Efficient spectral-element methods for electronic Schrödinger equation

Jie Shen, Yingwei Wang, and Haijun Yu

Abstract Two efficient spectral-element methods, based on Legendre and Laguerre polynomials respectively, are derived for direct approximation of the electronic Schrödinger equation in one spatial dimension. A spectral-element approach is used to treat the singularity in nucleus-electron Coulomb potential, and with the help of Slater determinant, special basis functions are constructed to obey the antisymmetric property of the fermionic wavefunctions. Numerical tests are presented to show the efficiency and accuracy of the proposed methods.
Key words spectral methods, electronic Schrödinger equation, sparse grids, Slater determinant, Coulomb potential.

1 Introduction

In this article we consider the *electronic Schrödinger equation* (ESE) in one spatial dimension

$$H\Psi(\mathrm{x}) = E\Psi(\mathrm{x}), \tag{1}$$

with the Hamiltonian operator

$$H = T + V_{ne} + V_{ee}, \tag{2}$$

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where the kinetic energy T, nucleus-electron potential V_{ne} and electron-electron potential V_{ee} operators are

$$T = -\frac{1}{2}\sum_{i=1}^{N}\partial_{x_i}^2, \quad V_{ne} = N\sum_{i=1}^{N}|x_i|, \quad V_{ee} = -\sum_{i=1}^{N}\sum_{j>i}|x_i - x_j|. \tag{3}$$

Here N denotes the number of electrons in this system, $x_i \in \mathbb{R}$ the position of the i-th electron, and the solution $\Psi(\mathrm{x})$, with $\mathrm{x} = (x_1, \cdots, x_N)$, describes the wave function associated to the total energy E, and satisfies the boundary condition

$$\Psi(x_1, x_2, \cdots, x_N) \to 0, \quad \text{as } |x_j| \to \infty, \ \ j = 1, \cdots, N. \tag{4}$$

The electronic Schrödinger equation, in three spatial dimension, results from Born-Oppenheimer approximation to the general Schrödinger equation for a system of electrons and nuclei, which is one of the core problems in computational quantum chemistry [23, 13, 5]. However, except for very simple cases, there is no analytical solution available. Hence, it is essential to develop efficient and accurate numerical algorithms for this problem. While most applications of the ESE are in three spatial dimension, the one-dimensional formulation above does inherits some essential features, such as high-dimensionality and singular behavior, of the three dimensional case. Hence, developing a solver in one dimension is an important preliminary and calibrating step that serves as a prototype for solving the ESE in two or three spatial dimensions.

There are several major difficulties for solving the ESE (1). We summarize them below and describe our strategies.

(i) It is an N dimensional problem so it suffers from the so-called *curse of dimensionality* if classical numerical methods are employed. Therefore, various model approximations have been developed in quantum chemistry to reduced the computational complexity. We intend to discretize the ESE directly using sparse grids [3] which have proven to be useful for a class of high-dimensional problems, including in particular the ESE [25, 26]. For example, M. Griebel and J. Hamaekers proposed sparse grid methods for ESE based on Meyer wavelets [7], Fourier functions [8], adaptive Gaussian type orbitals basis sets [9]. On the other hand, we propose to use spectral sparse grid methods based on hyperbolic cross approximations [19, 21, 22, 20] .

(ii) The singularities of the Coulomb potentials shown in (3), called "*Coulomb singularity*" or "*Kato cusp condition*" [6, 12], deteriorate the convergence rates of global spectral methods. In order to treat the singularity in V_{ne} more effectively, we propose a spectral element framework to design basis functions which provide better approximations to the singularity.

(iii) The wave function $\Psi(\mathrm{x})$ has the additional constraint that it must be *antisymmetric* under exchange of variables, according to Pauli exclusion principle. We shall construct, using the antisymmetrizer and Slater determinant, basis functions which obey the antisymmetric property. We also propose an efficient implementation of inner products with respect to antisymmetric functions.

In our previous attempt for solving ESE [22], we used a global spectral method whose convergence rate is severely affected by the *Coulomb singularity*, and we did not enforce the antisymmetry so it resulted in a much larger number of unknowns than actually needed by the physical problem. The main purpose of this paper is to develop efficient procedures to address these two issues.

The rest of the paper is organized as follows. In Sections 2 and 3, we propose two kinds of efficient spectral Galerkin methods based on Legendre and Laguerre polynomials respectively, including the basis functions for one or many electrons, full or sparse grids, and with or without the antisymmetric property. In Section 4, we present numerical results to illustrate the convergence of our methods for ESE calculations. Finally, some conclusions and possible directions for future research are presented in Section 5.

2 A spectral-element method for ESE

In this and next sections, we develop a spectral-element framework to discretize the ESE (1). First, we focus on the set of basis functions for one electron case. Then, we demonstrate the strategies for dealing with high dimensional problems and antisymmetric functions. In addition, we also briefly show how to generate the matrices required in Galerkin methods efficiently, involving mass, stiffness and various potential matrices.

2.1 One electron case

As a starting point, let us focus on the case with $N = 1$ in Eq. (1),

$$\begin{cases} -\dfrac{1}{2}\Psi''(x) + |x|\Psi(x) = E\Psi(x), \quad x \in \mathbb{R}, \\ \lim\limits_{x\to\pm\infty} \Psi(x) = 0. \end{cases} \tag{5}$$

Let ξ be a truncation parameter. After a truncation from the unbounded interval $(-\infty,+\infty)$ to bounded one $[-2\xi,2\xi], \xi > 0$, and further a linear map from general interval $[-2\xi,2\xi]$ to standard one $[-2,2]$, we arrive at

$$\begin{cases} -\dfrac{1}{2\xi^2}\tilde{\Psi}''(x) + \xi|x|\tilde{\Psi}(x) = E\tilde{\Psi}(x), \quad x \in [-2,2], \\ \tilde{\Psi}(\pm 2) = 0. \end{cases} \tag{6}$$

Galerkin formulation

Let X_n be an approximation space and ω be the weight function. The spectral Galerkin method for the problems (5) or (6) can all be casted in the following form: Find $u_n \in X_n$ such that

$$c_1 \langle \partial_x u_n, \partial_x(\phi_n \omega)\rangle + c_2 \langle |x| u_n, \phi_n\rangle_\omega = \lambda \langle u_n, \phi_n\rangle_\omega, \quad \forall \phi_n \in X_n. \tag{7}$$

Note that $c_1 = \frac{1}{2}, c_2 = 1$ for problem (5), $c_1 = \frac{1}{2\xi^2}, c_2 = \xi$ for problem (6), and λ is the numerical estimate of E.

Let $\{\phi_k\}_{k=-n}^n$ be a set of basis functions for X_n. We denote

$$u_n(x) = \sum_{k=-n}^{n} \hat{u}_k \phi_k(x), \qquad \mathrm{u} = (\hat{u}_{-n}, \cdots, \hat{u}_n)^T, \tag{8}$$

$$s_{lk} = \langle \phi_k', (\phi_l \omega)'\rangle, \qquad S = (s_{lk})_{-n\le l,k\le n}, \tag{9}$$

$$m_{lk} = \langle \phi_k, \phi_l\rangle_\omega, \qquad M = (m_{lk})_{-n\le l,k\le n}, \tag{10}$$

$$p^{ne}_{lk} = \langle |x|\phi_l, \phi_k\rangle_\omega, \qquad P^{ne} = (p^{ne}_{lk})_{-n\le l,k\le n}. \tag{11}$$

Thus, the Galerkin formulation (7) yields the following generalized eigenvalue problem

$$(c_1 S + c_2 P^{ne})\mathrm{u} = \lambda M \mathrm{u}, \tag{12}$$

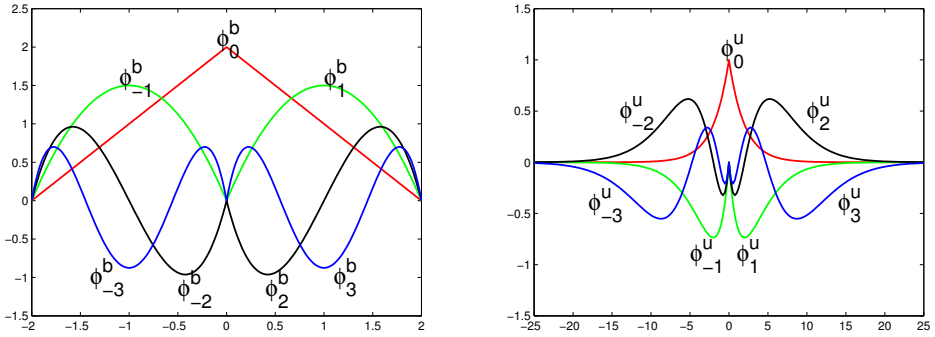
where λ is the eigenvalue and u is the corresponding eigenvector.

Basis functions

In classical spectral-Galerkin approach, Hermite functions are often served as the basis functions for the problem defined on the whole line [10, 18] while Legendre or Chebyshev polynomials are frequently used for the problem in bounded intervals [14, 15]. However, the nucleus-electron potential $V_{ne} = |x|$ in Eq. (5) and Eq. (6) is not differentiable at the origin. Thus, the convergence rates are rather limited if classical spectral methods are employed here. Therefore, we split the interval at the origin into two subintervals, and use a spectral-element method [4] to deal with the singularity at the origin. The basis functions for the (two-elements) spectral-element methods are as follows:

(i) For the problem (6) in bounded domain $[-2,2]$, the function space $X_n^b = \text{span}\{\phi_k^b : k = -n, \cdots, n\}$, the weight $\omega = 1$, and the basis functions $\{\phi_k^b\}_{k=-n}^n$ for one electron are chosen as

$$\phi_k^b(x) = \begin{cases} L_{k-1}(x-1) - L_{k+1}(x-1), & k > 0, \ \ x \in [0,2], \\ 2 - |x|, & k = 0, \ \ x \in [-2,2], \\ L_{|k|-1}(|x|-1) - L_{|k|+1}(|x|-1), & k < 0, \ \ x \in [-2,0], \end{cases} \tag{13}$$



(i) Legendre basis in bounded domain (ii) Laguerre basis in unbounded domain

Fig. 1 First few basis functions for one electron case: Legendre and Laguerre basis sets.

where $L_k(x), x \in [-1,1]$, is the *Legendre polynomial* of degree k. By the property of Legendre polynomials, we know that

$$\begin{aligned} &\phi_k^b(0) = \phi_k^b(2) = 0, && k > 0, \\ &\phi_0^b(0) = 1, \quad \phi_0^b(\pm 2) = 0, && k = 0, \\ &\phi_k^b(-2) = \phi_k^b(0) = 0, && k < 0. \end{aligned}$$

If the basis functions $\{\phi_k\}$ in Eq. (7) are chosen as $\phi_k(x) = \phi_k^b(x)$, then by using the properties of Legendre polynomials [17], the stiffness, mass and potential matrices defined in (9), (10) and (11) are diagonal, penta-diagonal and seven-diagonal matrices, respectively, and can be computed explicitly.

(ii) For the problem (5) in unbounded domain $(-\infty, +\infty)$, the function space $X_n^u = \text{span}\,\{\phi_k^u : k = -n, \cdots, n\}$, the weight $\omega = 1$, and the basis functions $\{\phi_k^u\}_{k=-n}^n$ for one electron are chosen as

$$\phi_k^u(x) = \begin{cases} \hat{L}_k(x) - \hat{L}_{k-1}(x), & k > 0, \quad x \in [0, +\infty), \\ \mathrm{e}^{-|x|/2}, & k = 0, x \in (-\infty, +\infty), \\ \hat{L}_{|k|}(|x|) - \hat{L}_{|k|-1}(|x|), & k < 0, \quad x \in (-\infty, 0], \end{cases} \tag{14}$$

where $\hat{L}_k(x), x \in [0, +\infty)$, is the *Laguerre function* of degree k. By the property of the Laguerre functions, we know that

$$\begin{aligned} &\phi_k^u(0) = 0, && k \neq 0, \\ &\phi_0^u(0) = 1, && k = 0, \\ &\lim_{x\to\infty} \phi_k^u(x) = \lim_{x\to-\infty} \phi_k^u(x) = 0, && \forall k. \end{aligned}$$

If the basis functions $\{\phi_k\}$ in Eq. (7) are chosen as $\phi_k(x) = \phi_k^u(x)$, then by using the properties of Laguerre polynomials [17], the stiffness, mass and potential matrices defined in (9), (10) and (11) are tri-diagonal, tri-diagonal and penta-diagonal matrices, respectively, and can be computed explicitly.

A few basis functions $\{\phi_k^b(x)\}$ and $\{\phi_k^u(x)\}$ for $k = -3,-2,-1,0,1,2,3$ defined above are illustrated in Figure 1.

2.2 *N*-electron case

We first introduce some notations:

- For $N \in \mathbb{N}$, we use boldface lowercase letters to denote N-dimensional multi-indices and vectors, e.g., $\mathrm{k} = (k_1, \cdots, k_N) \in \mathbb{Z}^N$. Besides, we need following norms: $|\mathrm{k}|_1 = \sum_{j=1}^N |k_j|$, $|\mathrm{k}|_\infty = \max_{1\le j\le N} |k_j|$, $|\mathrm{k}|_{mix} = \prod_{j=1}^N \max\{1, |k_j|\}$. Note that $|\mathrm{k}|_{mix} \ge 1$ for all $\mathrm{k} \in \mathbb{Z}^N$.
- $\Lambda \subset \mathbb{Z}^N$ is the set of indices and $|\Lambda|$ means its cardinality.

Now let us consider the ESE for the system with N electrons.

$$\begin{cases} -\dfrac{1}{2}\displaystyle\sum_{i=1}^N \partial_{x_i}^2 \Psi + N\sum_{i=1}^N |x_i|\Psi - \sum_{i=1}^N\sum_{j>i} |x_i - x_j|\Psi = E\Psi, \quad \mathrm{x} \in \mathbb{R}^N, \\ \lim\limits_{x_j \to \pm\infty} \Psi(\mathrm{x}) = 0, \quad \forall j = 1,2,\cdots N. \end{cases} \tag{15}$$

Similarly as in the one electron case, after truncation and linear mapping, the problem in the unbounded domain is equivalent to the following in a bounded domain:

$$\begin{cases} -\dfrac{1}{2\xi^2}\displaystyle\sum_{i=1}^N \partial_{x_i}^2 \Psi + N\xi\sum_{i=1}^N |x_i|\Psi - \xi\sum_{i=1}^N\sum_{j>i} |x_i - x_j|\psi = E\Psi, \quad \mathrm{x} \in \Omega, \\ \Psi(\mathrm{x})|_{\partial\Omega} = 0, \end{cases} \tag{16}$$

where $\Omega = [-2,2]^N$.

Galerkin formulation

Similarly as in previous subsection, let X_n be the approximation space. The spectral Galerkin method for the problems (15) or (16) can all be casted in the following form: Find $u_\mathrm{n} \in X_n$ such that $\forall \Phi_\mathrm{n} \in X_n$,

$$c_1 \sum_{j=1}^N \left\langle \partial_{x_j} u_\mathrm{n}, \partial_{x_j} \Phi_\mathrm{n} \right\rangle + c_2 \left\langle \sum_{j=1}^N |x_j| u_\mathrm{n}, \Phi_\mathrm{n} \right\rangle + c_3 \left\langle \sum_{i=1}^N\sum_{j>i} |x_i - x_j| u_\mathrm{n}, \Phi_\mathrm{n} \right\rangle = \lambda \left\langle u_\mathrm{n}, \Phi_\mathrm{n} \right\rangle, . \tag{17}$$

Note that for problem (15), $c_1 = \frac{1}{2}, c_2 = N, c_3 = -1$ while for problem (16), $c_1 = \frac{1}{2\xi^2}, c_2 = N\xi, c_3 = -\xi$. λ, to be solved, is an approximation of E in X_n.

Let $\{\Phi_{\mathrm{k}}\}_{\mathrm{k}\in\Lambda}$ be a set of basis functions for X_n, where Λ is the set of indices to be determined. We denote

$$u_{\mathrm{k}}(x) = \sum_{\mathrm{k}\in\Lambda} \hat{u}_{\mathrm{k}}\Phi_{\mathrm{k}}(x), \qquad \mathrm{u} = \mathrm{vec}\,(\hat{u}_{\mathrm{k}})_{\mathrm{k}\in\Lambda}, \tag{18}$$

$$s_{\hat{l},\hat{k}} = \sum_{j=1}^{N} \langle \partial_j\Phi_{\mathrm{k}}, \partial_j\Phi_{\mathrm{l}}\rangle, \qquad S = (s_{\hat{l},\hat{k}}), \tag{19}$$

$$m_{\hat{l},\hat{k}} = \langle \Phi_{\mathrm{k}}, \Phi_{\mathrm{l}}\rangle, \qquad M = (m_{\hat{l},\hat{k}}), \tag{20}$$

$$p^{ne}_{\hat{l},\hat{k}} = \langle \sum_{j=1}^{N} |x_j|\Phi_{\mathrm{k}}, \Phi_{\mathrm{l}}\rangle, \qquad P^{ne} = (p^{ne}_{\hat{l},\hat{k}}), \tag{21}$$

$$p^{ee}_{\hat{l},\hat{k}} = \langle \sum_{i=1}^{N}\sum_{j>i} |x_i - x_j|\Phi_{\mathrm{k}}, \Phi_{\mathrm{l}}\rangle, \qquad P^{ee} = (p^{ee}_{\hat{l},\hat{k}}). \tag{22}$$

where $\hat{k}$ is the corresponding order of $\mathrm{k} = (k_1, \cdots, k_N)$ in the set Λ and $\mathrm{u} = \mathrm{vec}\,(\hat{u}_{\mathrm{k}})_{\mathrm{k}\in\Lambda}$ is a column vector with entries $\{\hat{u}_k\}_{k\in\Lambda}$. Suppose the cardinality of the set Λ be $|\Lambda|$, then u defined in (18) is a $|\Lambda|$-by-1 column vector and the matrices defined in (19), (20), (21) and (22) are $|\Lambda|$-by-$|\Lambda|$ square matrices.

Thus, the Galerkin formulation (17) gives the following generalized eigenvalue problem

$$(c_1 S + c_2 P^{ne} + c_3 P^{ee})\mathrm{u} = \lambda M\mathrm{u}, \tag{23}$$

where λ is the eigenvalue and u is the corresponding eigenvector.

Full grid and sparse grid

The classical tensor-product basis function in N-dimensional space is

$$\Phi_{\mathrm{k}}(\mathrm{x}) = \prod_{j=1}^{N} \phi_{k_j}(x_j), \tag{24}$$

where $\mathrm{k} = (k_1, k_2, \cdots, k_N) \in \mathbb{Z}^N, \mathrm{x} = (x_1, x_2, \cdots, x_N) \in \mathbb{R}^N$, and $\phi_{k_j}(x_j)$ is the one-dimensional basis function considered in previous subsection, e.g. $\{\phi^b_k(x)\}$ defined in (13) or $\{\phi^u_k(x)\}$ defined in (14).

The approximation space in N-dimensional space is

$$X^N_n = \mathrm{span}\,\{\Phi_{\mathrm{k}}(\mathrm{x}) : \mathrm{k} \in \Lambda_n\}, \quad n \in \mathbb{N}.$$

For different set of indices Λ, we have different space.

- The set of indices for *full grid* is

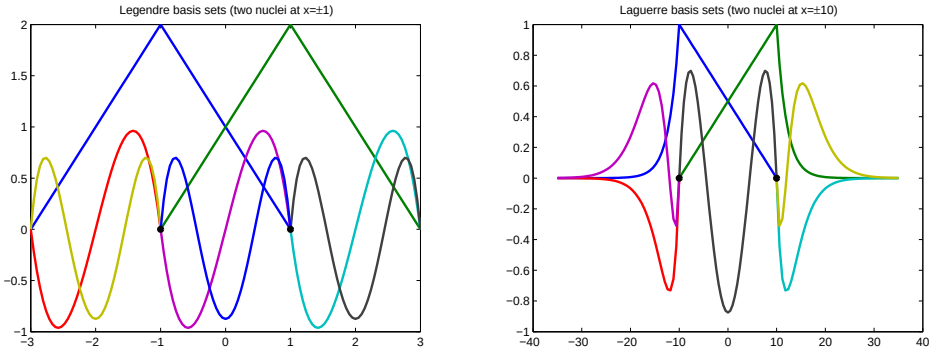
$$\Lambda_n^F = \{\mathrm{k} \in \mathbb{Z}^N : |\mathrm{k}|_\infty \le n\}, \quad n \in \mathbb{N}. \tag{25}$$

- The set of indices for *sparse grid* of hyperbolic cross type is

$$\Lambda_n^S = \{\mathrm{k} \in \mathbb{Z}^N : |\mathrm{k}|_\infty \le n, 1 \le |\mathrm{k}|_{mix} \le n\}, \quad n \in \mathbb{N}. \tag{26}$$

Here are several remarks on the spectral-element basis function sets we use.

- The electronic eigenfunctions are proved to decay exponentially as the spatial variable goes to infinity in the sense that there exist positive constants A and B for which $|\phi(x)| \le Ae^{-B\|x\|}$. (see Ref [1].) Hence, in the Legendre spectral method, the error caused by restriction from unbounded domain to bounded one would also be exponentially convergent as the parameter L goes to the infinity.
- The idea of spectal-element method to treat the nuclei-electron cusps could be easily generalized to the case with several nuclei. See Figure 2 for two nuclei case.
- For ESE in three spatial dimension, it is known that the sparse grids based on hyperbolic cross fit the smoothness property of the eigenfunctions [3, 25, 26]. However, for the ESE in one spatial dimension considered in this paper, there are no theoretical results available in the literature. In Section 4, we will compare the numerical results obtained from full grids (25) and sparse grids (26).



(i) Legendre basis in bounded domain (ii) Laguerre basis in unbounded domain

Fig. 2 Legendre and Laguerre basis sets for two nuclei case

3 Antisymmetry and antisymmetric inner product

The electronic wavefunction $\Psi(\mathrm{x})$ for many body system must be *antisymmetric* with respect to electron positions $\mathrm{x} = (x_1, \cdots, x_N)$, i.e.

$$\Psi(x_1,\cdots,x_i,\cdots,x_j,\cdots,x_N) = -\Psi(x_1,\cdots,x_j,\cdots,x_i,\cdots,x_N). \tag{27}$$

It is obvious that $\Phi_{\mathrm{k}}(\mathrm{x})$ defined in (24) does not obey the antisymmetric property. A main difficulty is how to construct basis functions which satisfy the antisymmetry, and how to efficiently compute the inner products between them.

3.1 Antisymmetrizer and Slater determinant

In order to enforce antisymmetry, we introduce a linear operator called *antisymmetrizer* [11], also called *skew symmetrization* or *alternation*, which is defined by

$$\mathscr{A} = \frac{1}{N!}\sum_{p\in S_N}(-1)^p\mathscr{P}, \tag{28}$$

where S_N is the permutation group on N elements. For the element $p \in S_N$, the operator $\mathscr{P}$ acts on a function by permuting its variables, as $\mathscr{P}\Psi(\gamma_1,\gamma_2,\cdots) = \Psi(\gamma_{p(1)},\gamma_{p(2)},\cdots)$. The sign $(-1)^p$ is -1 if p is an odd permutation and 1 if it is even. Applying $\mathscr{A}$ to the function $\Phi_{\mathrm{k}}(\mathrm{x})$ defined in (24) leads to the antisymmetric basis $\Phi^A_{\mathrm{k}}(\mathrm{x})$ expressed as a Slater determinant:

$$\begin{aligned}\Phi^A_{\mathrm{k}}(\mathrm{x}) :=& \mathscr{A}\Phi_{\mathrm{k}}(\mathrm{x})\\ =& \frac{1}{N!}\begin{vmatrix}\phi_{k_1}(x_1) & \phi_{k_1}(x_2) & \cdots & \cdots & \phi_{k_1}(x_N)\\ \phi_{k_2}(x_1) & \phi_{k_2}(x_2) & \cdots & \cdots & \phi_{k_2}(x_N)\\ \cdots & \cdots & \cdots & \cdots & \cdots\\ \phi_{k_N}(x_1) & \phi_{k_N}(x_2) & \cdots & \cdots & \phi_{k_N}(x_N)\end{vmatrix}.\end{aligned} \tag{29}$$

It is easy to check that the basis function $\Phi^A_{\mathrm{k}}(\mathrm{x})$ satisfies the antisymmetric property (27). Besides, if $k_i = k_j$, then the determinant in Eq.(29) would be zero. Thus, the set of indices for antisymmetric basis $\{\Phi^A_{\mathrm{k}}(\mathrm{x})\}_{\mathrm{k}\in\Lambda^A_n}$ should be

$$\Lambda^A_n = \{\mathrm{k}\in\mathbb{Z}^N : |\mathrm{k}|_\infty \le n, k_1 < k_2 < \cdots < k_N\}, \quad n\in\mathbb{N}. \tag{30}$$

It implies that the cardinality of antisymmetric basis set is about $\frac{1}{N!}$ times of the regular one.

Now we have four kinds of grids, namely *full grid* (**'F'**), *sparse grid* (**'S'**), *full grid with antisymmetric property* (**'FA'**) and *sparse grid with antisymmetric property* (**'SA'**). The cardinality of them are shown in the Table 1 and sketch for two dimensional case are shown Figure 3.

Table 1 Four kinds of grids for N-dimensional problems

Grids	Set of indices	Cardinality[a]
'F'	Λ_n^F	$(2n+1)^N$
'FA'	$\Lambda_n^F \cap \Lambda_n^A$	$\frac{(2n+1)^N}{N!}$
'S'	Λ_n^S	$O\big((2n+1)\log^{N-1}(2n+1)\big)$
'SA'	$\Lambda_n^S \cap \Lambda_n^A$	$O\Big(\frac{(2n+1)\log^{N-1}(2n+1)}{N!}\Big)$

[a] The cardinality of hyperbolic cross sparse grids can be found in [19].

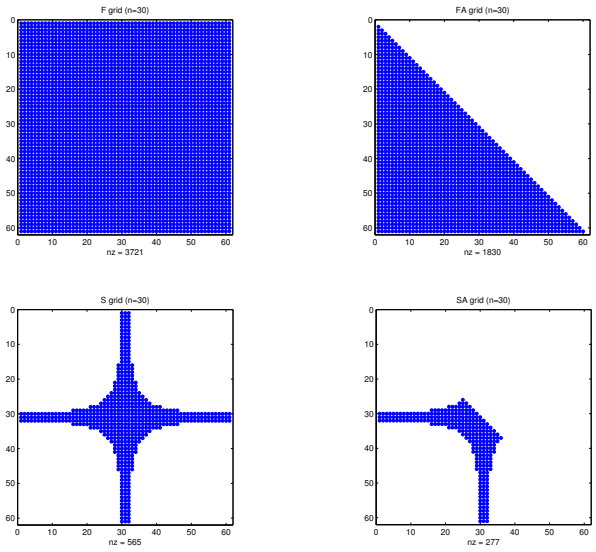


Fig. 3 Full/sparse grids without/with antisymmetric property: two dimensional case

3.2 Antisymmetric inner product and Löwdin's rule

One of the main difficulties in implementation of spectral type methods based on antisymmetric grids (**'FA'** and **'SA'**) is the calculation of inner products between two Slater determinants. In this subsection, we briefly show how to compute the entries in the matrices S, M, P^{ne} and P^{ee} defined in (19)-(22) with respect to the antisymmetric basis functions $\{\Phi_{\mathrm{k}}^A(\mathrm{x})\}_{\mathrm{k}\in\Lambda_n^A}$.

- For the mass matrix M, we need to construct the following auxiliary matrix

$$\tilde{M}_{\mathrm{k,l}} = \begin{pmatrix} \langle \phi_{k_1}, \phi_{l_1} \rangle & \cdots & \langle \phi_{k_1}, \phi_{l_N} \rangle \\ \vdots & \ddots & \vdots \\ \langle \phi_{k_N}, \phi_{l_1} \rangle & \cdots & \langle \phi_{k_N}, \phi_{l_N} \rangle \end{pmatrix} \quad \forall\, \mathrm{k,l} \in \Lambda_n^A. \tag{31}$$

Then each entry of M can be computed as

$$\langle \Phi_{\mathrm{k}}^A, \Phi_{\mathrm{l}}^A \rangle = \frac{1}{N!} \det(\tilde{M}_{\mathrm{k,l}}), \tag{32}$$

which is the so called *Löwdin's rule* [11]. Note that the matrix $\tilde{M}_{\mathrm{k,l}}$ defined above is a submatrix of the one-dimensional mass matrix M defined in (10), either tri-diagonal one in Laguerre case or penta-diagonal one in Legendre case, so its determinant can be computed efficiently. The denominator $N!$ need never be computed, since it will occur in every term in our equations and so cancels.

- For the stiffness matrix S and nucleus-electron potential matrix P^{ne}, we need to construct the following auxiliary matrices

$$\tilde{S}_{\mathrm{k,l},i} = \begin{pmatrix} \langle \phi_{k_1}, \phi_{l_1} \rangle & \cdots & \langle \phi'_{k_1}, \phi'_{l_i} \rangle & \cdots & \langle \phi_{k_1}, \phi_{l_N} \rangle \\ \vdots & \ldots & \vdots & \ldots & \vdots \\ \langle \phi_{k_N}, \phi_{l_1} \rangle & \cdots & \langle \phi'_{k_N}, \phi'_{l_i} \rangle & \cdots & \langle \phi_{k_N}, \phi_{l_N} \rangle \end{pmatrix},$$

$$\tilde{P}^{ne}_{\mathrm{k,l},i} = \begin{pmatrix} \langle \phi_{k_1}, \phi_{l_1} \rangle & \cdots & \langle |x| \phi_{k_1}, \phi_{l_i} \rangle & \cdots & \langle \phi_{k_1}, \phi_{l_N} \rangle \\ \vdots & \ldots & \vdots & \ldots & \vdots \\ \langle \phi_{k_N}, \phi_{l_1} \rangle & \cdots & \langle |x| \phi_{k_N}, \phi_{l_i} \rangle & \cdots & \langle \phi_{k_N}, \phi_{l_N} \rangle \end{pmatrix}.$$

for each $\mathrm{k,l} \in \Lambda_n^A$. Then each entry of S and P^{ne} can be computed as

$$\sum_{i=1}^{N} \langle \partial_{x_1} \Phi_{\mathrm{k}}^A, \partial_{x_i} \Phi_{\mathrm{l}}^A \rangle = \frac{1}{N!} \sum_{i=1}^{N} \det(\tilde{S}_{\mathrm{k,l},i}), \tag{33}$$

$$\sum_{i=1}^{N} \langle |x_i| \Phi_{\mathrm{k}}^A, \Phi_{\mathrm{l}}^A \rangle = \frac{1}{N!} \sum_{i=1}^{N} \det(\tilde{P}^{ne}_{\mathrm{k,l},i}). \tag{34}$$

- For the electron-electron interaction potential matrix P^{ee}, we use the methodology proposed by G.Beylkin [2]. To show the idea, we need more notations.

$$\Phi_{\mathrm{k}}(\mathrm{x}) = \prod_{i=1}^{N} \phi_{k_i}(x_i), \qquad \Phi_{\mathrm{k}}(\mathrm{x}) = \begin{pmatrix} \phi_{k_1}(x_1) \\ \phi_{k_2}(x_2) \\ \cdots \\ \phi_{k_N}(x_N) \end{pmatrix}, \tag{35}$$

$$\Phi_{\mathrm{l}}(\mathrm{x}) = \prod_{i=1}^{N} \phi_{l_i}(x_i), \qquad \Phi_{\mathrm{l}}(\mathrm{x}) = \begin{pmatrix} \phi_{l_1}(x_1) \\ \phi_{l_2}(x_2) \\ \cdots \\ \phi_{l_N}(x_N) \end{pmatrix}, \tag{36}$$

$$\Theta_{\mathrm{k,l}} = \tilde{M}^{-1}_{\mathrm{k,l}} \Phi_{\mathrm{k}} := \begin{pmatrix} \theta_1(x_1) \\ \theta_2(x_2) \\ \cdots \\ \theta_N(x_N) \end{pmatrix}. \tag{37}$$

Then the electron-electron inner products can be computed by

$$\langle \sum_{i=1}^{N} \sum_{j>i} W(x_i,x_j)\Phi_{\rm k}^A, \Phi_{\rm l}^A \rangle = \frac{\det(\tilde{M}_{\rm k,l})}{2N!} \sum_{i\neq j} \int W(x_i,x_j)\Phi_{l_i}(x_i)\Phi_{l_j}(x_j)\det(\Theta_{\rm k,l}^{i,j})\mathrm{d}x_i\mathrm{d}x_j, \tag{38}$$

where the weight $W(x_i,x_j) = |x_i - x_j|$ and

$$\Theta_{\rm k,l}^{i,j} = \begin{pmatrix} \theta_i(x_i) & \theta_i(x_j) \\ \theta_j(x_i) & \theta_j(x_j) \end{pmatrix}.$$

The formula (38) should be very efficient for large N. However, for many cases, the matrix $\tilde{M}$ is singular, that is to say we need to redefine the $\Theta_{\rm k,l}$ in (37) and $\det(\tilde{M})$. The detailed discussion can be found in [2]. We omit the details here for simplicity.

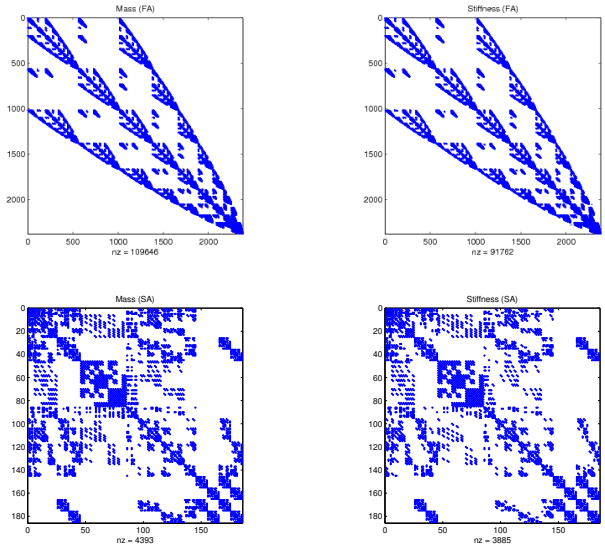


Fig. 4 Mass/stiffness matrices for Legendre basis in full/sparse antisymmetric grids: $N = 4, n = 8$

The mass and stiffness and matrices M, S based on antisymmetric Legendre and Laguerre bases for 4 electrons with $n = 8$ are shown in Figures 4-5. All of this matrices are symmetric and positive definite.

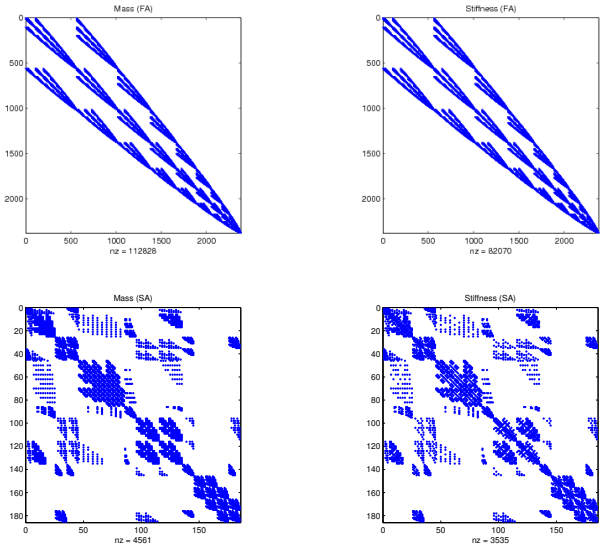


Fig. 5 Mass/stiffness matrices for Laguerre basis in full/sparse antisymmetric grids: $N = 4, n = 8$

4 Numerical results

It is well known that the performance of spectral methods in unbounded domains can be significantly enhanced by choosing a proper truncation or scaling parameter such that the extreme collocation points are at or close to the endpoints of the effective interval (outside of which the solution is essentially zero). For the mapped Legendre method, the scaling parameter is the parameter ξ in Eq. (6). For the Laguerre method, one usually needs to determine a suitable scaling parameter ζ [24, 16] and then make a coordinate transform $y = x/\zeta$. That is to say the basis function for problem (5) should be chosen as

$$\phi^u_{k,\zeta}(x) := \phi^u_k(x/\zeta), \quad \zeta > 0, \tag{39}$$

where ϕ^u_k is defined in (14).

We apply the efficient spectral methods proposed in the previous section to the ESE (1). More precisely, the methods used in this section are

- Antisymmetric full grids based on Legendre basis (**'Leg-FA'**) with parameters ξ and Laguerre basis (**'Lag-FA'**) with parameters ζ;
- Antisymmetric sparse grids based on Legendre basis (**'Leg-SA'**) with parameters ξ and Laguerre basis (**'Lag-SA'**) with parameters ζ.

Besides, we make the following notations: *DoF* means the total number of degrees of freedom; E is the first eigenvalue and ΔE denotes the relative difference between the two successive values of E.

The numerical results for $N = 1$ are shown in Tables 2-3. The exponential rates of convergence could be observed both in Legendre and Laguerre basis, since the singularity in the V_{ne} has been taken care of (However, this exponential convergence does not extend to the more electron cases, see below). Further, the best choice for parameters is $\xi = 4$ and $\zeta = 0.1$ for $N = 1$. Note that the Legendre method with $\xi = 2$ has a faster convergence rate than Legendre methods with larger ξ values, but it converges to an energy that is too far from the exact one. In Figure 6, we plot the convergence curves of our Legendre and Laguerre methods together with the results of **'Fourier'** method (hyperbolic cross sparse grid method based on Fourier basis, proposed in [8]). The significant advantages of the bases proposed here over the Fourier bases demonstrates the importance of handling the nucleus-electron singularity. From Figure 6, we also see that the Laguerre method is more sensitive to the scaling parameter than the Legendre method, although that an optimal scaled Laguerre method seems gives better solution than Legendre method.

The numerical results of **'Leg-FA'**, **'Lag-FA'**, **'Leg-SA'** and **'Lag-SA'** for $N = 2,4,6,8$ are shown in Tables 4-7 respectively. We see that the advantages of sparse grids over full grids is not significant for small N ($N \leq 4$). The reason might be that the sparse grids based on hyperbolic cross allow to treat the nucleus-electron cusps properly which are aligned to the particle coordinate axes of the system while does not fit well to the "diagonal" directions of the electron-electron cusps. However the sparse grids based on hyperbolic cross for six and eight dimensional case do give better results that the full grid cases. We observe also that carefully choice of parameters ξ and ζ is needed to obtain a decent accuracy for E. As showed in the one-dimensional case, the Legendre method is not very sensitive to the scaling parameter comparing to the Laguerre method. The results show that all our numerical methods have monotonic convergence property, which might be used to determine optimal scaling in practice through multiple runs.

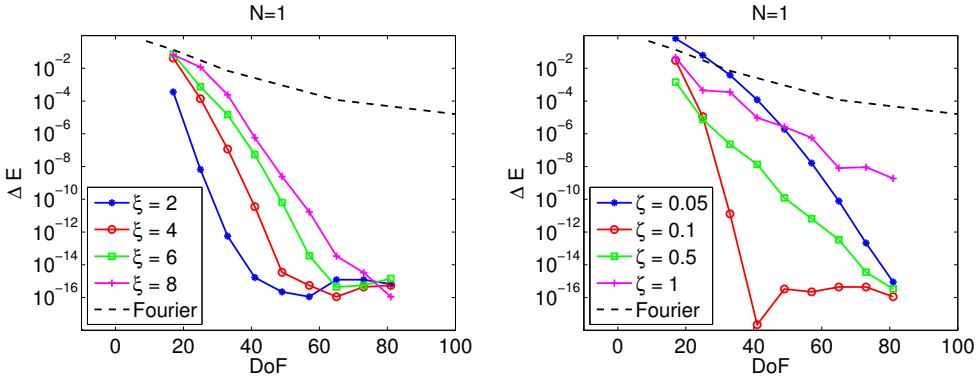
As a comparison with published results using a Fourier method in [8], we list in Table 8 our results with the "best" parameters and the corresponding results in [8]. We observe that our method gives much better results with significant less number of unknowns.

Table 2 First eigenvalues: Legendre basis for $N = 1$.

DoF	$\xi = 2$		$\xi = 4$		$\xi = 6$		$\xi = 8$	
	E	ΔE	E	ΔE	E	ΔE	E	ΔE
9	0.80898847		0.85120259		0.88298404		0.88823511	
17	0.80862555	4.49e-04	0.80875522	4.24e-02	0.80937787	9.09e-02	0.82066506	6.76e-02
25	0.80862554	8.19e-09	0.80861663	1.39e-04	0.80863141	9.23e-04	0.80885868	1.18e-02
33	0.80862554	6.97e-13	0.80861652	1.17e-07	0.80861657	1.84e-05	0.80861710	2.42e-04
41	0.80862554	2.06e-15	0.80861652	3.57e-11	0.80861652	6.61e-08	0.80861652	5.82e-07
49	0.80862554	2.75e-16	0.80861652	3.44e-15	0.80861652	7.90e-11	0.80861652	2.48e-09
57	0.80862554	1.37e-16	0.80861652	5.55e-16	0.80861652	4.39e-14	0.80861652	1.69e-11
65	0.80862554	1.51e-15	0.80861652	1.11e-16	0.80861652	5.49e-16	0.80861652	3.42e-14
73	0.80862554	1.51e-15	0.80861652	4.44e-16	0.80861652	6.86e-16	0.80861652	3.33e-15
81	0.80862554	8.24e-16	0.80861652	5.55e-16	0.80861652	1.78e-15	0.80861652	1.11e-16

Table 3 First eigenvalues: Laguerre basis for $N = 1$.

DoF	$\zeta = 0.05$		$\zeta = 0.1$		$\zeta = 0.5$		$\zeta = 1$	
	E	ΔE	E	ΔE	E	ΔE	E	ΔE
9	1.53707272		0.83910765		0.81007589		0.85464218	
17	0.87424212	7.58e-01	0.80862774	3.05e-02	0.80862429	1.80e-03	0.80943446	4.52e-02
25	0.81259311	7.59e-02	0.80861652	1.12e-05	0.80861676	9.31e-06	0.80898253	4.52e-04
33	0.80873830	4.77e-03	0.80861652	1.30e-11	0.80861653	2.83e-07	0.80862929	3.53e-04
41	0.80861843	1.48e-04	0.80861652	2.22e-18	0.80861652	1.67e-08	0.80861978	9.51e-06
49	0.80861653	2.35e-06	0.80861652	3.33e-16	0.80861652	1.51e-10	0.80861711	2.67e-06
57	0.80861652	2.01e-08	0.80861652	2.22e-16	0.80861652	8.05e-12	0.80861654	5.74e-07
65	0.80861652	9.65e-11	0.80861652	4.44e-16	0.80861652	4.20e-13	0.80861653	8.02e-09
73	0.80861652	2.63e-13	0.80861652	4.44e-16	0.80861652	4.39e-15	0.80861652	9.20e-09
81	0.80861652	1.10e-15	0.80861652	1.11e-16	0.80861652	4.12e-16	0.80861652	1.88e-09



(i) Legendre basis (ii) Laguerre basis

Fig. 6 Convergence rates for different scaling parameters ξ and ζ (one electron case)

Table 4 First eigenvalues: **'Leg-FA'** method for $N = 2,4,6,8$.

N	DoF	$\xi = 2$		$\xi = 4$		$\xi = 6$		$\xi = 8$	
		E	ΔE	E	ΔE	E	ΔE	E	ΔE
2	36	2.77064844		2.83934161		3.23853921		3.83477463	
2	136	2.75897331	4.23e-03	2.75962610	7.97e-02	2.78271494	1.64e-01	2.79743867	1.04e+00
2	300	2.75896782	1.99e-06	2.75853265	1.09e-03	2.75867580	8.71e-03	2.76007806	3.74e-02
2	528	2.75896776	2.02e-08	2.75852536	7.29e-06	2.75852924	5.31e-05	2.75856947	1.51e-03
2	820	2.75896776	1.98e-09	2.75852515	2.03e-07	2.75852540	1.39e-06	2.75852700	4.25e-05
2	1176	2.75896775	3.41e-10	2.75852513	2.53e-08	2.75852517	8.17e-08	2.75852535	1.65e-06
2	1596	2.75896775	8.62e-11	2.75852512	5.58e-09	2.75852513	1.34e-08	2.75852518	1.75e-07
2	2080	2.75896775	2.63e-11	2.75852512	1.65e-09	2.75852513	3.56e-09	2.75852514	3.72e-08
2	2628	2.75896775	3.59e-11	2.75852512	8.05e-10	2.75852512	4.76e-09	2.75852513	1.77e-08
2	3916	2.75896775	5.44e-12	2.75852512	1.15e-10	2.75852512	6.47e-10	2.75852512	2.22e-09
2	5460	2.75896775	1.09e-12	2.75852512	2.47e-11	2.75852512	1.32e-10	2.75852512	4.35e-10
2	7260	2.75896775	3.62e-13	2.75852512	6.53e-12	2.75852512	3.55e-11	2.75852512	1.14e-10
2	9316	2.75896775	3.62e-13	2.75852512	2.17e-12	2.75852512	1.16e-11	2.75852512	3.66e-11
4	35	11.3744684		14.6183222		19.5555592		25.2272328	
4	126	11.1529293	1.99e-02	12.5401722	2.08e+00	15.4303761	2.67e-01	19.0645225	6.16e+00
4	330	11.0906509	5.62e-03	11.4897741	1.05e+00	13.2777107	1.62e-01	15.5602812	3.50e+00
4	715	11.0387961	4.70e-03	11.1928180	2.97e-01	12.0181657	1.05e-01	13.5778359	1.98e+00
4	1365	11.0311564	6.93e-04	11.1503562	4.25e-02	11.3807587	5.60e-02	12.3383459	1.24e+00
4	2380	11.0309216	2.13e-05	11.0667169	8.36e-02	11.2139303	1.49e-02	11.5916733	7.47e-01
4	3876	11.0306460	2.50e-05	11.0150199	5.17e-02	11.1756559	3.42e-03	11.2803427	3.11e-01
4	5985	11.0305710	6.80e-06	11.0034337	1.16e-02	11.0953952	7.23e-03	11.2180070	6.23e-02
4	8855	11.0305636	6.76e-07	11.0025213	8.29e-05	11.0312699	5.81e-03	11.1718388	4.13e-03
4	12650	11.0305614	2.00e-07	11.0020105	4.64e-05	11.0076249	2.15e-03	11.0932904	7.08e-03
6	7	30.4774572	0.00e+00	41.7709865	0.00e+00	59.0079666	0.00e+00	77.4736697	0.00e+00
6	84	27.7191179	9.95e-02	34.4566265	2.12e-01	45.3580818	3.01e-01	58.2795553	3.29e-01
6	462	27.3018885	1.53e-02	30.7355475	1.21e-01	37.4024467	2.13e-01	46.1984215	2.62e-01
6	1716	27.0408367	9.65e-03	28.3071847	8.58e-02	33.0501800	1.32e-01	38.7185569	1.93e-01
6	5005	26.8872665	5.71e-03	27.3234899	3.60e-02	30.2367754	9.30e-02	34.2981982	1.29e-01
6	12376	26.8720859	5.65e-04	27.1394812	6.78e-03	28.3094643	6.81e-02	31.4814019	8.95e-02
8	9	58.97684862		75.48658360		104.9615300		137.2152993	
8	165	53.64284607	9.94e-02	65.09745212	1.60e-01	84.71660799	2.39e-01	108.4869011	2.65e-01
8	1287	52.91599468	1.37e-02	59.33803295	9.71e-02	72.01714565	1.76e-01	89.02662541	2.19e-01
8	6435	52.15277285	1.46e-02	54.85127080	8.18e-02	64.67355647	1.14e-01	76.12430898	1.69e-01
8	24310	51.83345874	6.16e-03	52.69663222	4.09e-02	59.72645435	8.28e-02	68.00062085	1.19e-01

5 Concluding remarks

We developed in this paper efficient spectral-element methods with Legendre and Laguerre basis sets for ESE in one spatial dimension. To achieve high-order approximation to the nucleus-electron cusps, we construct the basis sets in spectral-element type. For the system with N electrons, we proposed to use sparse grids of hyperbolic cross type to deal with high dimensionality.

We also presented efficient procedure to enforce the antisymmetry using Slater determinants which reflect the Pauli principle, and lead to antisymmetric basis sets for full/sparse grid spaces with a substantially reduced amount of degree of freedoms. We

Table 5 First eigenvalues: **'Lag-FA'** method $N = 2, 4, 6, 8$.

N	DoF	$\zeta = 0.05$		$\zeta = 0.1$		$\zeta = 0.5$		$\zeta = 1$	
		E	ΔE	E	ΔE	E	ΔE	E	ΔE
2	36	7.30379716		3.12261380		2.77777209		2.85513015	
2	136	3.34341896	1.18e+00	2.75950375	3.63e-01	2.75896094	6.82e-03	2.78956672	6.56e-02
2	300	2.82490601	1.84e-01	2.75852513	9.79e-04	2.75854050	1.52e-04	2.75986845	2.97e-02
2	528	2.76277165	2.25e-02	2.75852512	6.59e-09	2.75852626	5.16e-06	2.75897551	8.93e-04
2	820	2.75865751	1.49e-03	2.75852512	8.16e-10	2.75852547	2.85e-07	2.75858518	3.90e-04
2	1176	2.75852721	4.72e-05	2.75852512	2.76e-10	2.75852526	7.83e-08	2.75853935	4.58e-05
2	1596	2.75852514	7.51e-07	2.75852512	1.15e-10	2.75852519	2.53e-08	2.75852947	9.88e-06
2	2080	2.75852512	6.37e-09	2.75852512	5.55e-11	2.75852516	1.09e-08	2.75852635	3.12e-06
2	2628	2.75852512	6.41e-09	2.75852512	3.12e-11	2.75852514	1.64e-08	2.75852581	1.33e-06
2	3916	2.75852512	1.09e-12	2.75852512	9.79e-12	2.75852513	4.71e-09	2.75852535	1.65e-07
2	5460	2.75852512	3.63e-13	2.75852512	3.99e-12	2.75852512	1.79e-09	2.75852522	4.68e-08
2	7260	2.75852512	3.63e-13	2.75852512	1.81e-12	2.75852512	8.05e-10	2.75852517	1.74e-08
2	9316	2.75852512		2.75852512	1.09e-12	2.75852512	4.09e-10	2.75852515	8.05e-09
4	35	84.5261141		24.0010489		11.4543515		14.4696514	
4	126	48.1712017	7.55e-01	15.9511257	8.05e+00	11.3868658	5.93e-03	12.9426380	1.53e+00
4	330	32.5685850	4.79e-01	12.9989513	2.95e+00	11.2011807	1.66e-02	12.0343856	9.08e-01
4	715	24.4059885	3.34e-01	11.7815358	1.22e+00	11.0620997	1.26e-02	11.5559439	4.78e-01
4	1365	19.6523245	2.42e-01	11.2772003	5.04e-01	11.0168962	4.10e-03	11.3619089	1.94e-01
4	2380	16.6988902	1.77e-01	11.0837922	1.93e-01	11.0106396	5.68e-04	11.3091692	5.27e-02
4	3876	14.7880278	1.29e-01	11.0207238	6.31e-02	11.0084099	2.03e-04	11.2814318	2.77e-02
4	5985	13.5204842	9.37e-02	11.0046752	1.60e-02	11.0054217	2.72e-04	11.2304460	5.10e-02
4	8855	12.6679704	6.73e-02	11.0017149	2.69e-04	11.0033635	1.87e-04	11.1647721	5.88e-03
4	12650	12.0916290	4.77e-02	11.0013445	3.37e-05	11.0023306	9.39e-05	11.1040989	5.46e-03
6	7	488.968428		126.923387		30.8058940		44.1789048	
6	84	194.6512414	1.51e+00	55.6839778	1.28e+00	28.3194836	8.78e-02	37.5755909	1.76e-01
6	462	114.5606263	6.99e-01	38.0266025	4.64e-01	27.8526463	1.68e-02	34.1104499	1.02e-01
6	1716	79.2855548	4.45e-01	31.4021247	2.11e-01	27.5394558	1.14e-02	31.6957497	7.62e-02
6	5005	60.3655526	3.13e-01	28.5962373	9.81e-02	27.0880214	1.67e-02	29.9054490	5.99e-02
6	12376	49.0792283	2.30e-01	27.3804649	4.44e-02	26.7879171	1.12e-02	28.7231166	4.12e-02
8	9	862.24608230		225.04342820		61.42218240		89.76996256	
8	165	351.8825621	1.45e+00	101.6315296	1.21e+00	56.01728167	9.65e-02	77.38512422	1.60e-01
8	1287	211.4500817	6.64e-01	70.80521708	4.35e-01	54.10871261	3.53e-02	70.39360988	9.93e-02
8	6435	148.7485015	4.22e-01	59.17412032	1.97e-01	53.50632043	1.13e-02	65.88471983	6.84e-02
8	24310	114.6497701	2.97e-01	54.24858141	9.08e-02	52.65395877	1.62e-02	62.16347168	5.99e-02

performed numerical experiments which showed that our methods enjoy exponential convergence rate for the one electron case, and for multi-electron cases, can lead to a target accuracy with significantly fewer number of unknowns than other appraoches.

We only presented some preliminary numerical results with one-dimensional particles here. We believe that these preliminary results are very encouraging, and many techniques developed in this paper can be extended to solving ESE in two and three spatial dimensions. For example, we can construct special basis functions of spectral-element type that take care of the nuclei-electron singularities like $1/\|x\|$ in $\mathbb{R}^3$ and $\log(\|x\|)$ in $\mathbb{R}^2$. Such consideration and other issues are currently under investigation.

Table 6 First eigenvalues: **'Leg-SA'** method $N = 2, 4, 6, 8$.

N	DoF	$\xi = 2$		$\xi = 4$		$\xi = 6$		$\xi = 8$	
		E	ΔE	E	ΔE	E	ΔE	E	ΔE
2	30	2.77117360		2.85154776		3.29333192		4.00360881	
2	76	2.75907121	4.39e-03	2.77186894	7.97e-02	2.84618789	1.57e-01	2.98567403	1.02e+00
2	188	2.75898056	3.29e-05	2.75912734	1.27e-02	2.77101057	2.71e-02	2.79193494	1.94e-01
2	440	2.75896878	4.27e-06	2.75856637	5.61e-04	2.75897392	4.36e-03	2.76075915	3.12e-02
2	1016	2.75896792	3.11e-07	2.75852925	3.71e-05	2.75856020	1.50e-04	2.75873647	2.02e-03
2	2288	2.75896776	5.80e-08	2.75852531	1.43e-06	2.75852667	1.22e-05	2.75853155	7.43e-05
4	45	11.2855573		13.1270840		17.5972705		22.7581385	
4	185	11.0456316	2.17e-02	11.8762275	1.25e+00	14.1293533	2.45e-01	17.2075738	5.55e+00
4	685	11.0315868	1.27e-03	11.2689744	6.07e-01	12.3384003	1.45e-01	14.0281403	3.18e+00
4	2166	11.0306207	8.76e-05	11.0607111	2.08e-01	11.3668441	8.55e-02	12.1527206	1.88e+00
4	6438	11.0305668	4.89e-06	11.0050047	5.57e-02	11.0629403	2.75e-02	11.4151839	7.38e-01
4	18070	11.0305602	5.95e-07	11.0018297	2.89e-04	11.0111051	4.71e-03	11.1064143	2.78e-02
6	4	28.8667472	0.00e+00	40.2289337	0.00e+00	57.5510278	0.00e+00	74.9994059	0.00e+00
6	42	27.5001095	4.97e-02	34.8584080	1.54e-01	47.0333024	2.24e-01	60.8190456	2.33e-01
6	258	26.9802045	1.93e-02	31.3576095	1.12e-01	39.9539319	1.77e-01	50.1906803	2.12e-01
6	1240	26.8819947	3.65e-03	28.4995437	1.00e-01	32.8373715	2.17e-01	39.6716608	2.65e-01
6	4984	26.8682208	5.13e-04	27.0984039	5.17e-02	30.0298964	9.35e-02	34.9065789	1.37e-01
6	18232	26.8675138	2.63e-05	26.7326315	1.37e-02	28.4165043	5.68e-02	31.8035686	9.76e-02
8	4	59.40209940		76.68172385		107.3043916		140.4792744	
8	57	54.08534117	9.83e-02	62.51098600	2.27e-01	81.15357811	3.22e-01	103.7463664	3.54e-01
8	425	52.17333953	3.66e-02	57.86688923	8.03e-02	73.18590963	1.09e-01	91.50522209	1.34e-01
8	2425	51.81422944	6.93e-03	55.23428566	4.77e-02	67.37989091	8.62e-02	82.06933495	1.15e-01
8	11641	51.78818166	5.03e-04	53.37488078	3.48e-02	62.67868975	7.50e-02	74.35006938	1.04e-01

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Table 7 First eigenvalues: **'Lag-SA'** method $N = 2, 4, 6, 8$.

N	DoF	$\zeta = 0.05$		$\zeta = 0.1$		$\zeta = 0.5$		$\zeta = 1$	
		E	ΔE	E	ΔE	E	ΔE	E	ΔE
2	30	8.67617797		3.34484794		2.77827775		2.86808325	
2	76	4.95071500	7.53e-01	2.85047130	4.94e-01	2.75910728	6.95e-03	2.79510521	7.30e-02
2	188	3.56995225	3.87e-01	2.76696643	8.35e-02	2.75857016	1.95e-04	2.76032963	3.48e-02
2	440	2.97004425	2.02e-01	2.75854879	8.42e-03	2.75853604	1.24e-05	2.75890350	1.43e-03
2	1016	2.78412765	6.68e-02	2.75852514	2.36e-05	2.75852721	3.20e-06	2.75857819	3.25e-04
2	2288	2.75876032	9.20e-03	2.75852512	7.25e-09	2.75852561	5.80e-07	2.75853878	1.43e-05
4	45	86.6917450		24.7000085		11.4797932		13.0563335	
4	185	47.4767386	8.26e-01	15.7385648	8.96e+00	11.0834163	3.58e-02	11.9600581	1.10e+00
4	685	32.5716096	4.58e-01	12.9635893	2.77e+00	11.0087891	6.78e-03	11.3378162	6.22e-01
4	2166	22.7567084	4.31e-01	11.5596749	1.40e+00	11.0027861	5.46e-04	11.0910824	2.47e-01
4	6438	16.9797442	3.40e-01	11.0511325	5.09e-01	11.0015878	1.09e-04	11.0167019	7.44e-02
4	18070	14.1738357	1.98e-01	11.0034033	4.34e-03	11.0013648	2.03e-05	11.0045689	1.10e-03
6	4	952.185785		242.664898		31.7056642		40.9407131	
6	42	278.0484912	2.42e+00	75.6539917	2.21e+00	28.0048853	1.32e-01	35.2221880	1.62e-01
6	258	183.0644900	5.19e-01	52.9850239	4.28e-01	27.0791781	3.42e-02	31.7607206	1.09e-01
6	1240	118.8419089	5.40e-01	39.4694998	3.42e-01	26.7470351	1.24e-02	29.4671183	7.78e-02
6	4984	88.6458674	3.41e-01	33.3728721	1.83e-01	26.6316558	4.33e-03	28.1039769	4.85e-02
6	18232	62.0557435	4.28e-01	28.4594806	1.73e-01	26.6028587	1.08e-03	27.2593918	3.10e-02
8	4	1397.855236		358.1470801		63.17782097		90.38022455	
8	57	739.6581056	8.90e-01	194.9633013	8.37e-01	57.62889533	9.63e-02	69.29072364	3.04e-01
8	425	439.0533644	6.85e-01	123.6510866	5.77e-01	53.87219761	6.97e-02	64.08200887	8.13e-02
8	2425	291.0249117	5.09e-01	89.23827767	3.86e-01	51.68828658	4.23e-02	59.76006788	7.23e-02
8	11641	202.0154616	4.41e-01	69.31440411	2.87e-01	50.95865047	1.43e-02	57.05869814	4.73e-02

Table 8 Best results of first eigenvalues achieved by various methods for $N = 2, 4, 6, 8$.

Methods	$N = 2$		$N = 4$		$N = 6$		$N = 8$	
	DoF	E	DoF	E	DoF	E	DoF	E
'Leg-FA'	9316	2.75852512	12650	11.0020105	12376	26.872086	24310	51.83345874
'Leg-SA'	2288	2.75852531	18070	11.0018297	18232	26.867514	11641	51.78818166
'Lag-FA'	9316	2.75852512	12650	11.0013445	12376	26.787917	24310	52.65395877
'Lag-SA'	2288	2.75852512	18070	11.0013648	18232	26.602859	11641	50.95865047
'Fourier'	3409	2.758536	79498	11.011562	297605	27.571226	215864	60.838970

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