The Discrete Variable Representation

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Lecture notes of a four hours course during the
Post Graduate course on Theoretical Chemistry and Spectroscopy,
Domaine des Masures, Han-sur-Lesse, Belgium,
December 10-14, 2001.
These notes are available from www.theochem.kun.nl/~gerritg.

December 9, 2001

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1.1 Introduction

A common approach to solve a time-independent Schrödinger equation

$$\hat{H}\Psi = E\Psi \tag{1.1}$$

is the variational method. In this method one chooses a n-dimensional basis $\{\psi_1, \ldots, \psi_n\}$, in which one expands the wave function

$$\Psi = \sum_{i=1}^{n} c_i \psi_i. \tag{1.2}$$

The expansion coefficients c_i and the energy E are found by solving the matrix-eigenvalue problem

$$\mathbf{Hc} = E\mathbf{c}, \tag{1.3}$$

assuming that the basis is orthonormal, i.e., $\langle \psi_i | \psi_j \rangle = \delta_{ij}$. The column vector $\mathbf{c}$ contains the expansion coefficients, $\mathbf{c} = [c_1, c_2, \ldots, c_n]^T$, and $\mathbf{H}$ is a $n \times n$ matrix consisting of matrix elements H_{ij} of the Hamiltonian $\hat{H}$:

$$H_{ij} = \langle \psi_i | \hat{H} | \psi_j \rangle \tag{1.4}$$

In the context of the DVR method this matrix-representation is sometimes referred to as the variational basis representation (VBR).

In 1965, Harris, Engerholm, and Gwinn (HEG) from the University of Berkeley, California, published a paper with the title: *Calculation of Matrix Elements for One-Dimensional Quantum-Mechanical Problems and the Application to Anharmonic Oscillators* [1]. In this paper they consider a one-dimensional problem in which the Hamiltonian can be written as

$$\hat{H} = \hat{H}_0 + \hat{V} \tag{1.5}$$

where $\hat{H}_0$ is the harmonic oscillator Hamiltonian and $\hat{V}$ is some "complicated" potential energy operator. If one chooses a basis of harmonic oscillator eigenfunctions,

$$\hat{H}_0 \psi_i = \epsilon_i \psi_i \tag{1.6}$$

the hardest part of the calculation is computing the matrix elements

$$\langle \psi_i | V | \psi_j \rangle = \int \psi_i(x)^* V(x) \psi_j(x)\, dx. \tag{1.7}$$

HEG propose a convenient numerical method to approximate the integrals. Three years later, Dickinson and Certain [2] show that for any basis that consists of orthogonal polynomials (such as the harmonic oscillator eigenfunctions) the method of HEG is equivalent to Gaussian quadratures. When in a variational calculation the matrix elements are approximated with some quadrature of course the results, strictly speaking, need not be upper limits to the true eigenvalues. Therefore, such a representation of the potential energy operator is sometimes referred to as a *finite* basis representation (FBR) to distinguish it from a *variational* representation (VBR).

The term discrete variable representation (DVR) is introduced by Lill, Parker, and Light in 1982 [3]. In this representation the basis functions are associated with (quadrature) points and the potential energy operator is represented by a diagonal matrix, where the diagonal elements, apart from some weight factor, are simply the values of the potential in those points. Lill *et al.* point out that the approximation involved in the DVR is identical to the approximation involved in a FBR, and the FBR and DVR are related by a unitary transformation. This unitary transformation in fact already appeared in the paper of HEG, so that's where we'll start in the next section.

1.2 Computing matrix elements

To compute the potential energy matrix elements [Eq. (1.7)] HEG assume that the potential may be expanded in a Taylor series:

$$V(x) = v_0 + v_1 x + v_2 x^2 + \ldots. \tag{1.8}$$

For a harmonic oscillator basis the matrix elements $\langle \psi_i | x^n | \psi_j \rangle$ may be computed analytically. HEG propose to compute first

$$X_{ij} = \langle \psi_i | x | \psi_j \rangle. \tag{1.9}$$

Since the matrix X represents the multiplicative operator x, one may take the matrix X^n as a representation of the operator x^n. For a complete basis this procedure is exact. For example, to compute the matrix for x^2 we insert the resolution of identity:

$$\hat{I} = \sum_{n=0}^{\infty} |\psi_n\rangle\langle\psi_n| \tag{1.10}$$

into

$$\begin{aligned} \langle\psi_i|x^2|\psi_j\rangle &= \langle\psi_i|x\hat{I}x|\psi_j\rangle & (1.11)\\ &= \sum_{n=0}^{\infty}\langle\psi_i|x|\psi_n\rangle\langle\psi_n|x|\psi_j\rangle & (1.12)\\ &= \sum_{n=0}^{\infty} X_{in}X_{nj} & (1.13) \end{aligned}$$

We see that in a finite basis, where the summation is truncated to some finite value the procedure is, in general, not exact. Actually, since X turns out to be tri-diagonal we find for a N-dimensional basis, i.e., $i, j = 0, \ldots, N-1$ that matrix elements for x^n computed with this procedure are exact for $i + j \leq 2(N - n)$.

The potential matrix V can now be computed as

$$V = v_0 I + v_1 X + v_2 X^2 + \ldots \tag{1.14}$$

Since this involves many matrix multiplications, the amount of work may be reduced by diagonalization of the matrix X:

$$X\mathbf{u}_i = \lambda_i \mathbf{u}_i. \tag{1.15}$$

With

$$U = [\mathbf{u}_1\mathbf{u}_2 \ldots \mathbf{u}_n] \tag{1.16}$$

and

$$\mathbf{\Lambda} = \begin{bmatrix} \lambda_i & & \\ & \ddots & \\ & & \lambda_n \end{bmatrix} \tag{1.17}$$

we may write this in matrix notation as

$$XU = U\mathbf{\Lambda}. \tag{1.18}$$

Since X is a real symmetric matrix, U is unitary, i.e.,

$$U^\dagger U = UU^\dagger = I \tag{1.19}$$

and we have

$$X = U\mathbf{\Lambda}U^\dagger \tag{1.20}$$

and also

$$X^2 = U\mathbf{\Lambda}U^\dagger U\mathbf{\Lambda}U^\dagger \quad (1.21)$$
$$= U\mathbf{\Lambda}^2 U \quad (1.22)$$

and similarly for higher powers of X. Thus, we may write

$$V = U(v_0 I + v_1\mathbf{\Lambda} + v_2\mathbf{\Lambda}^2 + \ldots)U^\dagger \quad (1.23)$$

or

$$V = UV^{\text{diag}}U^\dagger \quad (1.24)$$

where V^{diag} is a diagonal matrix with diagonal elements

$$(V^{\text{diag}})_{ii} = v_0 + v_1\lambda_i + v_2\lambda_i^2 + \ldots = V(\lambda_i). \quad (1.25)$$

In the last step we see that with this method of computing the matrix V, we don't really need the Taylor expansion of the potential. If we assume that it exists it is sufficient to know the values of the potentials in the points λ_i. The transformation matrix U and the eigenvalues λ_i are determined by diagonalization of the x operator, which is independent of the potential.

1.3 Quadrature approximation

A straightforward method to compute potential energy matrix elements

$$V_{ij} = \int \psi_i^*(x)V(x)\psi_j(x)\,dx \quad (1.26)$$

is the use of a quadrature approximation. A n-point quadrature consisting of the abscissas $\{x_1, \ldots, x_n\}$ and the weights $\{w_1, \ldots, w_n\}$ gives

$$V_{ij} \approx V_{ij}^{FBR} = \sum_{k=1}^{n} w_k\psi_i^*(x_k)V(x_k)\psi_j(x_k). \quad (1.27)$$

Thus if we define

$$A_{ki} \equiv w_k^{\frac{1}{2}}\psi_i(x_k) \quad (1.28)$$

and the diagonal matrix

$$V_{kl}^{\text{diag}} = \delta_{kl}V(x_k), \quad (1.29)$$

we have

$$V_{ij}^{FBR} = \sum_{k=1}^{n} A_{ki}^* V_{kk}^{diag} A_{kj} \quad (1.30)$$

or, in matrix notation

$$V^{FBR} = A^\dagger V^{diag} A \quad (1.31)$$

This expression looks very similar to Eq. (1.24). We will show that they are indeed equivalent if a Gaussian quadrature approximation is used.

1.4 Orthogonal polynomials

The theory of Gaussian quadratures is intimately linked with the theory of orthogonal polynomials. For a given weight function $w(x) \geq 0$ on the interval $[a, b]$ (where a and b may be $\pm\infty$) we define the scalar product $\langle f|g\rangle$ between the real functions f and g as:

$$\langle f|g\rangle = \int_a^b w(x)f(x)g(x)\,dx. \tag{1.32}$$

Two functions are orthogonal if $\langle f|g\rangle = 0$. For each choice of a scalar product, i.e., an interval and a weight function, a set of orthogonal polynomials may be defined by

$$p_0(x) \equiv 1 \tag{1.33}$$

and the recursion relation

$$p_{i+1}(x) = xp_i(x) - \sum_{j=0}^{i} p_j(x)\frac{\langle p_j|x|p_i\rangle}{\langle p_j|p_j\rangle}. \tag{1.34}$$

One can easily see that $p_{i+1}(x)$ is orthogonal to all $p_k(x)$ with $k \leq i$ since

$$\langle p_k|p_{i+1}\rangle = \langle p_k|x|p_i\rangle - \sum_{j=0}^{i}\langle p_k|p_j\rangle\frac{\langle p_j|x|p_i\rangle}{\langle p_j|p_j\rangle}. \tag{1.35}$$

Thus, if we assume that for $kj \leq i$ the polynomials are already orthogonal, only the term with $j = k$ survives in the summation and we get

$$\langle p_k|p_{i+1}\rangle = \langle p_k|x|p_i\rangle - \langle p_k|p_k\rangle\frac{\langle p_k|x|p_i\rangle}{\langle p_k|p_k\rangle} = 0. \tag{1.36}$$

Furthermore, for $k > i + 1$ we have by definition

$$\langle p_k|p_{i+1}\rangle = 0 \tag{1.37}$$

hence we find, by substituting the recursion relation Eq. (1.34) into this expression:

$$0 = \langle p_k|x|p_i\rangle. \tag{1.38}$$

Because the scalar product is symmetric we find that

$$\langle p_i|x|p_j\rangle = 0, \quad \text{for } |i - j| > 1, \tag{1.39}$$

so the recursion relation for orthogonal polynomials simplifies to a three term recursion relation

$$p_{i+1}(x) = xp_i(x) - \alpha_i p_i(x) - \beta_i p_{i-1}(x) \tag{1.40}$$

with

$$\alpha_i = \langle p_i|x|p_i\rangle \tag{1.41}$$
$$\beta_i = \langle p_i|x|p_{i-1}\rangle. \tag{1.42}$$

If we take the weight function $w(x) = 1$ and the interval $[a, b] = [-1, 1]$ we obtain the Legendre polynomials and the weight function $w(x) = e^{-x^2}$ on $[-\infty, +\infty]$ gives the Hermite polynomials. Many more examples can be found in Chapter 22 of Abramowitz and Stegun [4].

1.5 Gaussian quadratures

With the definition of the scalar product Eq. (1.32), the integral

$$I[f] = \int_a^b w(x)f(x)\,dx \tag{1.43}$$

may be written as

$$I[f] = \langle p_0|f\rangle. \tag{1.44}$$

A Gaussian quadrature $\{(x_k, w'_k), k = 1, \ldots n\}$ is defined by the condition that

$$I[f] = \sum_{k=1}^{n} w'_k f(x_k) \tag{1.45}$$

is exact for the first $2n$ orthogonal polynomials $p_0, \ldots, p_{2n-1}$. This is possible since there are precisely $2n$ parameters (x_k, w'_k) that may be chosen.

In order to eliminate the weight function $w(x)$ from the definition of the scalar product we introduce the functions

$$\psi_i(x) = N_i w(x)^{\frac{1}{2}} p_{i-1}(x),\ i = 1, \ldots, n \tag{1.46}$$

where the normalization N_i is chosen such that, with the new definition of the scalar product,

$$\langle\psi_i|\psi_j\rangle \equiv \int_a^b \psi_i(x)\psi_j(x)\,dx = \delta_{ij} \tag{1.47}$$

Note that in the case of Hermite polynomials the functions $\psi_i(x)$ are harmonic oscillator eigenfunctions. By adjusting the Gaussian quadrature weights

$$w_k = \frac{w'_k}{w(x_k)} \tag{1.48}$$

we find that the quadrature approximation to the overlap matrix

$$\langle\psi_i|\psi_j\rangle = \sum_{k=1}^{n} w_k \psi_i(x_k)\psi_j(x_k) \tag{1.49}$$

is exact. In fact, since the Gaussian quadrature is exact for polynomials of degree $2n-1$ we find that also the quadrature approximations of the matrix elements

$$X_{ij} = \langle \psi_i | x | \psi_j \rangle = \sum_{k=1}^{n} w_k \psi_i(x_k) x_k \psi_j(x_k) \tag{1.50}$$

are exact.

If we substitute the definition of the matrix A [Eq. (1.28)] into Eq. (1.49) we find

$$\sum_{k=1}^{n} A_{ki} A_{kj} = \sum_{k=1}^{n} w_k \psi_i(x_k) \psi_j(x_k) = (A^\dagger A)_{ij} = \delta_{ij} \tag{1.51}$$

Thus, the matrix A is unitary and $A^\dagger = A^{-1}$.

Furthermore, from Eq. (1.50) we have

$$X_{ij} = \sum_{k=1}^{n} A_{ki} x_k A_{kj} \tag{1.52}$$

or, in matrix notation

$$X = A^\dagger X^{\text{diag}} A \tag{1.53}$$

where $X^{\text{diag}}_{kl} = x_k \delta_{kl}$, i.e.,

$$X A^\dagger = A^\dagger X^{\text{diag}}. \tag{1.54}$$

By comparing this with Eq. (1.18) we see that indeed the HEG method is equivalent to the Gaussian quadrature approximation of the matrix elements, with $A^\dagger = U$ and $x_k = \lambda_k$.

It may be of interest to point out that the Gaussian quadrature points x_k happen to be the roots or the orthogonal polynomial $p_n(x)$. Also, the recursion relation Eq. (1.34) shows that the matrix X is a tridiagonal matrix. Diagonalizing this matrix is actually one of the easiest ways to find the roots of $p_n(x)$. Finally, note that we can find the (unadjusted) Gaussian quadrature weights w'_k from

$$A_{k,1} = w_k^{\frac{1}{2}} \psi_1(x_k) = \left(\frac{w'_k}{w(x_k)} \right)^{\frac{1}{2}} N_1 w(x_k)^{\frac{1}{2}} p_0(x) \tag{1.55}$$

i.e, $w'_k = |A_{k,1}/N_1|^2$.

A mathematically more rigorous—and still quite readable—treatment of Gaussian quadratures can be found in Stoer and Bulirsch[5].

1.6 DVR

So far, we have seen that the method of HEG to compute potential energy matrix elements is equivalent to using a Gaussian quadrature in the case of

a basis of orthogonal polynomials. In this so called FBR (finite basis representation) the potential matrix can be written as a unitary transformation of a diagonal matrix. The idea of a DVR (discrete variable representation), as proposed by Lill, Parker, and Light[3], is to apply the unitary transformation to the basis such that the potential matrix is diagonal:

$$\phi_k(x) \equiv \sum_{i=1}^{n} A_{ki}\psi_i(x). \tag{1.56}$$

Evaluating the DVR functions $\phi_k(x)$ in the quadrature points gives

$$\phi_k(x_l) = \sum_{i=1}^{n} A_{ki}\psi_i(x_l) = \sum_{i=1}^{n} A_{ki}A_{li}w_l^{-\frac{1}{2}} = \delta_{kl}w_l^{-\frac{1}{2}}. \tag{1.57}$$

Thus, we can easily verify that any multiplicative operator is diagonal in this basis if the quadrature approximation is used:

$$\langle\phi_i|V|\phi_j\rangle = \sum_{k=1}^{n} w_k\phi_i(x_k)V(x_k)\phi_j(x_k) = \sum_{k=1}^{n}\delta_{ik}V(x_k)\delta_{jk} = V(x_k)\delta_{ij} \tag{1.58}$$

Clearly, the kinetic energy matrix is not diagonal in a DVR. Thus, in one-dimensional problems there is no clear advantage of this Gaussian-quadrature based DVR over the FBR.

1.7 Multi-dimensional DVRs

The main advantage of discrete representations becomes evident in multi-dimensional problems. In a two-dimensional problem we may take the direct product of two one-dimensional DVR bases to obtain a $N = n_x \times n_y$ dimensional basis:

$$\chi_{ij}(x,y) = \phi_i^{(x)}(x)\phi_j^{(y)}(y),\ i = 1,\ldots,n_x,\ j = 1,\ldots,n_y. \tag{1.59}$$

In this basis the potential energy matrix is diagonal:

$$V_{ij,i'j'} = \langle\phi_i^{(x)}\phi_j^{(y)}|\hat{V}|\phi_{i'}^{(x)}\phi_{j'}^{(y)}\rangle = \delta_{ii'}\delta_{jj'}V(x_i,y_j). \tag{1.60}$$

When the kinetic energy operator has the form

$$\hat{T} = -\frac{1}{2m_x}\frac{\partial^2}{\partial x^2} - \frac{1}{2m_y}\frac{\partial^2}{\partial y^2} = \hat{T}^{(x)} + \hat{T}^{(y)}, \tag{1.61}$$

the corresponding matrix is sparse, i.e., has many zeros:

$$T_{ij,i'j'} = T_{ii'}^{(x)}\delta_{jj'} + \delta_{ii'}T_{jj'}^{(y)}. \tag{1.62}$$

Hence we see that in the DVR the calculation of the Hamiltonian matrix is very cheap compared to the diagonalization. In a conventional matrix diagonalization we need memory in the order of N^2, while the cpu-time scales as N^3, which becomes not practical for N in the order of 10^4. In iterative methods, which are typically more efficient if we are interested in only a few eigenvalues/eigenvectors, however, we only need to compute matrix vector multiplications $H\mathbf{x}$. This is also true for wave-packet propagation methods that may be used for either time-dependent or time-independent methods.

If the kinetic energy operator has cross-terms like

$$T^{(xy)} = \frac{\partial^2}{\partial x \partial y} = \hat{t}_x \hat{t}_y, \tag{1.63}$$

the kinetic energy matrix is not sparse, since,

$$T^{(xy)}_{ij,i'j'} = t^{(x)}_{ii'} t^{(y)}_{jj'} \tag{1.64}$$

Still, the factorization helps to compute matrix-vector products. To compute

$$y_{ij} = \sum_{i'j'} t^{(x)}_{ii'} t^{(y)}_{jj'} x_{i'j'} \tag{1.65}$$

for all (ij) we don't need $N^2 = n_x^2 n_y^2$ operations. Instead, we apply one factor at a time:

$$z_{i'j} = \sum_{j'} t^{(y)}_{jj'} x_{i'j'} \tag{1.66}$$

which costs $n_x n_y^2 = N n_y$ operations, and then

$$y_{ij} = \sum_{i'} t^{(x)}_{ii'} z_{i'j}, \tag{1.67}$$

which costs $n_x^2 n_y = N n_x$.

For complicated kinetic energy operators there are sometimes different possibilities to represent it. An example of how to treat such a case can be found in Ref. [6].

1.8 Changing representations, the pseudospectral method

In a one-dimensional problem changing between a localized (DVR) and a delocalized (FBR) representation costs $N^3 = n_x^3$ operations. For example, if

$$\Psi(x) = \sum_i \psi_i(x) c_i = \sum_k \phi_k(x) d_k \tag{1.68}$$

and ϕ_k and ψ_i are related via the unitary transformation $A = U^\dagger$ [Eq. (1.56)] then

$$c_i = \sum_k \langle \psi_i | \phi_k \rangle d_k = \sum_k A_{ki} d_k = \sum_k U_{ik} d_k. \tag{1.69}$$

In two-dimensional problems the transformation factorizes for a direct product basis

$$c_{ij} = \sum_{i'j'} U^{(x)}_{ii'} U^{(y)}_{jj'} d_{i'j'}, \tag{1.70}$$

and we can apply the same one-coordinate-at-a-time transformation as before. Thus, going back and forth between a representation where the potential matrix is diagonal (the DVR) and another representation in which the kinetic energy is diagonal, or at least simple, is affordable. These transformations are discussed in some detail in a paper by Bramley and Tucker Carrington [7].

It is even possible to have more points than functions, in which case the transformation matrices become rectangular. Although the inverse of a rectangular matrix does not exist we can still go from the pointwise representation to the delocalized basis by projecting onto the basis. In this case it is important to use the delocalized basis as the *primary* representation, i.e., to use this basis to represent the Hamiltonian. This approach is called the *pseudo spectral* method.

A very nice example of the power of this method is the calculation of a number of bound states of the water-dimer by Leforestier *et al.*[8]. In this calculation the monomers were rigid, which still leaves six degrees of freedom. This paper also explains how to treat the rotational part of the problem, which does not have a direct product structure, and how to use symmetry.

The idea of switching representations is also used in the Fourier method[9]. For a periodic coordinate the wave function may be represented on an equally spaced grid, which may be transformed to a Fourier expansion for which the kinetic energy operator is diagonal. In this case, fast Fourier transformation (FFT) can be used, which scales more favorable than matrix multiplication, although for a small number of points per coordinate this advantage is not very important.

1.9 Potential-optimized DVR

When the potential is not at all harmonic a Gauss-Hermite DVR may not be the best option. In the case of a multi-dimensional problem we may try to construct the best possible DVR for each coordinate separately, and then use a direct product of these one-dimensional DVRs. One way to do this is the potential optimized DVR (PO-DVR) [10].

This method follows almost exactly the original HEG method. However, the delocalized basis the HEG method starts with is not a set of orthogonal polynomials, but rather a set of functions that was computed with a DVR

method. The idea is to start with a grid of many (n_0) points which gives essentially fully converged one-dimensional eigenfunctions. Then all (n_1) eigenfunctions with eigenvalues below a certain cut-off energy $E_{\max}$ are used in the HEG procedure to construct a $n_1 (< n_0)$ point grid representation. This grid is subsequently used to construct a direct product grid.

1.10 Sinc-function DVR

This DVR was first presented in 1985 by Charles Schwartz of the physics department of UC Berkeley[11] and reinvented in 1992 by Colbert and Miller[12] of the chemistry department of the same university. Here we give an alternative derivation of Groenenboom en Colbert [13], which shows where the name "sinc"-function DVR comes from. This last paper also shows how to implement efficiently a multidimensional DVR when points in a direct product grid are eliminated, e.g., because the potential in those points is above a specified cutoff energy $V_{\max}$.

This DVR is not derived from orthogonal polynomials. It is most convenient to define the sinc-function basis set $\{|n>, n = -\infty, \ldots, \infty\}$ in frequency (ω) space and then use a Fourier transform to get the x-representation of the basis set.

In ω-space we have a Fourier basis on the interval $-\omega_{\max} \ldots \omega_{\max}$:

$$\phi_n(\omega) =< \omega|n >= \begin{cases} \frac{1}{\sqrt{2\omega_{\max}}} e^{in\pi\frac{\omega}{\omega_{\max}}} & \text{for } |\omega| \leq \omega_{\max} \\ 0 & \text{otherwise.} \end{cases} \tag{1.71}$$

After Fourier transformation we obtain a basis that is complete for all band-limited functions, i.e. functions that have no frequency components above a certain frequency $\omega_{\max}$:

$$\phi_n(x) =< x|n > = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-i\omega x} < \omega|n > d\omega \tag{1.72}$$

$$= \frac{1}{2\sqrt{\pi\omega_{\max}}} \int_{-\omega_{\max}}^{\omega_{\max}} e^{-i\omega x} e^{in\pi\frac{\omega}{\omega_{\max}}} d\omega \tag{1.73}$$

$$= \sqrt{\frac{\omega_{\max}}{\pi}} \text{sinc}(\omega_{\max} x - n\pi), \tag{1.74}$$

where

$$\text{sinc}(x) \equiv \frac{\sin(x)}{x}. \tag{1.75}$$

Hence, with

$$\omega_{\max} = \frac{2\pi}{\lambda} = \frac{\pi}{\Delta}, \tag{1.76}$$

we get:

$$\phi_n(x) = \frac{1}{\sqrt{\Delta}} \text{sinc}[\pi(\frac{x}{\Delta} - n)]. \tag{1.77}$$

Since $\mathrm{sinc}(n\pi) = \delta_{n,0}$ it is easy to verify that the quadrature $x_i = i\Delta, \quad i = -\infty, \ldots, +\infty$ and weights $w_i = \Delta$ is exact for the overlap integrals:

$$< n|m > = \int \phi_n(x)\phi_m(x)dx \tag{1.78}$$

$$= \sum_{i=-\infty}^{\infty} \Delta \frac{\mathrm{sinc}[\pi(i-n)]}{\sqrt{\Delta}} \frac{\mathrm{sinc}[\pi(i-m)]}{\sqrt{\Delta}} \tag{1.79}$$

$$= \sum_{i=-\infty}^{\infty} \delta_{i,n}\delta_{i,m} = \delta_{n,m}. \tag{1.80}$$

To calculate matrix elements of the $\frac{\partial}{\partial x}$ and $\frac{\partial^2}{\partial x^2}$ operators we can use the fact that the derivatives of band limited functions are also band limited, i.e. if

$$f(x) = \int_{-\infty}^{\infty} h(\omega)e^{i\omega x}d\omega \quad \text{with} \quad h(\omega) = 0 \quad \text{for} \quad |\omega| > \omega_{\max}, \tag{1.81}$$

then

$$\frac{\partial^n}{\partial x^n} f(x) = \int_{-\infty}^{\infty} h(\omega)(i\omega)^n e^{i\omega x}d\omega \tag{1.82}$$

$$= \int_{-\infty}^{\infty} g(\omega)e^{i\omega x}d\omega \tag{1.83}$$

and so the derivatives are also band limited, with the same bandwidth:

$$g(\omega) = h(\omega)(i\omega)^n = 0 \quad \text{for} \quad |\omega| > \omega_{\max}. \tag{1.84}$$

This means that we can use the quadrature to evaluate the matrix elements:

$$< n|\frac{\partial^k}{\partial x^k}|m > = \int_{-\infty}^{\infty} dx \frac{1}{\Delta}\mathrm{sinc}[\pi(\frac{x}{\Delta} - n)]\frac{\partial^k}{\partial x^k}\mathrm{sinc}[\pi(\frac{x}{\Delta} - m)] \tag{1.85}$$

$$= \sum_{i=-\infty}^{\infty} \mathrm{sinc}[\pi(i-n)]\frac{\partial^k}{\partial x^k}\mathrm{sinc}\,[\pi(\frac{x}{\Delta} - m)]\Big|_{x=i\Delta} \tag{1.86}$$

$$= \frac{\partial^k}{\partial x^k}\mathrm{sinc}\,(\pi\frac{x}{\Delta})\Big|_{x=(n-m)\Delta}. \tag{1.87}$$

This gives for $k = 1$:

$$< n|\frac{\partial}{\partial x}|m >= \begin{cases} 0 & n = m \\ \frac{1}{\Delta}\frac{(-1)^{n-m}}{n-m} & n \neq m \end{cases} \tag{1.88}$$

and for $k = 2$ we get:

$$< n|\frac{\partial^2}{\partial x^2}|m >= \begin{cases} -\frac{1}{3}\frac{\pi^2}{\Delta^2} & n = m \\ -\frac{2}{\Delta^2}\frac{(-1)^{n-m}}{(n-m)^2} & n \neq m \end{cases}. \tag{1.89}$$

Note that for the diagonal term we need the second derivative of the sinc function at $x = 0$, which is most easily done by using Taylor series:

$$\frac{\partial^2}{\partial x^2}\left.\frac{\sin(x)}{x}\right|_{x=0} = \frac{\partial^2}{\partial x^2}\left.\frac{x - \frac{1}{3!}x^3 + \frac{1}{5!}x^5 - \ldots}{x}\right|_{x=0} = -\frac{1}{3}. \tag{1.90}$$

If we have the boundary condition $\psi(0) = 0$ we can use (for $n = 1, 2, \ldots, \infty$):

$$\phi_n^-(x) = < x|n^- > \;=\; \phi_n(x) - \phi_n(-x) \tag{1.91}$$

$$\;=\; \frac{1}{\sqrt{\Delta}}\left\{\mathrm{sinc}[\pi(\frac{x}{\Delta} - n)] - \mathrm{sinc}[\pi(\frac{x}{\Delta} + n)]\right\}. \tag{1.92}$$

This basis is orthonormal on the range $0 \ldots \infty$ and:

$$\phi_n^-(x_i) = \frac{1}{\sqrt{\Delta}}(\delta_{i,n} - \delta_{i,-n}) = \frac{1}{\sqrt{\Delta}}\delta_{i,n}, \quad (i, n > 0). \tag{1.93}$$

Thus, we have the quadrature points $x_i = i\Delta, \quad i = 1, 2, \ldots, \infty$ and weights $w_i = \Delta$.

For the matrix elements of the $\frac{\partial}{\partial x}$ operator we can not use the quadrature since:

$$\frac{\partial}{\partial x}\phi_n^-(x)|_{x=0} \neq 0 \tag{1.94}$$

but for $\frac{\partial^2}{\partial x^2}$ we get:

$$< n^-|\frac{\partial^2}{\partial x^2}|m^- > \;=\; \sum_{k=1}^{\infty}\{\mathrm{sinc}[\pi(k-n)] - \mathrm{sinc}[\pi(k+n)]\}\frac{\partial^2}{\partial x^2}\phi_m^-(x_k) \tag{1.95}$$

$$\;=\; \frac{\partial^2}{\partial x^2}\{\mathrm{sinc}[\pi(\frac{x}{\Delta} - m)] - \mathrm{sinc}[\pi(\frac{x}{\Delta} + m)]\}_{x=n\Delta}. \tag{1.96}$$

Hence,

$$< n^-|\frac{\partial^2}{\partial x^2}|m^- >= \begin{cases} -\frac{1}{3}\frac{\pi^2}{\Delta^2} + \frac{2}{\Delta^2}\frac{(-1)^{n+m}}{(n+m)^2} & n = m \\ -\frac{2}{\Delta^2}\left[\frac{(-1)^{n-m}}{(n-m)^2} - \frac{(-1)^{n+m}}{(n+m)^2}\right] & n \neq m \end{cases} \tag{1.97}$$

Beware of the sign-mistakes in the corresponding equation in Ref. [13].

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