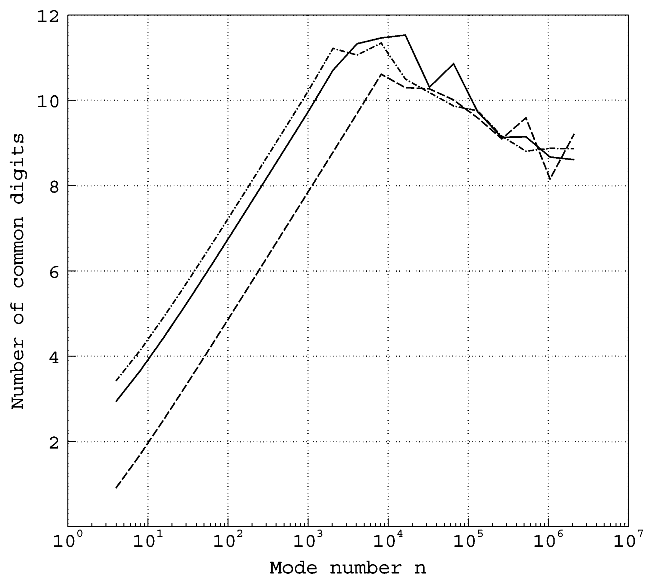

Fig. 1. Number of common digits (defined in Eq. (57)) with respect to the mode number n. Straight line: $p = s = 3$; Dash-dot: $p = 5, s = 3$; Dashed line: $p = 9$, $s = 3$.

from the exact formula are not accurate. This precision problem is conveniently revealed in Fig. 1 where the number of common digits (n.c.d.) between the second order asymptotic expression and the computed formula (56) are plotted against n. By convention, n.c.d. is evaluated as the real quantity

$$\text{n.c.d.} = \left|\log \frac{|\text{Second order} - \text{Analytical}|}{\text{Leading order}}\right|. \tag{57}$$

Below a certain threshold $n < n_t$, the progression is in agreement with the $\mathcal{O}(\epsilon^3)$ approximation error. For larger values, the exact expression (56) cannot be computed properly and the loss of accuracy gets progressively worse as n increases.

Since (55) has to be used for moderately small exponent p, corrective terms A_1 and A_2 as well as the binomial coefficients $\mathcal{C}_\sigma^p$ can be computed and stored once and for all at very small cost, and then the asymptotic expression (55) can be computed extremely rapidly. Here the gain is clear when compared with the cost of the full computation of the sum in (56) for each value of n. It is believed that this should have some important applications in quantum chemistry and physics programs since in many cases of practical interest the wave functions are expanded in the harmonic oscillator basis [6,7]. We end this section by noting that more elaborate formulae could be developed for taking into account higher order correctives terms; we only restricted ourselves to a second order expansion for the sake of clarity.

4.2. Legendre polynomials and associated Legendre functions

We extend the method to the associated Legendre functions of the first kind, P_n^ν, defined for $n \geqslant \nu$ and obtained from the Legendre polynomials as $P_n^\nu(x) = (-1)^\nu(1-x^2)^{\nu/2}(\mathrm{d}^\nu/\mathrm{d}x^\nu) P_n^0(x)$ where, by convention, we put $P_n \equiv P_n^0$. Though the functions P_n^ν are not polynomials (except when ν is even) they satisfy the two-term recurrence relation (see p. 334 in [9]):

$$(2n+1)x P_n^\nu(x) \\ = (n+\nu)P_{n-1}^\nu(x) + (n+1-\nu)P_{n+1}^\nu(x) \tag{58}$$

as well as the orthogonality relation

$$\int_{-1}^{1} P_n^\nu(x)P_m^\nu(x)\,\mathrm{d}x = \frac{2}{2n+1}\frac{(n+\nu)!}{(n-\nu)!}\delta_{n,m}. \tag{59}$$

So, if we define the associated normalized functions $\psi_{n,\nu}^L$ as

$$\psi_{n,\nu}^L(x) = \left(\frac{2(n+\nu)+1}{(n+2\nu)!}\frac{n!}{2}\right)^{1/2} P_{n+\nu}^\nu(x), \tag{60}$$

then $\psi_{n,\nu}^L$ satisfy (30) with

$$a_n = \frac{1}{2}\left(\frac{(n+\nu+1)^2-\nu^2}{(n+\nu+1)^2-1/4}\right)^{1/2}. \tag{61}$$

These coefficients have the striking properties of having a relatively simple asymptotic form, namely

$$a_{n+l} = \frac{1}{2}\left(1 - \epsilon^2\frac{4\nu^2-1}{8} + \cdots\right) \\ \text{with } \epsilon = \frac{1}{n+\nu+1}. \tag{62}$$

So $\alpha_l = 0$, and β_l is *independent* of l and

$$\beta_l = \beta = \frac{1}{8}(1-4\nu^2). \tag{63}$$

It is easy to show that $f_1 = g_1 = 0$, $f_2(s) = s\beta$ and $g_2(\sigma, p) = 2\beta\sigma$ and hence we end up with the explicit formula

$$\int_{-1}^{1} x^p \psi_{n,\nu}^L(x)\psi_{n+s,\nu}^L(x)\,\mathrm{d}x \\ = \frac{\mathcal{C}_\sigma^p}{2^p}\left(1+\epsilon^2\beta p + \mathcal{O}(\epsilon^3)\right) \quad \text{where } \sigma \in \mathbb{N}. \tag{64}$$

This last result is useful for certain quantum physics computations. For the sake of illustration, we consider the interaction of a three dimensional quantum wave field due a rotation-invariant potential with an axisymmetric perturbation. Interactions between the spherical harmonics are conveniently described by the transition matrix elements

$$T_{0\nu-\nu}^{qnm} = \int Y_q^0(\Omega)Y_n^\nu(\Omega)Y_m^{-\nu}(\Omega)\,\mathrm{d}\Omega, \quad m \geqslant n \geqslant \nu \geqslant 0, \tag{65}$$

where $Y_n^\nu(\Omega)$ is a spherical harmonic, $\mathrm{d}\Omega = \sin\theta\,\mathrm{d}\theta\,\mathrm{d}\phi$ is the element of the solid angle and the integral covers the entire surface area of the unit sphere. These quantities are usually computed with the aid of the Wigner $3j$ symbols as

$$T^{qnm}_{0\nu-\nu} = \sqrt{\frac{(2q+1)(2n+1)(2m+1)}{4\pi}} \times \begin{pmatrix} q & n & m \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} q & n & m \\ 0 & \nu & -\nu \end{pmatrix}. \tag{66}$$

For large orders n and m, the Wigner $3j$ symbols are known to be both difficult and time consuming to evaluate numerically [3,4]. To overcome this difficulty, we shall use the asymptotic form (64). Since, by definition,

$$Y^{\nu}_n(\Omega) = \frac{e^{i\nu\phi}}{\sqrt{2\pi}} \psi^L_{n-\nu,\nu}(\cos\theta) \quad \text{and}$$
$$Y^{-\nu}_m(\Omega) = (-1)^{\nu} \frac{e^{-i\nu\phi}}{\sqrt{2\pi}} \psi^L_{m-\nu,\nu}(\cos\theta), \tag{67}$$

it may be shown that we have the alternative form

$$T^{qnm}_{0\nu-\nu} = (-1)^{\nu} \sqrt{\frac{2q+1}{4\pi}} \int_{-1}^{1} P_q(x) \psi^L_{n-\nu,\nu}(x) \psi^L_{m-\nu,\nu}(x)\, dx. \tag{68}$$

Expanding $P_q(x)$ in the polynomial basis x^r, i.e.

$$P_q(x) = 2^{-q} \sum_{r=0}^{[q/2]} (-1)^r \mathcal{C}^q_r \mathcal{C}^{2q-2r}_q x^{q-2r}, \tag{69}$$

together with (64) yields the asymptotic form for the non-zero transition matrix elements

$$T^{qnm}_{0\nu-\nu} = \frac{(-1)^{\nu}}{4^q} \sqrt{\frac{2q+1}{4\pi}} \sum_{r=0}^{\bar{\sigma}} (-4)^r \mathcal{C}^q_r \mathcal{C}^{2q-2r}_q \mathcal{C}^{q-2r}_{\bar{\sigma}-r} \times \left(1 + \epsilon^2 \beta(q-2r) + \mathcal{O}(\epsilon^3)\right), \tag{70}$$

where

$$\bar{\sigma} = \frac{q-(m-n)}{2} \in \mathbb{N} \quad \text{and} \quad \epsilon = \frac{1}{n+1}. \tag{71}$$

Thus, up to the first order in ϵ, the transition matrix element amplitude only depends on q and the difference $m-n$. Here again, the second order expression (70) can be computed extremely rapidly with increasing accuracy for moderately small values of q.

4.3. Gegenbauer and Chebyshev polynomials

The leading and first order asymptotic expressions for the Gegenbauer polynomials can be shown to be identical to those of the previous section. Indeed, by rearranging the terms, the recurrence coefficients have the following form

$$a_n = \frac{1}{2} \left(\frac{(n+\alpha+1/2)^2 - (\alpha^2-\alpha+1/4)}{(n+\alpha+1/2)^2 - (\alpha+1/4)} \right)^{1/2}. \tag{72}$$

So, if we define the small parameter

$$\epsilon = \frac{1}{n+\alpha+1/2}, \tag{73}$$

we get the relatively simple asymptotic form

$$a_{n+l} = \frac{1}{2} \left(1 - \epsilon^2 \frac{\alpha}{2}(\alpha-2) + \cdots \right). \tag{74}$$

Here again, $\alpha_l = 0$ and β_l is independent of l, namely $\beta_l = -\alpha(\alpha-2)/2$. After some calculation we end up with the explicit formula for the non-zero transition matrix elements

$$\int_{-1}^{1} x^p \psi^G_n(x) \psi^G_{n+s}(x)\, dx = \frac{\mathcal{C}^p_{\sigma}}{2^p} \left(1 - \epsilon^2 \frac{\alpha}{2}(\alpha-2)p + \mathcal{O}(\epsilon^3) \right). \tag{75}$$

The integration formula for the Chebyshev polynomial of the second kind is extremely straightforward as the recurrence coefficients are constant with $a_n = 1/2$. This yields the *exact* formula

$$\int_{-1}^{1} x^p \psi^C_n(x) \psi^C_{n+s}(x)\, dx = \frac{\mathcal{C}^p_{\sigma}}{2^p}. \tag{76}$$

Thus, the normalized functions ψ_n associated with Legendre, Gegenbauer and Chebyshev polynomials share the same striking property; that is, to leading order the integral formula in all three cases is $I^p_{n,m} = 2^{-p} \mathcal{C}^p_{\sigma} (1 + \mathcal{O}(1/n^2))$.

5. Conclusion

In this article we have presented an algebraic method for evaluating typical transition matrix elements arising in a wide range of quantum mechanical problems. The technique allows the accurate and fast numerical treatment of transition matrix elements for large quantum numbers. We have strong reasons to believe that the idea can be extended to a wider class of wave functions and this will be the subject of future work.

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References

[1] L.D. Landau, E.M. Lifshitz, Quantum Mechanics (Non-Relativistic Theory), third ed., Pergamon Press Ltd., Oxford, 1977.
[2] J. Tennyson, On the calculation of matrix elements between polynomial basis functions, Comput. Phys. Comm. 38 (1985) 39–41.
[3] I.N. Kozin, J. Tennyson, M.M. Law, Effective computation of matrix elements between polynomial basis functions, Comput. Phys. Comm. 165 (2005) 10–14.
[4] J. Rasch, A.C.H. Yu, Efficient storage scheme for precalculated Wigner $3j$, $6j$, and Gaunt coefficients, SIAM J. Sci. Comput. 25 (4) (2003) 1416–1428.

[5] N.B. Delone, S.P. Goreslavsky, V.P. Krainov, Dipole matrix elements in the quasi-classical approximation, J. Phys. B: Atom. Molec. Phys. 27 (1994) 4403–4419.
[6] S.-T. Lai, P. Palting, Y.-N. Chiu, One-dimensional Schrödinger equation in the harmonic oscillator basis with various potentials, Comput. Phys. Comm. 82 (1994) 221–232.
[7] V. Martin, L.M. Robledo, Numerical and symbolic calculation of the multipole matrix elements in the axial and triaxial harmonic oscillator basis, Comput. Phys. Comm. 99 (1996) 113–127.
[8] J.-L. Basdevant, J. Dalibard, Quantum Mechanics, Springer-Verlag, Berlin, Heidelberg, 2002.
[9] M. Abramowitz, I.A. Stegun, Handbook of Mathematical Functions, tenth ed., Appl. Math. Ser., vol. 55, National Bureau of Standards, U.S. Government Printing Office, Washington, DC, 1972.
[10] A.K. Mitra, On the interaction of the type $\lambda x^2/(1+gx^2)$, J. Math. Phys. 19 (10) (1978) 2018–2022.
[11] W. Duch, Matrix elements of x^k and $e^{\alpha x}x^k$ in the harmonic oscillator basis, J. Phys. A: Math. Gen. 16 (1983) 4233–4326.
[12] E. Perrey-Debain, I.D. Abrahams, A diffusion analysis approach for multimode random optical waveguides, in: Proc. 7th Internat. Conf. Mathematical and Numerical Aspects of Wave Propagation, WAVES 2005, Brown University, U.S., pp. 267–269.