Pseudospectral Tools Notes

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Contents

1 Mathematical Preliminaries

1.1 The General Problem

This section overviews the general mathematical framework the code is built upon. These notes are largely derived from Boyd's 2001 book (Ref. [1]).

The general form of the partial differential equation we want to solve is a non-linear Sturm-Liouville problem of the form,

$$\hat{h}[\psi_\alpha]\psi_\alpha(x) = E_\alpha \psi_\alpha(x) \tag{1}$$

where $x \in \mathbb{R}^3$, $\hat{h}$ is a mean-field Hamiltonian that depends on orbitals $\psi_\alpha(x)$. For static problems we must enforce boundary conditions $\psi_\alpha(x) \to 0$ as $|x| \to \infty$ for all α. Due to

these boundary conditions, the domain of the solutions ψ_α must be $(-\infty, \infty) \times (-\infty, \infty) \times (-\infty, \infty)$.

To solve Eq. (1) we use a spectral method. The details of this method are very nicely explained in Ref. [1]. We will briefly overview the fundamental mathematics of the approach however we will not show all the details of these methods here. References will be provided for anyone that wants more detail where appropriate.

Since the domain of our solution is infinite 3-dimensional space, Ref. [1] suggests there are only a few basis sets one could use to represent functions numerically on infinite domains. One such choice are what are generally called "Hermite functions" or as physicists would call "Harmonic Oscillator functions". We take these to be defined as

$$\phi_n(x) = \frac{1}{\sqrt{\pi}2^n n!} e^{-\frac{m\omega}{2\hbar}x^2} H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right) \tag{2}$$

Just for brevity, we will define the oscillator constant as

$$\gamma = \sqrt{\frac{m\omega}{\hbar}} \tag{3}$$

so that

$$\phi_n(x) = \frac{1}{\sqrt{\pi}2^n n!} e^{-\gamma^2 x^2/2} H_n(\gamma x) \tag{4}$$

As we will discuss later, the choice of optimal scale parameter γ will depend on the number of grid points and domain truncation. For now we will keep γ as defined above. The main idea of a spectral method is to expand the solution $\psi_\alpha(x)$ as a linear combination of basis functions. In 1-dimension, an orbital is approximated by

$$\psi_\alpha(x) = \sum_{n=0}^{N_x} c_{n\alpha}\phi_n(x) \tag{5}$$

In 3 dimensions, we use a tensor product basis,

$$\psi_\alpha(x, y, z) = \sum_{n_x=0}^{N_x} \sum_{n_y=0}^{N_y} \sum_{n_z=0}^{N_z} c_{n_x n_y n_z \alpha}\phi_{n_x}(x)\phi_{n_y}(y)\phi_{n_z}(z) \tag{6}$$

For short hand, define

$$|n_x, n_y, n_z\rangle = \phi_{n_x}(x)\phi_{n_y}(y)\phi_{n_z}(z) \tag{7}$$

We define the full basis set of Hermite functions as $\mathcal{B} = \{\phi_{n_x}(x)\phi_{n_y}(y)\phi_{n_z}(z)\}$ for all (n_x, n_y, n_z). The dimension of this set is $\dim(\mathcal{B}) = N_x N_y N_z$ which grows as N^3.

1.2 Basis State Selection

What is very commonly done in nuclear physics is to select a subset of the basis set $\mathcal{B}$. We define the "Harmonic oscillator" basis $\mathcal{B}_{HO} \subset \mathcal{B}$ by

$$\mathcal{B}_{HO}(N_{max}) = \{|n_x, n_y, n_z\rangle \in \mathcal{B} : N_{max} \geq n_x + n_y + n_z, \forall n_x, n_y, n_z \in \mathbb{Z}^+\} \tag{8}$$

N_{max} is referred to as the maximum shell number. Why is this subset selection more desirable than the full basis set $\mathcal{B}$ for nuclear DFT problems? There are a few points to consider

1. If we believe the ground state of the nucleus we are interested in is not too different from the harmonic oscillator, $\mathcal{B}_{HO}$ might be a much more reasonable basis set. That is, if the ground state is roughly $E \sim \hbar\omega(N_{max} + 3/2)$ for some ω, the harmonic oscillator basis provides a reasonable energy scale for the nuclear system. For example, for $N_{max} = 30$ in the full basis set $\mathcal{B}$, we could include states like $|30, 30, 30\rangle$ which corresponds to a state that would be included in the $N_{shell} = 90$ shell. This state has a corresponds to a very high energy harmonic oscillator state which is completely negligible for approximating a ground state.

2. Scaling: Since the full basis set $\mathcal{B}$ would include high energy states, we can reduce the number of basis elements included in our expansion by truncating based on oscillator shells. $\dim(\mathcal{B}_{HO})$ grows roughly as $\frac{N^3}{6}$ instead of N^3 (I found this out just from empirical computation).

As a side note, we can equivalently label each basis element with an integer $n \in [1, N_{states}]$ where $N_{states} = \dim(\mathcal{B}_{HO})$. This is the notation we will adopt.

1.3 Galerkin/Spectral Representation

Let $N_{states} = \dim(\mathcal{B}_{HO}(N_{max}))$ for a given N_{max}. Let $|n\rangle, |m\rangle \in \mathcal{B}_{HO}(N_{max})$. Using the expansion defined in Eq. (6) (except using labels n and m) and substituting it into Eq. (1), we have

$$\hat{h} \sum_{n=0}^{N_{states}} c_{\alpha,n} |n\rangle = E_\alpha \sum_{n=0}^{N_{states}} c_{\alpha,n} |n\rangle \tag{9}$$

To derive the Galerkin/spectral representation, we simply take the inner product of both sides with an arbitrary basis element, $|m\rangle$

$$\sum_{n=0}^{N_{max}} c_{\alpha n} \langle m | \hat{h} | n\rangle = E_\alpha \sum_{n=0}^{N_{max}} c_{\alpha n} \delta_{mn} = E_\alpha c_{\alpha n} \tag{10}$$

or in vector form,

$$h\vec{c}_\alpha = E_\alpha \vec{c}_\alpha \tag{11}$$

where the matrix elements of h are given by integrals

$$h_{mn} = \langle m | \hat{h} | n\rangle \tag{12}$$

This defines the Galerkin representation of Eq. (1).
Advantages:

1. Curse of Dimensionality: In coordinate space/pseudospectral representation, the matrix dimension of h is set by the dimension of the tensor basis set which is on the scale of $N^3 \times N^3$ where N is the number of lattice sites. While h is this representation is typically sparse, it has a very high dimension. The spectral representation typically results in a much smaller but dense representation.

2. Good basis functions with boundary conditions naturally imposed are known.

Disadvantages:

1. The matrix h is constructed by integration which can be computationally expensive. This can be mediated by parallel computational routines.

2. Evaluation of non-linear terms is very difficult in spectral space.

Considering the advantages and disadvantages, we use a spectral method where Eq. (1) is represented and diagonalized in spectral space (Eq. (11)). Once we solve Eq. (11), we transform to pseudospectral space to evaluate non-linear terms, then transform back to spectral space. The transformations to and from spectral space add computational cost. Since we do not have an operation like the Fast Fourier transform which is $O(N \log(N))$, for the Hermite basis, the transformations will be slower. There is some work on Fast Hermite transforms which might get close to $O(N \log(N))$ but will ultimately be slower (See Matrix Multiplication Transform (MMT) in Ref. [1]). Since we will be switching back and forth between pseudospectral and spectral representations, we will also review the essentials of the pseudospectral representation.

1.4   Pseudospectral/Collocation Representation

Since we will be dealing with non-linear terms in Eq. (1), we need to discuss the pseudospectral representation. Note, this representation goes by many different names however they are all the same: "pseudospectral" aka "collocation" aka "discrete variable representation (DVR)" aka "method of selected points" and there probably exist others. We will be using these names synonymously however Ref. [1] ascribes a more rigorous naming scheme.

To describe the pseudospectral representation properly, one needs to talk about interpolation. This is described very well in Ref. [1]. We will skip to the point here. We do however need some definitions so that everything will be clear enough.

Definition 1.1 (Interpolating Approximation From Ref. [1]:). *An interpolating approximation of a function $f(x)$ is an expression $P_{N-1}(x)$ whose N degrees of freedom are determined by the requirement that the interpolant agree with $f(x)$ at each N interpolation points*

$$P_{N-1}(x_i) = f(x_i), \forall i = 1, ..., N \tag{13}$$

Note that the interpolation points x_i are also called collocation points. More generally, we can express any interpolant in the form,

$$P_N(x) = \sum_{i=0}^{N} f(x_i)C_i(x) \tag{14}$$

where $C_i(x)$ are called a Cardinal function satisfying

$$C_i(x_j) = \delta_{ij} \tag{15}$$

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There are a few choices for the Cardinal function and they depend on the problem under consideration. One common choice for polynomial interpolation is the "Lagrange" Cardinal function (aka "polynomials of piece-wise interpolation"):

$$C_i(x) = \prod_{j=0, N \neq i}^{N} \frac{x - x_j}{x_i - x_j} \tag{16}$$

As we will see in the next section, there are a large number of Cardinal functions one can chose for interpolation and these functions are intimately related to the Galerkin representation we saw in the previous section.

1.5 Equivalence between Galerkin and Pseudospectral Representations

One question we have is the following: what are the appropriate grid points x_j to interpolate a function $f(x)$ on. We motivate a particular choice by example. Consider the function

$$f(x) = \frac{1}{1 + x^2}, \quad x \in [-5, 5] \tag{17}$$

It turns if we try to interpolate $f(x)$ on a uniform grid in the domain $[-5, 5]$, the interpolant $P_N(x)$ does not converge to the true function $f(x)$ as $N \to \infty$. Ref. [1] has more discussion on this point. But what this example shows is one must chose collocation points with care. As a side note, we know $f(x)$ above has poles at $x = \pm i$. This means the Taylor series converges for $|x| \leq 1$. But interpolation can extend this domain of convergence beyond $|x| = 1$. But the trade off is, the interpolation fails spectacularly at the boundaries of the domain. Since we know uniform grids do not work here, one could as the following: if we move the collocation points around, can we reduce interpolation errors? The answer is given by two theorems.

Theorem 1.1. *Let $f(x)$ be at least $N+1$ differentiable and let $P_N(x)$ it's Lagrange interpolant of degree N. Then,*

$$f(x) - P_N(x) = \frac{1}{N + 1!} f^{(N+1)}(\xi) \prod_{i=0}^{N} (x - x_i) \tag{18}$$

for some ξ in the domain of f spanned by x and interpolation points.

Note that ξ depends on N, x, interpolation points x_i. So what this theorem says is, if we want to minimize the error of interpolation, we need to optimize $\prod_{i=0}^{N}(x - x_i)$ for some chosen set of collocation points. So which set of x_i gives the smallest possible error in magnitude over the interval of interest. The answer to this is given by the following theorem:

Theorem 1.2 (Chebyshev Minimal Amplitude Theorem). *Let $T_N(x)$ be the Nth degree Chebyshev polynomial. All polynomials with leading coefficient $1x^N$, the unique polynomial which is the smallest maximum on [-1,1] is $T_N(x)/2^{N-1}$. That is,*

$$\max_{x \in [-1,1]} |P_N(x)| \geq \max_{x \in [-1,1]} \left| \frac{T_{N+1}(x)}{2^{N-1}} \right| \tag{19}$$

From this theorem, since $T_N(x)$ is a polynomial, we can factor,

$$\frac{1}{2^N}T_{N+1}(x) = \prod_{i=1}^{N+1}(x - x_i) \tag{20}$$

So, on a bounded domain, *the optimal collocation points are roots of $T_{N+1}(x)$*. Now this solves the interpolation problem on a closed interval $[a, b]$. Similar results can be extended to problems with different boundary conditions and basis elements (see Ref. [1]). How does this relate to a spectral/Galerkin representation? Turns out making the optimal choice of interpolation makes pseudospectral methods *identical* to Galerkin representation. This equivalence is shown clearly through "Gaussian integration".

Numerical integration and Lagrangian interpolation are very closely related. The standard formula for integration is

$$\int_a^b f(x)dx \approx \sum_{i=0}^{N}w_if(x_i) \tag{21}$$

$$w_i = \int_a^b C_i(x)dx \tag{22}$$

where x_i are collocation points and $C_i(x)$ are Cardinal functions. Note: in numerical integration literature, the collocation points $\{x_i\}$ are often called "interpolation points" or "abscissa" and w_i are called "weights".

To minimize the error in numerical integration, we have the following theorem,

Theorem 1.3 (Gauss-Jacobi Integration). *If $N + 1$ collocation points are chosen to be zeros of an orthogonal polynomial $P_{N+1}(x)$ over the interval $[a, b] \ni x$ with respect to weight function $\rho(x)$, then*

$$\int_a^b f(x)\rho(x)dx = \sum_{i=1}^{N}w_if(x_i) \tag{23}$$

is exact for all f which are polynomials of most degree $2N + 1$.

From this result, the inner products used to derive the Galerkin representation are of the form,

$$\langle f, g \rangle = \int_a^b f(x)g(x)\rho(x)dx \approx \sum_{i=1}^{N}f(x_i)g(x_i)w_i \tag{24}$$

Why do we care? Since the quadrature formulas, like the one above, are obtained by analytic integration of the interpolation polynomial, the best choice of collocation points are also the best quadurature points. Thus *collocation points must be chosen in association with a basis set*. So integrals that define matrix elements for the Galerkin representation are evaluation by numerical quadruture at the collocation points associated to a given basis, i.e. roots of the basis.

Theorem 1.4 (Galerkin with Quadruture). *If matrix elements are evaluated with quadrature then, the spectral coefficients $\{c_n\}$ in*

$$u_{N,G} = \sum_{n=0}^{N} c_n \phi_n(x) \tag{25}$$

as calculated by the Galerkin method will be identical with those computed with collocation/pseudospectral methods.

Proof. Let the pseudospectral equation be

$$\vec{\vec{L}}\vec{c} = \vec{f} \tag{26}$$

where $L_{ij} = \hat{L}\phi_j(x_i)$, $f_i = f(x_i)$ where $\hat{L}$ is a linear operator and $\phi_j(x)$ is an element of an orthonormal basis set. If we multiply both sides by $w_i\phi_n(x_i)$, then we have

$$\sum_{i=0}^{N} w_i\phi_n(x_i)\hat{L}\phi_j(x_i) = \sum_{i=0}^{N} w_i\phi_n(x_i)f(x_i). \tag{27}$$

Define

$$H_{nj} = \langle \phi_n, \hat{L}\phi_j(x_i) \rangle \tag{28}$$

and

$$g_n = \sum_{i=0}^{N} w_i\phi_n(x_i)f(x_i) = \langle \phi_n, f \rangle \tag{29}$$

This gives us,

$$\vec{\vec{H}}\vec{c} = \vec{g} \tag{30}$$

This is exactly the Galerkin/spectral representation of the problem. This shows that a pseudospectral method with quadrature points chosen to be the same as the collocation points *must* inherit a Galerkin representation. □

So to represent a function $f(x)$ as a spectral series, we don't really need to do any integrals. Instead we can just multiply

$$\vec{c} = M\vec{f}, \quad M_{ij} = \phi_i(x_j)w_j \tag{31}$$

where x_j are roots of $\phi_{N+1}(x)$.

Now we return to interpolation and selection of a Cardinal function. Recall, if we want to approximate a function $f(x)$, we expand it as

$$f(x) = \sum_{i=0}^{N} f(x_i)C_i(x) \tag{32}$$

where $C_i(x_j) = \delta_{ij}$. The Cardinal functions depends on the choice of basis. In our case, we want to use solutions to Sturm-Liouville problems. These are typically functions that are products of a decaying functions and polynomials such as the Harmonic Oscillator basis. In this case, the Cardinal functions are of the form,

$$C_j(x) = \frac{\phi_{N+1}(x)}{\phi_{N+1}(x_j)(x - x_j)} \tag{33}$$

Note there also exists a "Lobatto" form of the Cardinal function (See Ref. [1] for details). So to define a pseudospectral representation of a differential equation, one needs to know how derivatives act on Eq. (32). These can be done analytically. For detail derivation of derivative matrices in spectral and pseudospectral space, see Appendix A. We will just list the first two derivative matrices here

$$D_{ij}^{(1)} = \begin{cases} \frac{\phi'_{N+1}(x_i)}{\phi'_{N+1}(x_j)(x_i - x_j)} & i \neq j \\ \frac{1}{2}\frac{\phi''_{N+1}(x_i)}{\phi'_{N+1}(x_i)} & i = j \end{cases} \tag{34}$$

$$D_{ij}^{(2)} = \begin{cases} \frac{\phi''_{N+1}(x)}{\phi'_{N+1}(x_j)(x - x_j)} - \frac{2\phi'_{N+1}(x)}{\phi'_{N+1}(x_j)(x - x_j)^2} + \frac{2\phi_{N+1}(x)}{\phi'_{N+1}(x_j)(x - x_j)^3} & i \neq j \\ \frac{\phi'''_{N+1}(x_i)}{3\phi'_{N+1}(x_j)} & i = j \end{cases} \tag{35}$$

It is important to note that $D^{(1)}D^{(1)} \neq D^{(2)}$ and neither of these matrices are hermitian.

1.6 Convergence Properties

The convergence properties of global Hermite function approximations were worked out in one dimension by Hu and Yu in their 2024 paper in Ref. [2]. We will overview their results and then extend to 3 dimensions. Let the unscaled Hermite functions be defined by

$$\hat{H}_n(x) = \mathcal{N}e^{-x^2/2}H_n(x) \tag{36}$$

where $\mathcal{N}$ is a normalization constant and $H_n(x)$ is a Hermite polynomial. Let $\{x_j\}_{j=0}^N$ be roots of $\hat{H}_n(x)$ with order $x_0 < \ldots < x_N$. In Shen (2011) (Ref. [3]) it was shown that

$$\max_j |x_j| \sim \sqrt{2N} \tag{37}$$

For an interval $[x_0, x_N]$, we have a scaling of $[-\sqrt{2N}, \sqrt{2N}]$.

Suppose we introduce a scaling parameter γ, we can define scaled Hermite functions $\hat{H}_n(\gamma x)$. The interval then becomes, $[-\frac{\sqrt{2N}}{\gamma}, \frac{\sqrt{2N}}{\gamma}]$. Tang (1993) [4] showed for functions with gaussian asymptotics, a choice of

$$\gamma = \frac{\sqrt{2N}}{M} \tag{38}$$

for some positive real number M guaranteed exponential convergence an negligible error near the boundary of the interval. However, if we want to approximate a function $f(x)$ that has

asymptotics $f(x) \sim e^{-c|x|^p}$ for $p < 2$ we cannot expect a good approximation using Hermite functions since they decay as $e^{-x^2/2}$. This means the error beyond $[-\frac{\sqrt{2N}}{\gamma}, \frac{\sqrt{2N}}{\gamma}]$ is large.

Is there an optimal γ we can choose that will reduce error arising from an asymptotics mismatch? Ref [2] showed that we can construct an upper bound on the global accuracy of the Hermite function approximation error using the Fourier transform of $\hat{H}_n(\gamma x)$ basis and we will overview their proof here. Approximating a function $u(x)$ by $\{\hat{H}_n(\gamma x)\}$ is equivalent to approximating it's Fourier transform $\tilde{u}$ by $\{\hat{H}_n(\frac{k}{\gamma})\}$. Truncation on the spatial domain $[-\frac{\sqrt{2N}}{\gamma}, \frac{\sqrt{2N}}{\gamma}]$ is equivalent to a truncation in Fourier space $[-\gamma\sqrt{2N}, \gamma\sqrt{2N}]$. Now here is their main theorem from Ref. [2],

Theorem 1.5. *Let $a = b = \frac{1}{2\sqrt{2}}$ and $c = \frac{1}{16}$. Define $f \lesssim g$ to be $f < Cg$ for some positive constant C. Define $\widehat{\Pi}_N$ to denote projection on to the Hermite function basis of order N. Define $\hat{I}_{x\in D}$ be an indicator function for domain D. Then,*

$$\left| u(x) - \widehat{\Pi}_N u(x) \right|_{L^2} \lesssim \left| u \cdot \hat{I}_{|x|>\frac{a\sqrt{N}}{\gamma}} \right|_{L^2} + \left| \mathcal{F}[u] \cdot \hat{I}_{|k|>b\sqrt{N}\gamma} \right|_{L^2} + |u|_{L^2} \, e^{-cN} \tag{39}$$

See Ref. [2] for the proof. This theorem shows that the global error of the Hermite approximation is bounded above by the L^2 error of the function outside the spatial and Fourier intervals. We also notice that the error bound is a function of scale γ. This implies that we must balance both the spatial and Fourier cutoff errors in order to get the most optimal convergence possible with this expansion of $u(x)$.

1.6.1 HF/HFB Specific Case

In our case of interest, we know, in the presence of Coulomb interactions, the particle densities have asymptotic behaviour [5]

$$\rho(r) \sim e^{-\kappa_q r} \ as \ r \to \infty \tag{40}$$

where κ_q is related to the proton or neutron separation energies S_q, $\kappa_q \sim \sqrt{2m_q S_q/\hbar}$. From this we can see the Hermite function basis has the wrong asymptotics but the rate of the solution decay is set by κ_q. It is also very clear that as we approach dripline nuclei where S_q approaches 0, the convergence rate of the approximation is extremely miserable. Since we know the asymptotic behavior we expect from our orbitals, we can estimate the convergence rate of the Hermite approximation from Theorem 1.5. We will evaluate the error at the boundary of the spatial and Fourier intervals. First we note that we will assume $u \sim e^{-\kappa|x|}$. The Fourier transform is then

$$\mathcal{F}[u] = \frac{\kappa_q^2}{k^2 \kappa_q^2} \sim \frac{1}{k^2} \ as \ k \to \infty \tag{41}$$

Using this result we have

$$\left| u(x) - \widehat{\Pi}_N u(x) \right|_{L^2} \lesssim e^{-\kappa_q \frac{\sqrt{2N}}{\gamma}} + \frac{1}{(\gamma\sqrt{2N})^2} \tag{42}$$

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Since $e^{-\sqrt{N}}$ and $1/N$ terms are larger than the e^{-N} term, we throw it out in the limit as $N \to \infty$. If we want to minimize the error on the right hand side, we want to find a γ such that the error contributions are comparable. So we need to solve

$$e^{-\kappa_q \frac{\sqrt{2N}}{\gamma}} \approx \frac{1}{2\gamma^2 N} \tag{43}$$

$$-\kappa_q \frac{\sqrt{2N}}{\gamma} \approx \ln(2\gamma^2 N)$$

$$-\kappa_q \frac{\sqrt{2N}}{\gamma} \approx 2\ln(\gamma)$$

where we threw out subdominate terms. If we expand about $\gamma = 1$ (the default value of the scaled basis), we have

$$-\kappa_q \frac{\sqrt{2N}}{\gamma} \approx \ln(2\gamma^2 N) \tag{44}$$

$$-\kappa_q \frac{\sqrt{2N}}{\gamma} \approx 2(\gamma - 1)$$

Solving for γ, we get the optimal choice for scaling parameter γ,

$$\gamma = N^{1/4}\sqrt{\kappa_q}. \tag{45}$$

Plugging this back into the error bound, we get

$$\left| u(x) - \widehat{\Pi}_N u(x) \right|_{L^2} \lesssim e^{-\kappa_q^{1/2} N^{1/4}\sqrt{2}} + \frac{1}{2\kappa_q N^{3/2}} \tag{46}$$

Thus, we arrive at our convergence rate,

$$\left| u(x) - \widehat{\Pi}_N u(x) \right|_{L^2} \lesssim \frac{1}{2\kappa_q N^{3/2}} \tag{47}$$

This is the best possible convergence rate for the Hermite approximation of u given that the function decays exponentially. It is not exponential but rather algebraic and shows that global approximations of functions that have asymptotics of $e^{-\kappa|x|}$ as $|x| \to \infty$ converge very slowly.

In three dimensions, we do not faire much better. The error bound in three dimensions with spherical symmetry is given by

$$\left| u(\vec{r}) - \widehat{\Pi}_N u(\vec{r}) \right|_{L^2} \lesssim \frac{R}{\kappa} e^{-\kappa_q R} + \frac{1}{\sqrt{5} R_k^{5/2}} \tag{48}$$

where

$$R = a\sqrt{\frac{2N_x}{\gamma_x^2} + \frac{2N_y}{\gamma_y^2} + \frac{2N_z}{\gamma_z^2}} \tag{49}$$

$$R_k = a\sqrt{2N_x\gamma_x^2 + 2N_y\gamma_y^2 + 2N_z\gamma_z^2} \tag{50}$$

By fixing a single direction, and finding the optimal γ similar to the 1d case gives a global error bound of

$$\left| u(\vec{r}) - \widehat{\Pi}_N u(\vec{r}) \right|_{L^2} \lesssim N^{1/4} e^{-\kappa_q^{1/2} N^{1/4}} + \frac{1}{\kappa_q N^{15/8}} \tag{51}$$

which is a little bit better than $N^{3/2}$ but still not good. Also note again, as $\kappa_q \to 0$, the error diverges as expected. How do we mitigate this problem?

1. Transformed Harmonic Oscillator (THO) basis: This strategy applies a coordinate transform to recover the proper asymptotics. (See for example [6])

2. Domain Truncation.

We take the domain truncation approach due to it's simplicity and has a chance to improve convergence. The domain strategy is summarized below:

1. Select a the length of the intervals making up your domain. This should be selected based on the magnitude of a typical one-body density near the boundary defined by the interval $[-\frac{\sqrt{2N_i}}{\gamma}, \frac{\sqrt{2N_i}}{\gamma}]$ where $i = x, y, z$.

2. Since we know the density decays roughly as $\rho(r) = e^{-\kappa_q r}$ for large r, we can choose a domain length based on the magnitude of ρ. Let R_{eff} be defined such that

$$\varepsilon = e^{\kappa_q R_{eff}} \tag{52}$$

where ε is chosen to be a number $\varepsilon \ll 1$. This means the effective domain size needs to be

$$R_{eff} = -\frac{\ln(\varepsilon)}{\kappa_q} \tag{53}$$

Since the domain size is set by N_i and R_{eff} is constant,

$$R_{eff} \sim \frac{\sqrt{2N_{i,min}}}{\gamma} \tag{54}$$

implies that $\gamma \sim \frac{\sqrt{2N_{i,min}}}{R_{eff}}$.

2 Numerical Method

3 Code

A Derivative Matrices

A.1 Spectral Space

A.2 Pseudospectral Space

From Ref. [1], the Cardinal functions near the collocation points of an orthonormal polynomial set are approximately

$$C_j(x) = \frac{\phi_{N+1}(x)}{\phi'(x_j)(x - x_j)} \tag{55}$$

In our case, ϕ is taken to be a Hermite function. To find the matrix representation of derivatives in pseudospectral space, we take derivatives of this expression and then evaluate them at the collocation points.

A.3 First Derivative Matrix

$$\frac{dC_j}{dx} = \frac{\phi'_{N+1}(x)}{\phi'_{N+1}(x_j)(x - x_j)} - \frac{\phi_{N+1}(x)}{\phi_{N+1}(x_j)(x - x_j)^2} \tag{56}$$

Now we need to consider cases as $x \to x_i$.

1) $x_i \neq x_j$:

$$\frac{dC_j}{dx}(x_i) = \frac{\phi'_{N+1}(x_i)}{\phi'_{N+1}(x_j)(x_i - x_j)} \tag{57}$$

2) $x_i = x_j$:

We evaluate the limit as $x \to x_i$ by L'Hopital's Rule for both terms,

1.

$$\lim_{x \to x_i} \frac{\phi'_{N+1}(x)}{\phi_{N+1}(x_j)(x - x_i)} = \lim_{x \to x_i} \frac{\phi''_{N+1}(x)}{\phi'_{N+1}(x_j)} = \frac{\phi''_{N+1}(x_i)}{\phi'_{N+1}(x_j)} \tag{58}$$

2.

$$\lim_{x \to x_i} -\frac{\phi_{N+1}(x)}{\phi_{N+1}(x_j)(x - x_j)^2} = -\frac{\phi''_{N+1}(x_i)}{2\phi'_{N+1}(x_j)} \tag{59}$$

So we have

$$\frac{dC_j}{dx}(x_i) = \frac{\phi''_{N+1}(x_i)}{2\phi'_{N+1}(x_j)} \tag{60}$$

The 1st derivative matrix is then

$$\frac{dC_j(x_i)}{dx} = D^{(1)}_{ij} = \begin{cases} \frac{\phi'_{N+1}(x_i)}{\phi'_{N+1}(x_j)(x_i - x_j)} & i \neq j \\ \frac{1}{2}\frac{\phi''_{N+1}(x_i)}{\phi'_{N+1}(x_i)} & i = j \end{cases} \tag{61}$$

It is important to note that $D^{(1)}_{ij}$ is not hermitian.

A.4   Second Derivative Matrix

$$\frac{d^2C_j}{dx^2} = \frac{\phi''_{N+1}(x)}{\phi'_{N+1}(x_j)(x - x_j)} - \frac{2\phi'_{N+1}(x)}{\phi'_{N+1}(x_j)(x - x_j)^2} + \frac{2\phi_{N+1}(x)}{\phi'_{N+1}(x_j)(x - x_j)^3} \tag{62}$$

1) $x_i \neq x_j$:

$$\frac{d^2C_j}{dx^2} = \frac{\phi''_{N+1}(x_i)}{\phi'_{N+1}(x_j)(x_i - x_j)} - \frac{2\phi'_{N+1}(x_i)}{\phi'_{N+1}(x_j)(x_i - x_j)^2} \tag{63}$$

1) $x_i \neq x_j$:
Using L'Hopital's Rule for all three terms results in

$$\frac{d^2C_j}{dx^2} = \frac{\phi'''_{N+1}(x_i)}{\phi'_{N+1}(x_j)} - \frac{\phi'''_{N+1}(x_i)}{\phi'_{N+1}(x_j)} + \frac{\phi'''_{N+1}(x_i)}{3\phi'_{N+1}(x_j)} \tag{64}$$

$$= \frac{\phi'''_{N+1}(x_i)}{3\phi'_{N+1}(x_j)} \tag{65}$$

The derivative matrix is then

$$\frac{d^2C_j(x_i)}{dx^2} = D^{(2)}_{ij} = \begin{cases} \frac{\phi''_{N+1}(x)}{\phi'_{N+1}(x_j)(x - x_j)} - \frac{2\phi'_{N+1}(x)}{\phi'_{N+1}(x_j)(x - x_j)^2} + \frac{2\phi_{N+1}(x)}{\phi'_{N+1}(x_j)(x - x_j)^3} & i \neq j \\ \frac{\phi'''_{N+1}(x_i)}{3\phi'_{N+1}(x_j)} & i = j \end{cases} \tag{66}$$

The matrix $D^{(2)}_{ij}$ is not hermitian. It is also important to note that $D^{(1)}D^{(1)} \neq D^{(2)}$

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