Lagrange-Lobatto interpolating polynomials in the discrete variable representation

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(Received 2 April 2007; published 21 August 2007)

The discrete variable representation (DVR) is a well known and widely used computational technique in many areas of physics. Recently, the Lagrange-Lobatto basis has attracted increasing attention, especially for radial Hamiltonians with a singular potential at the origin and finite element DVR constructions. However, unlike standard DVR functions, the Lagrange-Lobatto basis functions are not orthogonal. The overlap matrix is usually approximated as the identity using the same quadrature approximation as for the potential. Based on the special properties of overlap matrix of Lagrange-Lobatto polynomials, an explanation of the success of the identity approximation, including error bounds, is presented. Results for hydrogen and the more nontrivial potentials of self-consistent all-electron density functional atomic calculations are also given.

DOI: 10.1103/PhysRevE.76.026704 PACS number(s): 02.70.−c

I. INTRODUCTION

In many areas of computational science and engineering the discretization of the relevant fundamental equations (choice of basis) is of critical importance to efficiently obtain a stable and accurate solution. The discrete variable representation (DVR) [1] has its origins in the works of Harris *et al.* [2] and Dickinson and Certain [3]. Since then it has become a widely used and developed method in several areas of physics with a huge amount of literature describing different DVR schemes tailored to specific problems. A review of the DVR is given in Ref. [4] and a selection of recent work, from atomic physics to electronic structure calculations, in Refs. [5–12].

Work presented in [13] notes the high accuracy of the Lagrange-Lobatto basis in singular central potential problems. These basis functions have also been used for accurate density functional atom calculations [14,15]. To our knowledge, this basis was first suggested in [16]. A combination of the Lagrange-Lobatto functions and the finite element method was also suggested in [17].

Usually the basis sets in the DVR are tailored to satisfy a given Gauss quadrature rule exactly and are therefore formally orthogonal. However, the Lagrange-Lobatto basis is not formally orthogonal due to the *preassigning* of two of the quadrature nodes and the resulting loss of accuracy in the quadrature rule. However, the Lagrange-Lobatto basis has been used many times in the past for a range of problems and has proven accurate even when the overlap is approximated as the identity matrix.

The main aim of this work is to place the "identity approximation" (treating the overlap as the identity matrix) when using the Lagrange-Lobatto basis on a firm theoretical foundation. It is also hoped this work will encourage research into the possibilities of basis sets with *special* nonorthogonality in which a relaxation of the formal orthogonality conditions can bring significant flexibility to the basis yet some of the extra difficulties may be circumvented.

II. BACKGROUND

First, a brief description of the Lagrange-Lobatto basis and the DVR approximation will be given. For a more complete discussion of the DVR method, see Ref. [4].

A. DVR basis

The general underlying methodology used in this work has been referred to as the DVR and the Lagrange-mesh method. For the most general definition of these methods we may assert we use a basis set that obeys the cardinality condition

$$u_i(x_j) = \frac{\delta_{ij}}{\sqrt{A_i}}, \tag{1}$$

and approximate a matrix of a function of x by the function of the matrix representation of x. This leads to the potential matrix being diagonal in the DVR basis. In this work we consider basis functions that take the form of Lagrange interpolating polynomials (up to a constant weighting factor)

$$u_i(x) = \frac{1}{\sqrt{A_i}} \prod_{k=0}^{n+1} \frac{x - x_k}{x_i - x_k}, \quad k \neq i. \tag{2}$$

Clearly, these functions satisfy the condition given in Eq. (1). The sets $\{A_k\}$ and $\{x_k\}$ may be chosen to coincide with the weights and abscissas, respectively, of a Gauss quadrature rule. We shall refer to the basis sets by the quadrature rule used to construct them; for example, Fig. 1 displays what we shall refer to as the "Lagrange-Lobatto" basis. In what follows the notation $\mathcal{P}^{(n)}$ will be used to denote an arbitrary polynomial of degree n when it is only the degree of the polynomial that is of interest [for example, the functions in Eq. (2) are in $\mathcal{P}^{(n+1)}$].

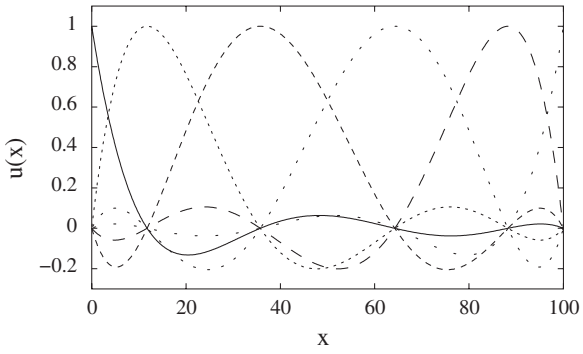

FIG. 1. The Lagrange-Lobatto basis functions for $n=4$.

We start with the Gauss quadrature rule for a positive weight function $p(x)$,

$$\int_a^b p(x)f(x)dx \simeq \sum_{k=0}^{n+1} A_k f(x_k), \tag{3}$$

where the weights $\{A_k\}$ and abscissas $\{x_k\}$ may be evaluated to make the quadrature exact if $f(x)$ is a polynomial of degree $\leq 2n+3$ $[f(x) \in \mathcal{P}^{(2n+3)}(x)]$. If $p(x)=1$ then Eq. (3) is termed Gauss-Legendre quadrature with weights and abscissas we shall denote by $\{A_k^{(1)}\}$ and $\{x_k^{(1)}\}$, respectively. The abscissas are real, distinct, and lie within $[a,b]$. Clearly, a basis of the form (2), defined in terms of $\{A_k^{(1)}\}$ and $\{x_k^{(1)}\}$, will diagonalize polynomial operators up to unitary degree (i.e., x^n, $n \leq 1$). In other words, the basis is orthogonal on $[a,b]$,

$$\int_a^b u_i(x)u_j(x)dx = \int_a^b \mathcal{P}^{(2n+2)}(x)dx = \sum_k A_k^{(1)} u_i(x_k^{(1)})u_j(x_k^{(1)}) = \delta_{ij}, \tag{4}$$

and diagonalizes the coordinate operator on $[a,b]$, in the *true spirit* of the DVR,

$$\int_a^b u_i(x)xu_j(x)dx = \int_a^b \mathcal{P}^{(2n+3)}(x)dx = \sum_k A_k^{(1)} u_i(x_k^{(1)})x_k^{(1)}u_j(x_k^{(1)}) = \delta_{ik}\delta_{jk}x_k^{(1)} = x_i^{(1)}\delta_{ij}. \tag{5}$$

However, for many physical problems, such as the radial Schrödinger equation, we may wish to specify our boundary conditions—which is not possible with the Gauss-Legendre quadrature rule.

B. Quadrature rules with preassigned nodes

For the sake of completeness some of the general ideas of preassigned quadrature nodes will be briefly introduced before moving to the specific case of Gauss-Lobatto quadrature that fixes two points at the limits of the integration range. For a more extensive discussion of these topics, see Ref. [18]. In general, we may construct a quadrature rule with m preassigned nodes and allow n points to be determined to make the quadrature rule exact for an integrand of highest polynomial degree,

$$\int_a^b p(x)f(x)dx = \sum_{k=1}^{n} A_k f(x_k) + \sum_{l=1}^{m} \tilde{A}_l f(\tilde{x}_l). \tag{6}$$

Equation (6) is exact if $f(x) \in \mathcal{P}^{(2n+m-1)}$.

In Gauss-Lobatto quadrature the limits of integration are preassigned to be abscissas in the quadrature formula. The Gauss-Lobatto quadrature rule, with weights $\{A_k\}$ and abscissas $\{x_k\}$ reads

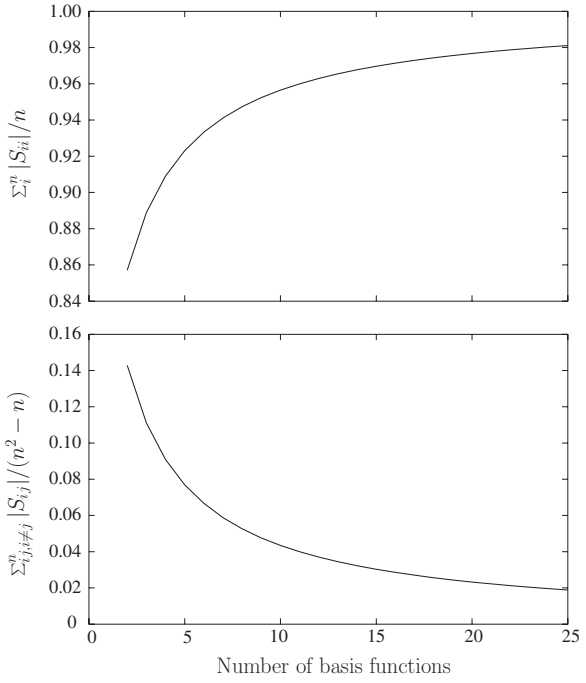

FIG. 2. Average absolute value of diagonal (upper) and off-diagonal (lower) overlap matrix elements with increasing number of basis functions.

$$\int_a^b p(x)f(x)dx \simeq A_0[f(a)+f(b)] + \sum_{k=1}^{n} A_k f(x_k), \tag{7}$$

which is exact for $f(x) \in \mathcal{P}^{(2n+1)}(x)$. This reduction in accuracy destroys the formal orthogonality of the basis functions defined in terms of $\{x_k\}$ [using Eq. (2)] as each basis function is a polynomial of degree $n+1$ leading to the integrand of the overlap integral $[(u_i(x)u_j(x))]$ being a polynomial of degree $2n+2$. For Gauss-Lobatto quadrature the remainder is given by

$$R_n^{[a,b]}(f) = \frac{f^{(2n+2)}(\tau)}{(2n+2)!}\int_a^b p(x)(x-a)(x-b)[w_n(x)]^2\,dx, \tag{8}$$

where $a<\tau<b$ and $f^{(2n+2)}$ is the integrand differentiated $(2n+2)$ times. For $p(x)=1$ on the range $[-1,1]$ the function $w(x)$ differs from the Jacobi polynomial $P_n^{(1,1)}(x)$ in a simple way,

$$w_n(x) = \frac{2^n n!\,\Gamma(n+3)}{\Gamma(2n+3)} P_n^{(1,1)}(x), \tag{9}$$

and the quadrature weights may be expressed in terms of Jacobi polynomials in the following way:

$$A_k = \frac{8(n+1)}{(n+2)(1-x_k^2)^2[P_n^{(1,1)'}(x_k)]^2}, \tag{10}$$

$$A_0 = \frac{2}{(n+1)(n+2)}. \tag{11}$$

The weights and abscissas on the interval $[-1,1]$ can be trivially scaled for an interval of arbitrary length $[a,b]$ using

$$A_i \leftarrow \frac{1}{2}(b-a)A_i, \tag{12}$$

$$x_i \leftarrow \frac{1}{2}[(b+a)x_i + (b-a)]. \tag{13}$$

Often the Gauss quadrature rule is used to justify approximating the overlap as the identity. However, Fig. 2 (evaluated using accurate numerical integration) shows just how poor the quadrature approximation is, and how slowly the overlap converges to the identity matrix with increasing basis size. The overlap of the basis functions given in Eq. (2) on $[a,b]$ is

$$S_{ij} = \int_a^b u_i(x)u_j(x)dx = \int_a^b \mathcal{P}^{(2n+2)}(x)dx$$
$$= \sum_{k=1}^{n} A_k u_i(x_k)u_j(x_k) + \epsilon_{ij} = \delta_{ij} + \epsilon_{ij}, \tag{14}$$

where ϵ_{ij} is the error in the quadrature approximation. Ignoring this error term has been used successfully in a number of calculations [13–17]. These works all approximate the overlap as the identity (using the Gauss approximation) and obtain very accurate results despite what is shown in Fig. 2. We now turn to examine in detail why this approximation has proven so successful.

III. OVERLAP OF LAGRANGE-LOBATTO POLYNOMIALS

For basis functions defined as in Eq. (2) the overlap matrix is

$$S_{ij} = \frac{1}{\sqrt{A_i A_j}} \int_a^b \prod_{k=0,\neq i}^{n+1} \frac{(x-x_k)}{(x_i-x_k)} \prod_{l=0,\neq j}^{n+1} \frac{(x-x_l)}{(x_j-x_l)} dx. \tag{15}$$

For our purposes we may make the simplification

$$u_i(x)u_j(x) = \frac{1}{\sqrt{A_i A_j}} \prod_{k=0,\neq i}^{n+1} \frac{1}{(x_i-x_k)} \prod_{l=0,\neq j}^{n+1} \frac{1}{(x_j-x_l)}$$
$$\times [x^{2n+2} + \mathcal{P}^{(2n+1)}]. \tag{16}$$

Due to the basis functions being defined in terms of the quadrature weights and abscissa there is no integration range dependence in the true overlap integral (and hence in the error term). Therefore, we may limit our analysis of ϵ_{ij} to the range $[-1,1]$. On this range the quadrature weights for internal nodes are given by Eq. (10). Therefore, we may write the remainder for the overlap matrix element S_{ij} [from the integrand $u_i(x)u_j(x)$] using Eq. (8) as

$$R_n^{[-1,1]}(u_i(x)u_j(x)) = \frac{(n+2)}{8(n+1)} \frac{|(1-x_i^2)P_n^{(1,1)'}(x_i)(1-x_j^2)P_n^{(1,1)'}(x_j)|}{\prod_{k=0,\neq i}^{n+1}(x_i-x_k) \prod_{l=0,\neq j}^{n+1}(x_j-x_l)} \int_{-1}^{1} [w_n(x)]^2(x^2-1)dx, \tag{17}$$

with the τ dependence in Eq. (8) differentiated out as our overlap integrand is always a polynomial of degree $2n+2$. Given that,

$$P_n^{(1,1)'}(x_i) = \frac{\Gamma(2n+3)}{2^n n!\,\Gamma(n+3)} \prod_{k=1,\neq i}^{n}(x_i-x_k), \tag{18}$$

the magnitude of the error has no i,j dependence, and the error may be written

$$R_n^{[-1,1]}(u_i(x)u_j(x)) = \chi_{ij}\frac{(n+2)}{8(n+1)} \int_{-1}^{1} [P_n^{(1,1)}(x)]^2(x^2-1)dx,$$

$$\chi_{ij} = \begin{cases} 1 & \text{if } |i-j| = 0 \text{ or is even} \\ -1 & \text{if } |i-j| \text{ is odd.} \end{cases} \tag{19}$$

Therefore, for a given basis size n the overlap has the very simple form

$$S_{ij} = \delta_{ij} - \epsilon_{ij}, \quad \epsilon_{ij} = (-1)^{j-i}\alpha_n, \tag{20}$$

where α_n is the magnitude of the quadrature error between basis functions of degree $n+1$. The reason for this structure is given by the formula for the error in the Gauss-Lobatto quadrature rule

$$R_n(f) = -\gamma_n \frac{f^{(2n+2)}(\tau)}{(2n+2)!}, \tag{21}$$

where for our purposes γ_n may be regarded as a constant as our overlap integrands are all of the same degree. The leading term in our integrand will have the form, for example (for $i,j \neq 1, i,j \neq 2$),

$$\frac{x^{(2n+2)}}{(x_i-x_1)(x_i-x_2)\cdots(x_j-x_1)(x_j-x_2)\cdots}. \tag{22}$$

The sign of the denominator determines the sign of the remainder. If $i=j$ then the denominator is positive, hence the error is negative. Therefore on the diagonal we have ele-

ments with the value $1-\alpha_n$. The overlap with the next basis function changes the sign of the denominator, and so on. Therefore, we obtain the oscillatory structure described in Eq. (20). The matrix with elements ϵ_{ij} is an example of a product matrix that can be written as the outer product of a vector with itself and has appeared previously in the literature [19]. A matrix of this structure must possess a highly oscillating normalized eigenvector of the form

$$\langle v^n| = (1/\sqrt{n}, -1/\sqrt{n}, 1/\sqrt{n}, -1/\sqrt{n}, \cdots). \tag{23}$$

If a vector $|\tilde{v}^n\rangle$ is orthogonal to $|v^n\rangle$ then

$$\langle v^n|\tilde{v}^n\rangle = \frac{1}{\sqrt{n}}\left[\sum_i (-1)^i \tilde{v}_i^n\right] = 0. \tag{24}$$

Therefore, the matrix-vector product of the overlap, or a function of the overlap as $F(S)=\Sigma_{k=0}^{\infty} S^k$, on $\tilde{v}^n$ yields

$$\sum_j S_{ij}\tilde{v}_j^n = \sum_j \{\delta_{ij} - (-1)^{j-i}\alpha_n\}\tilde{v}_j^n$$
$$= \tilde{v}_i^n - (-1)^i \alpha_n \sum_j (-1)^j \tilde{v}_j^n = \tilde{v}_i^n. \tag{25}$$

Therefore all other $n-1$ eigenvectors of the overlap, other than $|v^n\rangle$, have eigenvalues of unity. The above results are very revealing about the effect of approximating the overlap by the identity matrix. Essentially, if the solution vector has a small overlap with the most rapidly oscillating function the basis can represent, which is the case in most physically motivated calculations interested in low-lying energy states, then the identity approximation will have a negligible effect on the result.

IV. ERROR BOUNDS FOR THE IDENTITY APPROXIMATION

In what follows we are interested solely in the additional error brought by the identity approximation, therefore it will be assumed the Hamiltonian matrix elements are evaluated exactly (i.e., the DVR approximation is not used). Let us define

$$H_{ij}^{\{u^n\}} = \int u_i^n(x)\hat{H}u_j^n(x)dx, \tag{26}$$

$$S_{ij}^{\{u^n\}} = \int u_i^n(x)u_j^n(x)dx. \tag{27}$$

We may construct a linearly independent basis set $\{\phi_i^{n-1}\}$ that spans the space $\mathcal{P}^{(n)}$ and obeys

$$\langle v^n|\phi_i^{n-1}\rangle = 0, \quad i = 1, \ldots, n-1. \tag{28}$$

We may solve the eigenvalue problem

$$H^{\{\phi^{n-1}\}}|\psi_i^{\{\phi^{n-1}\}}\rangle = \lambda_i^{(n-1)} S^{\{\phi^{n-1}\}}|\psi_i^{\{\phi^{n-1}\}}\rangle, \tag{29}$$

and then project the solution $|\psi_i^{\{\phi^{n-1}\}}\rangle$ onto the basis set $\{u_i^n\}$, which we shall denote $|\psi_i^{\{\phi^{n-1}\}\to\{u^n\}}\rangle$. This projection satisfies, by construction,

TABLE I. Lowest eigenvalues for $l=0$ [Eq. (37)] with $R=50$ a.u. radius (see Sec. V explanation). For each eigenvalue given the upper value was calculated approximating the overlap as the identity, the middle and lower values include the full overlap calculated with a basis size of N and $N-1$, respectively. The potential matrix is exactly diagonal in the Lagrange-Lobatto basis for $l=0$.

n	$N=10$	$N=20$	$N=40$	Exact
1	−0.39428839	−0.49997882	−0.50000000	−0.50000000
	−0.40940653	−0.49998630	−0.50000000	
	−0.36928276	−0.49995041	−0.50000000	
2	−0.11142228	−0.12500000	−0.12500000	−0.12500000
	−0.11390159	−0.12500000	−0.12500000	
	−0.10504517	−0.12499998	−0.12500000	
3	−0.05165408	−0.05555555	−0.05555555	−0.05555555
	−0.05237384	−0.05555555	−0.05555555	
	−0.04890620	−0.05555555	−0.05555555	
4	−0.02957707	−0.03120434	−0.03120434	−0.03120434
	−0.02985518	−0.03120434	−0.03120434	
	−0.02804866	−0.03120434	−0.03120434	
5	−0.01651543	−0.01786476	−0.01786476	−0.01786476
	−0.01671341	−0.01786476	−0.01786476	
	−0.01472896	−0.01786476	−0.01786476	
6	−0.00060937	−0.00226590	−0.00226590	−0.00226590
	−0.00062789	−0.00226590	−0.00226590	
	+0.00332111	−0.00226590	−0.00226590	

$$\langle v^n|\psi_i^{\{\phi^{n-1}\}\to\{u^n\}}\rangle = 0, \quad i = 1, \ldots, n-1. \tag{30}$$

As a consequence of this and Eq. (25) we may write

$$|R_i\rangle = (\mathcal{H}^{\{u^n\}} - \tilde{\lambda}_i^n I)|\psi_i^{\{\phi^{n-1}\}\to\{u^n\}}\rangle = (H^{\{u^n\}} - \tilde{\lambda}_i^n S)|\psi_i^{\{\phi^{n-1}\}\to\{u^n\}}\rangle, \tag{31}$$

where

$$\mathcal{H}^{\{u^n\}} = [S^{\{u^n\}}]^{-1/2} H^{\{u^n\}} [S^{\{u^n\}}]^{-1/2}, \tag{32}$$

and

$$\tilde{\lambda}_i^n = \langle \psi_i^{\{\phi^{n-1}\}\to\{u^n\}}|\mathcal{H}|\psi_i^{\{\phi^{n-1}\}\to\{u^n\}}\rangle$$
$$= \langle \psi_i^{\{\phi^{n-1}\}\to\{u^n\}}|H|\psi_i^{\{\phi^{n-1}\}\to\{u^n\}}\rangle. \tag{33}$$

If $\langle R_i|R_i\rangle \neq 0$ then a given eigenvalue obtained using the identity approximation $\bar{\lambda}_i^n$ must obey the following:

$$\lambda_i^{n-1} > \bar{\lambda}_i^n > \lambda_i^n. \tag{34}$$

due to the Hylleraas-Undheim theorem. So, the error incurred by making the identity approximation is bounded by the additional error introduced by reducing the basis size by a single function in a calculation including the full overlap. This is demonstrated numerically in Table I where lower and middle entry for each eigenvalue was obtained from calculations including the full overlap. The lower and middle values for each eigenvalue was obtained using a basis of size N

TABLE II. Lowest eigenvalues for $l=1$ [Eq. (37)] with a $R=50$ a.u. radius. For each eigenvalue, given the upper value was calculated approximating the overlap as the identity and using the diagonal potential approximation, the lower value includes the full overlap and potential matrix.

n	$N=10$	$N=20$	$N=40$	Exact
1	−0.12653295	−0.12500000	−0.12500000	−0.12500000
	−0.12015014	−0.12500000	−0.12500000	
2	−0.05590431	−0.05555555	−0.05555555	−0.05555555
	−0.05361762	−0.05555555	−0.05555555	
3	−0.03129115	−0.03121650	−0.03121650	−0.03121650
	−0.03027894	−0.03121650	−0.03121650	
4	−0.01817683	−0.01817594	−0.01817594	−0.01817594
	−0.01734238	−0.01817594	−0.01817594	
5	−0.00316197	−0.00331888	−0.00331888	−0.00331888
	−0.00197214	−0.00331888	−0.00331888	
6	+0.01755777	+0.01653870	+0.01653870	+0.01653870
	+0.01988709	+0.01653870	+0.01653870	

-1 and N, respectively. The upper value (obtained from N basis functions using the identity approximation) is shown to satisfy Eq. (34).

It is uncertain whether other nonorthogonal basis sets obtained from a Gauss quadrature rule in a similar manner to the Lagrange-Lobatto functions used here yield similar pleasing results, though results from some alternative basis sets have been successful [12]. This may prove an interesting topic for future research.

V. NUMERICAL EXAMPLES

In what follows the size of the radial computational dimension R is given in atomic units and the number of basis functions is denoted by N. All energies given are also in atomic units. The kinetic matrix elements T_{ij} can be evaluated exactly using the Gauss-Lobatto quadrature rule in the following way:

$$T_{ij} = \sum_{k=0}^{N+1} \omega_k u_i'(x_k) u_j'(x_k), \tag{35}$$

where

$$u_i'(x_j) = \frac{1}{(x_i - x_j)} \prod_{k=0,\neq i,j}^{N+1} \frac{(x_j - x_k)}{(x_i - x_k)}, \quad j \neq i, \tag{36}$$

resulting in the kinetic integral being a polynomial of degree $2N$.

A. Hydrogen

First, results for the radial Schrödinger equation for hydrogen are presented:

$$\left[-\frac{1}{2}\frac{d^2}{dr^2} + \frac{l(l+1)}{2r^2} - \frac{1}{r} \right] R_{nl}(r) = E_{nl} R_{nl}(r), \tag{37}$$

TABLE III. All-electron self-consistent density functional atom calculations (spin-averaged, exchange-correlation functional given in [20]) using the Lagrange-Lobatto basis with the identity approximation and diagonal potential matrix. Total energies (E_{tot}) were converged to within 1 meV of accepted results [21].

Atom	N	R (a.u.)	E_{tot} (a.u.)
H	10	9.1	−0.4456740
C	32	9.9	−37.4257391
O	43	8.1	−74.4730447
Si	63	12.1	−288.1983740
Er	202	14.6	−12494.7182679

where $R_{nl}(0)=0$ and $R_{nl}(\infty)=0$ and we consider the problem in a finite volume by setting $R_{nl}(R)=0$. This test problem provides simplicity, a singular Hamiltonian, and has been used by previous authors [12,13] as a benchmark so results from this work may be compared directly. Some of the results in Table I reproduce those given by Schneider and Nygaard [13] and are included for ease of comparison. However, the operator r^{-1} is exactly diagonal in the Lagrange-Lobatto basis if $a=0$, therefore the results presented in [13] do not elucidate the accuracy of the method in relation to the potential evaluation as only results for $l=0$ were presented.

Tables I and II show results for the solution of Eq. (37) for $l=0$ and $l=1$, respectively. The case for $l=0$ (Table I), using the diagonal potential matrix, is exact and therefore the effects of the identity approximation are clearly highlighted. For $l=1$ (Table II) the *exact* potential matrix is full, therefore the results for diagonal potential with the identity approximation are compared to the full calculation of the potential matrix (using highly converged numerical integration) including the overlap. In both cases it can be seen that the DVR approximation with the identity approximation, while not variational, converges very rapidly.

B. Density functional atom calculations

We now present results for the more nontrivial case of solving the Kohn-Sham equations self-consistently in a radial potential. The Hamiltonian is given by

$$H = -\frac{1}{2}\frac{d^2}{dr^2} + \frac{l(l+1)}{2r^2} - \frac{Z}{r} + V_{\text{H}}(r) + V_{\text{xc}}(r), \tag{38}$$

where Z is the charge on the nucleus, V_H is the Hartree potential, and V_{xc} is the local density approximation to the exchange-correlation potential (in this work the functional presented in Ref. [20] is used). Table III shows the results for a selection of elements. As well as elements that are very common in simulations, erbium is also given as a stringent test of the convergence. All calculations were converged with respect to the radial computational dimension R and then with respect to the number of basis functions.

VI. CONCLUSION

The Lagrange-Lobatto basis set used in numerous studies in the past has been examined. The reason behind the success of approximating the overlap as the identity in these calculations has also been explained rigorously, adding weight to calculations using these functions. Furthermore, results for all-electron density functional atom calculations have been given.

ACKNOWLEDGMENTS

This work was supported by the European Commission within the Sixth Framework Programme through NEST-BigDFT (Contract No. BigDFT-511815).

[1] Some authors use the term "Lagrange mesh" method to refer to a specific subset of the DVR. For the purposes of this work the two names may be used interchangeably.
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