Extrapolation of Elliptic Eigenvalue Calculations on the Whole Space by the Virial Theorem

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Abstract

The calculations of eigenvalues of partial differential operators posed on the whole space are important in many applications. A typical model is the Schrödinger equation with various types of potentials in chemical physics where the eigenvalues are energy levels of an atom or molecule. The partial differential operator normally consists of sums of Laplacians signifying the quantized kinetic energy, and the potential energy operators can take various forms. The eigenvalues are then sums of the respective kinetic and potential energies. A common feature of these systems is that the kinetic and potential energy operators often have power law scaling properties such that the virial theorem is applicable. In this paper, we propose and prove extrapolation schemes that can be used to improve the accuracy of eigenvalue calculations by utilizing the virial theorem. Concrete data and examples from the finite element computation of the hydrogen atom and a quartic harmonic oscillator in three-dimensions are illustrated.

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1 Introduction

Eigenvalue calculations constitute an important part of numerical linear algebra and scientific computing. A majority of computation of matrix eigenvalue problems originates from differential equations as boundary value problems: mechanical vibrations, heat conduction, linear and nonlinear wave propagation, fluids, etc. Most of such boundary value problems are posed on \textit{bounded domains}, which are then further discretized by finite elements, finite differences, boundary elements, spectral methods, etc.

On the other hand, there is also a large class of differential eigenvalue problems posed on \textit{unbounded domains}. Many of such problems can be found in quantum mechanics, where the Schrödinger equation with various types of potentials is a standard model, with the underlying domain being the entire space. For example, in chemical physics, the Schrödinger equation with Coulomb potentials is the model for atoms and molecules. The determination of their electronic and molecular rotation and vibration \textit{energy levels} is crucial in chemical and physical applications. Such \textit{energy levels are exactly the eigenvalues of the Schrödinger operator}. In order to compute these eigenvalue problems by the standard finite element or finite difference methods, the unbounded domain (almost) inevitably need to be truncated down to a finite size. With the use of boundary elements or spectral methods, one might be able to get away without having to do such domain truncation sometimes.

For partial differential equations posed on the entire space, there is a great advantage that the \textit{methods of invariant transformations} may be applied, leading to invaluable theoretical information about the solution behavior and the assessment of the quality of numerical data. Almost without question the most important invariant transformation is the \textit{scaling (or dilation) of the spatial variables}. In mathematical physics, application of the scaling transformation will lead to the \textit{virial theorem}, a relation between the \textit{kinetic and potential energies} due to the different homogeneity degree of the kinetic
and potential energy operators when the scaling transformation is applied. For the case of the Schrödinger equation with a Coulomb potential in chemical physics (cf. Example 2.1 in Section 2), the virial theorem gives

$$2KE + PE = 0, \quad (KE = \text{kinetic energy}, PE = \text{potential energy}),$$

i.e.,

$$PE/KE = -2.$$  

The energy levels (or eigenvalues) $E$ are related to $KE$ and $PE$ by

$$E = KE + PE.$$  

Assume that now we are computing numerical eigenvalues $E$ by any numerical scheme, let the computed values be $E_h$, $KE_h$, and $PE_h$, where $h$ is the discretization parameter. We have

$$E_h = KE_h + PE_h.$$  

If the numerical values $KE_h$ and $PE_h$ have ratios $PE_h/KE_h$ deviating very much from $-2$, then we know a priori in general that the numerical eigenvalue $E_h$ cannot be very accurate. In this sense, the virial theorem provides a useful means for assessing the quality of numerical results or even numerical methods. In another instance (cf. Example 2.3, Section 2), we also see that the virial theorem can be used to establish the non-existence of eigenvalues.

These nice applications of the virial theorem in the above paragraph are somewhat or reasonably familiar to researchers in the quantum mechanics and mathematical physics communities, but not necessarily so to those doing scientific computation and other branches of applied mathematics. As a matter of fact, the virial theorem can be used in an even more constructive way to improve the accuracy of numerical eigenvalues. This is the main objective we wish to call attention to in this paper.

The organization of the paper is arranged as follows. In Section 2, we present a proof of the virial theorem in order to make the paper sufficiently
self-contained, and offer many concrete examples. In Section 3, we prove theorems for the application of the virial theorem to eigenvalue computation. The main idea is to \textit{extrapolate by projection and/or reflection} utilizing the virial equation. In Section 4, concrete numerical data from two computational examples of the hydrogen atom and a quartic harmonic oscillator are discussed as illustrations.

2 The Virial Theorem and Applications in Quantum Mechanics

Our study of elliptic eigenvalue problems on the whole space is motivated by the multi-particle Schrödinger equation in non-relativistic quantum mechanics, which can be written as

\[ i\hbar \frac{\partial}{\partial t} \psi(\mathbf{r}, t) = H \psi(\mathbf{r}, t), \quad t > 0; \hbar > 0, \]  

(2.1)

where

\[ \mathbf{r} = (\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N) \in \mathbb{R}^{3N}, \]  

(2.2)

is the collective position vector of \( N \) particles, with \( \mathbf{r}_j \in \mathbb{R}^3 \) denoting the position of the \( j^{\text{th}} \) particle, for \( j = 1, 2, \ldots, N \). The operator \( H \) in (2.1) is the \textit{Hamiltonian}, consisting of the kinetic and potential energy operators:

\[ H = K + P, \]  

(2.3)

where

\[ K \equiv \sum_{j=1}^{N} \frac{p_j^2}{2m_j} = -\frac{1}{2} \sum_{j=1}^{N} \frac{\hbar^2}{m_j} \nabla_j^2 \]  

(2.4)

\[ (p_j = \frac{\hbar}{i} \nabla_j, \nabla_j = \left( \frac{\partial}{\partial x_1^{(j)}}, \frac{\partial}{\partial x_2^{(j)}}, \frac{\partial}{\partial x_3^{(j)}} \right), \quad \mathbf{r}_j = (x_1^{(j)}, x_2^{(j)}, x_3^{(j)}), \]  

\[ \nabla_j^2 = \frac{\partial^2}{\partial x_1^{(j)^2}} + \frac{\partial^2}{\partial x_2^{(j)^2}} + \frac{\partial^2}{\partial x_3^{(j)^2}}, \quad m_j = \text{the mass of the } j^{\text{th}} \text{ particle } > 0 \), \]

\[ P \equiv V(\mathbf{r}) \cdot \mathbf{r}; \quad V(\cdot) \text{ is a real-valued function.} \]  

(2.5)
The function $\psi(r, t)$ in (2.1) is the wave function, satisfying the normalization condition
\[
\int_{\mathbb{R}^{3N}} |\psi(r, t)|^2 dr = \|\psi(\cdot, t)\|_{L^2(\mathbb{R}^{3N})}^2 = 1, \text{ signifying total probability 1. } (2.6)
\]
For steady states, the time and space variables can be separated: Write
\[
\psi(r, t) = e^{iEt/\hbar} \Psi(r),
\]
and substitute it into (2.1), yielding
\[
H \Psi(r) = E \Psi(r), \text{ on } \mathbb{R}^{3N}. \quad (2.7)
\]
This constitutes a second order linear elliptic eigenvalue problem over the entire space $\mathbb{R}^{3N}$, which is the main object of investigation in this paper. The underlying Hilbert space for (2.7) is
\[
\mathcal{H} = L^2(\mathbb{R}^{3N}), \text{ over } \mathbb{C}.
\]
We refer to Lieb and Loss [8] and Chen, et al. [5] for some basic properties of the Schrödinger operator $H$. The second order equation (2.7) induces a bilinear form
\[
a(u, v) \equiv \sum_{j=1}^N \frac{\hbar^2}{2m_j} \int \nabla_j u^* \cdot \nabla_j v \, dr + \int V(\cdot) u^* v \, dr, \\
\equiv a_K(u, v) + a_P(u, v), \quad (2.8)
\]
where "*" denotes the complex conjugate (a notation being inherited from physics), the integrals are over $\mathbb{R}^{3N}$, and
\[
u, v \in \mathcal{V} \equiv \left\{ \psi \in H^1(\mathbb{R}^{3N}) \mid \int V(\cdot) |\psi|^2 \, dr < \infty \right\}, \quad (2.9)
\]
where $H^1(\mathbb{R}^{3N})$ is the usual Sobolev space on $\mathbb{R}^{3N}$. The eigenvalue problem (2.7) thus has a weak form
\[
a(\Psi, v) = E \langle \Psi, v \rangle_{L^2(\mathbb{R}^N)} = E \int \Psi^* v \, dr, \quad \forall v \in \mathcal{V}, \quad (2.10)
\]
subject to
\[ \|\Psi\|_{L^2(\mathbb{R}^{3N})}^2 = 1. \]  
(2.11)

The inner products of functions in (2.8) and (2.10) involve complex conjugates of functions. Such complex conjugation actually is not needed because (for a large variety of concrete applications) \( H \) is a Hermitian operator, implying that all eigenvalues \( E \) are real and all eigenstates \( \Psi \) are real-valued. Thus, from now on we will drop “\(*\)" in (2.8) and (2.10) without further mention.

\section{2.1 Proof of the Virial Theorem}

Here, we derive the virial property of an eigenstate \( \Psi \). Such a proof is available in [5, 14], for example. Since the idea is of fundamental importance in this paper, for the sake of self-containedness and as a convenience for the reader, we include the proof below.

\textbf{Theorem 2.1 (The Virial Theorem). Let \( \Psi \) be an eigenstate satisfying (2.10) and (2.11). Then}
\[-2a_K(\Psi, \Psi) + \int r \frac{\partial V(r)}{\partial r} \Psi(r)^2 \, dr = 0.\]  
(2.12)

\textit{Proof}. In (2.10) and (2.11), choose \( v = \Psi(kr) \), where \( k > 0 \). Then we have
\[ \sum_{j=1}^{N} \frac{\hbar^2}{2m_j} \int \nabla \Psi(r) \cdot \nabla \Psi(kr) dr + \int V(r) \Psi(r) \Psi(kr) dr = E \int \Psi(r) \Psi(kr) dr.\]  
(2.13)

On the other hand, making the change of variable \( r \mapsto kr \) in (2.10), we obtain
\[ \frac{1}{k^2} \sum_{j=1}^{N} \frac{\hbar^2}{2m_j} \int \nabla \Psi(kr) \cdot \nabla v(kr) dr + \int V(kr) \Psi(kr) v(kr) dr = E \int \Psi(kr) v(kr) dr.\]  
(2.14)

Since \( v(kr) \) in (2.14) is arbitrary, we choose \( v(r) = \Psi(r/k) \) so that \( v(kr) = \psi \).
\[ \Psi(kr/k) = \Psi(r), \text{ and obtain} \]
\[
\frac{1}{k^2} \sum_{j=1}^{N} \frac{\hbar^2}{2m_j} \int \nabla \Psi(kr) \cdot \nabla \Psi(r) \, dr + \int V(kr) \Psi(kr) \Psi(r) \, dr = E \int \Psi(kr) \Psi(r) \, dr. \quad (2.15)
\]
Subtracting (2.13) from (2.15), dividing by \( k - 1 \) and letting \( k \) tend to 1, we obtain
\[
\lim_{k \to 1} \left( \frac{1}{k^2} \frac{1}{k-1} \right) \cdot \lim_{k \to 1} \int \nabla \Psi(kr) \cdot \nabla \Psi(r) \, dr + \int \lim_{k \to 1} \left[ \frac{V(kr) - V(r)}{k - 1} \right] \cdot \lim_{k \to 1} [\Psi(kr) \Psi(r)] \, dr = 0. \quad (2.16)
\]
Note that
\[
\lim_{k \to 1} \frac{V(kr) - V(r)}{k - 1} = \left. \frac{d}{dk} V(kr) \right|_{k=1} = r \frac{\partial V(r)}{\partial r}. \quad (2.17)
\]
So (2.16) and (2.17) yield (2.12).

**Remark 1.** If the quantum-mechanical potential \( V(r) \) is homogeneous of degree \( \alpha \in \mathbb{R} \), i.e.,
\[
V(kr) = k^\alpha V(r) \quad \text{for any } k > 0, \quad (2.18)
\]
then (2.17) gives
\[
\lim_{k \to 1} \frac{V(kr) - V(r)}{k - 1} = \left( \left. \frac{d}{dk} k^\alpha \right|_{k=1} \right) V(r) = \alpha V(r) \left( = r \frac{\partial V(r)}{\partial r} \right). \quad (2.19)
\]
Thus (2.12) can be written as
\[
-2a_K(\Psi, \Psi) + \alpha a_P(\Psi, \Psi) = 0. \quad (2.20)
\]
Define the kinetic energy (\( KE \)) and potential energy (\( PE \)) by
\[
KE \equiv a_K(\Psi, \Psi), \quad PE = a_P(\Psi, \Psi).
\]
Then
\[
PE/KE = 2/\alpha, \quad (2.21)
\]
a simple relation between the kinetic energy \( a_K(\Psi, \Psi) \) and the potential energy \( a_P(\Psi, \Psi) \).
Applications of the virial theorem in the literature involves mainly the case of homogeneity (2.18). Our treatment in this paper deals with the general case.

2.2 Application of the Virial Theorem to a Variety of Potentials

We now mention a collection of examples as applications and extensions of the virial theorem.

Example 2.1 (Atoms and molecules: the Schrödinger equation with a Coulomb potential). Every atom and (simple) molecule can be modeled by the Schrödinger equation with a Coulomb potential. In (2.4) and (2.5), let

\[ N = N_1 + N_2; \quad N_1 = \text{number of electrons}, \quad N_2 = \text{number of nuclei}, \quad (2.22) \]

and

\[ m_j = m = \text{the mass of the electron}, \quad j = 1, 2, \ldots, N_1; \]
\[ m_j = M_J = \text{the mass of the } J^{th} \text{ nucleus}, \quad J = 1, 2, \ldots, N_2; \quad j = N_1 + J; \]
\[ r_j = (x_1^{(j)}, x_2^{(j)}, x_3^{(j)}) = \text{the position of the } j^{th} \text{ electron}, \quad j = 1, 2, \ldots, N_1; \]
\[ r_j \equiv R_J = (X_1^{(J)}, X_2^{(J)}, X_3^{(J)}) = \text{the position of the } J^{th} \text{ nucleus}, \quad J = 1, 2, \ldots, N_2, \quad j = N_1 + J; \]
\[ r = (r_1, r_2, \ldots, r_{N_1}, R_1, R_2, \ldots, R_{N_2}). \]

Further, let

\[ e = \text{the electric change of the electron}, \]
\[ Z_J e = \text{the (positive) electric charge of the } J^{th} \text{ nucleus}, \quad J = 1, 2, \ldots, N_2, \]
\[ Z_J = \text{a positive integer}. \]

Then (2.7) and (2.8) can be written as

\[ -\left[ \frac{\hbar^2}{2m} \sum_{j=1}^{N_1} \nabla_j^2 \Psi(r) + \frac{\hbar^2}{2} \sum_{J=1}^{N_2} \frac{\nabla_J^2}{M_J} \Psi(r) \right] + V(r) \Psi(r) = E \Psi(r), \quad (2.23) \]
with
\[ V(\mathbf{r}) = \sum_{1 \leq j,j' \leq N_1} \left[ -\frac{Z_j e^2}{|\mathbf{R}_j - \mathbf{r}_j|} + \frac{Z_j Z_{j'} e^2}{|\mathbf{R}_j - \mathbf{R}_{j'}|} + \frac{e^2}{|\mathbf{r}_j - \mathbf{r}_{j'}|} \right], \quad (2.24) \]
and
\[ a(u,v) = \left[ \sum_{j=1}^{N_1} \frac{\hbar^2}{2m} \int \nabla_j u \cdot \nabla_j v \, d\mathbf{r} + \sum_{J=1}^{N_2} \frac{\hbar^2}{2M_J} \int \nabla_J u \cdot \nabla_J v \, d\mathbf{r} \right] \]
\[ + \left[ \int V(\cdot) uv \, d\mathbf{r} \right] \equiv a_K(u,v) + a_P(u,v), \quad (2.25) \]
respectively.

Note that the potential \( V \) in (2.24) satisfies (2.18) with \( \alpha = -1 \). Therefore for an eigenstate \( \Psi \), we have, by (2.20),
\[-2a_K(\Psi, \Psi) - a_P(\Psi, \Psi) = 0. \quad (2.26)\]
Then (2.21) gives the ratio between \( PE \) and \( KE \) as
\[ PE/KE = -2. \quad (2.27) \]
From (2.10) and (2.11),
\[ a(\Psi, \Psi) = a_K(\Psi, \Psi) + a_P(\Psi, \Psi) = KE + PE = E, \quad (2.28) \]
\[ E = KE + PE = KE - 2KE = -KE. \quad (2.29) \]
But \( KE = a_K(\Psi, \Psi) > 0 \) by (2.11). Therefore \( E < 0 \), i.e., an important by-product of the virial theorem is that all eigenvalues \( E \) of (2.23) are negative. \( \square \)

**Example 2.2** (The hydrogen atom). The hydrogen atom is the simplest atom in the universe for Example 2.1, with \( N_1 = 1 \), \( N_2 = 1 \), \( N = 2 \), \( Z_1 = 1 \), and
\[ V(\mathbf{r}) = -\frac{e^2}{|\mathbf{r}_1 - \mathbf{R}_1|}. \]
By using the center-of-mass coordinates (procedure omitted), one can separate the nuclear and electronic motions. (The nucleus of the hydrogen atom
consists of a proton only.) The electronic wave function can be shown to satisfy
\[-\frac{\hbar^2}{2m} \nabla^2 \Psi(r) - \frac{e^2}{r} \Psi(r) = E' \Psi(r), \quad r \in \mathbb{R}^3. \quad (2.30)\]
The various coefficients $\hbar, m$ and $e^2$ can be normalized by using atomic units:
\[\frac{\hbar^2}{me^2} = 1.\]
Thus, (2.30) becomes
\[-\frac{1}{2} \nabla^2 \Psi(r) - \frac{1}{r} \Psi(r) = E \Psi(r); \quad (E \equiv E'/e^2), \quad r \in \mathbb{R}^3. \quad (2.31)\]
It is well known that exact eigenvalues $E$ and eigenfunctions $\Psi$ of (2.31) are given by
\[
\begin{cases}
E = E_n = -\frac{1}{2n^2}, & n = 1, 2, 3, \ldots, \\
\Psi(r) = \left(\frac{2}{n}\right) \left\{ \frac{(n - \ell - 1)!}{2n[(n + \ell)!]^3} \left(\frac{2r}{n}\right)^\ell L_{2\ell+1}^{2\ell+1} \left(\frac{2r}{n}\right) e^{-r/n} \right\} P_{\ell}^{[m]}(\cos \theta)(e^{\pm im\phi}/\sqrt{2\pi}) \\
n = 1, 2, \ldots, \ell = 0, 1, 2, \ldots, n - 1; m = -\ell, -\ell + 1, \ldots, 0, 1, \ldots, \ell - 1, \ell,
\end{cases}
\quad (2.32)
\]
$P_{\ell}^{[m]}$: the associated Legendre function; $L_{n+\ell}^{2\ell+1}$: the associated Laguerre polynomials,
\quad (2.33)
where each $E_n$ has multiplicity $n^2$ [3, p. 72] due to the strong symmetry of the PDE (2.31). For (2.31), we have
\[
\begin{cases}
E = KE + PE, \\
2KE + PE = 0,
\end{cases}
\quad (2.34)
\]
following (2.26) and (2.28).

Finite element computational aspects of (2.31) will be discussed in Section 4.

\[\square\]

**Example 2.3** (Non-existence of eigenvalues and eigenfunctions for a $P^+e^+$-configuration). Return to Example 2.2, but assume that the hydrogen
nucleus (i.e., a proton P\(^+\)) is surrounded by a positron (\(e^+\), the anti-particle of electron, carrying a positive charge). Then because of the change of sign of the electric charge, equation (2.31) now becomes
\[
-\frac{1}{2} \nabla^2 \Psi(r) + \frac{1}{r} \Psi(r) = E \Psi(r), \quad r \in \mathbb{R}^3.
\] (2.35)
The two properties in (2.34) remain valid. However, (2.34)\(_2\) now reads
\[
0 = 2KE + PE = 2 \cdot \left(\frac{1}{2}\right) \int |\nabla \Psi|^2 \, dr + \int \frac{1}{r} |\Psi|^2 \, dr > 0,
\] (2.36)
for \(\Psi\) satisfying (2.11), a contradiction.

Therefore, equation (2.35) does not have any eigensolutions. Physically, this implies that the P\(^+\)e\(^+\)-configuration is unstable—the positron will be repelled by the proton to infinity. \(\square\)

**Example 2.4** (The Lennard–Jones (L-J) potential). A pair of neutral atoms or molecules experiences two distinct types of forces as a function of separation distance: repelling when the distance is small (called the Pauli repulsion due to the overlapping of electron orbitals), and attracting when the distance is large (called the van der Waals force); c.f. e.g. [12]. The L-J potential is a simple mathematical model providing an accurate empirical fit:
\[
V_{LJ}(r) = 4\epsilon \left[ \left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right]; \quad \epsilon, \sigma > 0,
\] (2.37)
\(\epsilon = \) depth of the potential well; \(\sigma = (2)^{-16}. \) minimum of the potential well, \(r = \) inter-particle separation distance; \(r = |r|, r \in \mathbb{R}^3.\)

Then for the case of two interacting particles with masses \(m_1\) and \(m_2\), the Schrödinger equation is given by
\[
\left[-\frac{\hbar^2}{2} \left(\frac{1}{m_1} + \frac{1}{m_2}\right) \nabla^2 + V_{LJ}(r)\right] \Psi(r) = E \Psi(r); \quad r \in \mathbb{R}^3.
\] (2.38)
In this case, \(V_{LJ}(\cdot)\) does not satisfy (2.18) for any \(\alpha.\) Nevertheless, by defining
\[
KE = a_K(\Psi, \Psi)
\]
in the same way as before, and letting

\[ PE_1 \equiv \int 4\varepsilon \left( \frac{\sigma}{r} \right)^{12} |\Psi(r)|^2 \, dr, \quad PE_2 \equiv -4\varepsilon \int \left( \frac{\sigma}{r} \right)^6 |\Psi(r)|^2 \, dr, \quad (2.39) \]

we then obtain from Theorem 2.1

\[
\begin{cases}
E = KE + PE_1 + PE_2, \\
KE + 6PE_1 + 3PE_2 = 0.
\end{cases} \quad (2.40)
\]

**Example 2.5** (The harmonic oscillator). The one-dimensional harmonic oscillator

\[-\hbar^2 \frac{d^2}{2m dx^2} \Psi(x) + \frac{\hbar}{m} \omega^2 x^2 \Psi(x) = E \Psi(x), \quad x \in \mathbb{R}, \quad (2.41)\]

is a basic model for single-mode electromagnetic waves (photons) in a cavity [13]. Its parabolic potential can be further used to approximate any potential, locally, in the neighborhood of a stable equilibrium position. More generally, a quartic polynomial may also be used as a potential:

\[ V(x) = a_1 x + a_2 x^2 + a_3 x^3 + a_4 x^4, \quad a_j \in \mathbb{R}, j = 1, 2, 3, 4; a_4 > 0. \]

For the Schrödinger equation

\[-\hbar^2 \frac{d^2}{2m dx^2} \Psi(x) + (a_1 x + a_2 x^2 + a_3 x^3 + a_4 x^4) \Psi(x) = E \Psi(x), \quad x \in \mathbb{R}, \quad (2.42)\]

we define

\[ KE = a_K(\Psi, \Psi) \quad \text{as usual}, \]

and

\[ PE_j \equiv \int a_j x^j |\Psi(x)|^2 \, dx, \quad j = 1, 2, 3, 4. \]

Then Theorem 2.1 gives

\[
\begin{cases}
E = KE + \sum_{j=1}^{4} PE_j \\
-2KE + \sum_{j=1}^{4} jPE_j = 0.
\end{cases} \quad (2.43)
\]
Three-dimensional versions of (2.42)

\[
\begin{cases}
\left[-\frac{1}{2}\nabla^2 + V(r)\right] \Psi(r) = E \Psi(r), & r = (x_1, x_2, x_3) \in \mathbb{R}^3, \\
V(r) \text{ is a polynomial of degree 4 of the variables } x_1, x_2 \text{ and } x_3,
\end{cases}
\]  

(2.44)

have also been used by chemists to model molecular vibrational motions [2, 6, 7], and an analogue of (2.43) remains valid. For more discussions and calculations, see Subsection 4.3

Example 2.6 (An ODE eigenvalue problem on the whole or half line). Consider an ODE

\[
\sum_{j=1}^{N_1} a_j (-1)^j \frac{d^2}{dx^j} \Psi(x) + \sum_{j=1}^{2N_2} b_j x^j \Psi(x) = E \Psi(x), \quad x \in \mathbb{R},
\]

(2.45)

where \(N_1 > 0, b_{2N_2} > 0\). The underlying space is \(\mathcal{H} = L^2(\mathbb{R})\). Define a bilinear form

\[
a(u, v; \mu) \equiv \sum_{j=1}^{N_1} a_j \int u^{(j)} v^{(j)} dx + \sum_{j=1}^{2N_2} b_j \int x^j uv dx \\
+ \mu \int uv dx; \quad u, v \in \mathcal{V}, \quad \text{for given } \mu \in \mathbb{R},
\]

(2.46)

\[
\mathcal{V} \equiv \{ \psi \in H^{N_1}(\mathbb{R}) \mid \int \sum_{j=1}^{2N_2} b_j x^j |\psi(x)|^2 dx < \infty \}.
\]

Then for \(\mu > 0\) sufficiently large, \(a(\cdot, \cdot; \mu)\) is positive definite. The weak form of (2.45) is

\[
a(\Psi, v; \mu) = (E - \mu) \langle \Psi, v \rangle_{L^2(\mathbb{R})}, \quad \forall v \in \mathcal{V}.
\]

The proof of Theorem 2.1 can be easily carried over to (2.45) and (2.46). Here, for \(\Psi \in \mathcal{V}, \|\Psi\|_{L^2(\mathbb{R})} = 1\), we define

\[
KE_j = a_j \int |\Psi^{(j)}|^2 dx, \quad j = 1, 2, \ldots, N_1,
\]

(2.47)

\[
PE_j = b_j \int x^j |\Psi|^2 dx, \quad j = 0, 1, 2, \ldots, 2N_2, \quad b_0 \equiv \mu.
\]

(2.48)
Then we have

\[
\begin{align*}
E &= \sum_{j=1}^{N_1} KE_j + \sum_{j=1}^{2N_2} PE_j, \\
\sum_{j=1}^{N_1} (-2j) KE_j + \sum_{j=1}^{2N_2} j PE_j &= 0.
\end{align*}
\]  

(2.49)

The virial equations (2.49) remain valid if, instead of considering (2.45) on the entire real line, we consider it on the half line \( \mathbb{R}_+ \equiv (0, \infty) \) or \( \mathbb{R}_- \equiv (-\infty, 0) \), with the Dirichlet boundary condition

\[
\Psi(0) = \Psi'(0) = \Psi''(0) = \cdots = \Psi^{(N_1-1)}(0) = 0,
\]

(2.50)

or the Neumann boundary condition

\[
\Psi^{(2N_1-1)}(0) = \Psi^{(2N_1-3)}(0) = \cdots = \Psi^{(N_1+1)}(0) = 0,
\]

(2.51)

or a mixture of (2.50) and (2.51) as long as the boundary condition at \( x = 0 \) is properly posed. However, Robin-type boundary conditions would lead to extra boundary terms at \( x = 0 \) in addition to the integrals (2.47) and (2.48).

This example also indicates that all of our discussions in this paper can be extended to half-space domains. \( \square \)

In the preceding Examples 2.1–2.6, the potentials \( V(\cdot) \) are all polynomial or rational functions of \( r \). In the subsequent two examples, we look at \( V(\cdot) \) that are transcendental functions.

**Example 2.7** (The Morse potential). The Morse potential is a useful, accurate model for the vibration of diatomic molecules \([4, 9]\). The Schrödinger equation here is

\[
\left[ -\frac{\hbar^2}{2m} \nabla^2 + V_M(\mathbf{r}) \right] \Psi(\mathbf{r}) = E \Psi(\mathbf{r}), \quad \mathbf{r} \in \mathbb{R}^3,
\]

(2.52)

with the Morse potential

\[
V_M(\mathbf{r}) \equiv D(e^{-2\alpha \tilde{r}} - 2e^{-\alpha \tilde{r}}), \quad \tilde{r} = \frac{r - r_0}{r_0},
\]

(2.53)
where $D, \alpha, r_0$ are positive constants. Note that $V_M(\cdot)$ decays exponentially with respect to $r$.

Define the kinetic and potential energies $KE$ and $PE$ in the same way as before, and apply Theorem 2.1. Then we obtain

$$
\begin{align*}
E &= KE + PE, \\
-2KE - 2\alpha D \int r(e^{-2\alpha \hat{r}} - e^{-\alpha \hat{r}})|\Psi(r)|^2 \, dr = 0.
\end{align*}
$$

(2.54)

□

**Example 2.8** (The logarithmic potential). The logarithmic potential can be used to stipulate confining potential between quarks in quantum chromodynamics (QCD) [11], given by

$$
V(r) = \gamma^2 \ln r, \quad r \in \mathbb{R}^3; \quad \gamma \in \mathbb{R} \text{ is given.}
$$

(2.55)

Then for the Schrödinger equation

$$
-\frac{\hbar^2}{2m} \nabla^2 \Psi(r) + \gamma^2 \ln r \Psi(r) = E \Psi(r), \quad r \in \mathbb{R}^3,
$$

(2.56)

the kinetic and potential energies are

$$
KE = a_K(\Psi, \Psi), \quad PE = a_P(\Psi, \Psi)
$$

as before, and we have

$$
\begin{align*}
E &= KE + PE, \\
-2KE + \gamma^2 &= 0,
\end{align*}
$$

(2.57)

where (2.57)$_2$ is the virial equation derived from $\|\Psi\|_{L^2(\mathbb{R}^3)}^2 = 1$. □

3 Utilizing the Virial Equation to Extrapolate and Improve the Accuracy of Eigenvalue Computations by Projection and Reflection

Through Examples 2.1–2.8 in Section 2, we see that the virial theorem provides an equation as extra information for various terms comprising the
kinetic and potential energies $KE$ and $PE$. In this section, we devise a projection method to utilize this virial equation to extrapolate the computed values of eigenvalue $E$, from the finite element computational point of view.

3.1 Synthesis for the Eigenvalue Problem Modeling in a Finite-Dimensional Framework by the Virial Equation

We revisit Examples 2.1, 2.2, and 2.4–2.6 in Subsection 2.2.

**Synthesis:** In these examples, we can cast the virial equations into the form

$$ \nu \cdot \hat{x} = 0, \quad (\cdot: \text{the dot product}) \tag{3.1} $$

where $\nu$ and $\hat{x}$ are vectors in a finite-dimensional space $\mathbb{R}^m$ for some positive integer $m$, and $\nu$ is known from the virial. Without loss of generality, we can assume $\nu$ to be a unit vector:

$$ \nu \cdot \nu = 1. \tag{3.2} $$

The eigenvalue $E$ can be obtained as

$$ E = \lambda \cdot \hat{x} \tag{3.3} $$

for some $\lambda \in \mathbb{R}^m$; $\lambda$ is also known. The vector $\hat{x} \in \mathbb{R}^m$ is unknown, yet to be computed. But approximations $x_j \in \mathbb{R}^m$, $j = 1, 2, \ldots, \ell$, are known from actual computations. We call (3.3) the eigenvalue equation.

(i) **Example 3.1** (Coulomb potentials). Let

$$ \hat{x} = (x_1, x_2) \equiv (KE, PE), \quad \nu = \frac{1}{\sqrt{5}}(2, 1); \quad \nu \in \mathbb{R}^2, \quad m = 2. \tag{3.4} $$

Then (2.27) gives

$$ \nu \cdot \hat{x} = 0, \tag{3.5} $$

while (2.28) gives

$$ E = \lambda \cdot \hat{x}, \quad \text{with} \quad \lambda = (1, 1) \in \mathbb{R}^2. \tag{3.6} $$
(ii) **Example 3.2** (The hydrogen atom). This is a special case of Example 3.1. So (3.4)–(3.6) remain valid from (2.34).

(iii) **Example 3.3** (Nonexistence). Skipped.

(iv) **Example 3.4** (The Lennard–Jones potential).

\[ \hat{x} = (x_1, x_2, x_3) \equiv (KE, PE_1, PE_2) \in \mathbb{R}^m; \quad m = 3. \]

Here (2.40)\textsubscript{2} gives

\[ \nu \cdot \hat{x} = 0 \quad \text{with} \quad \nu \equiv \frac{1}{\sqrt{46}}(1, 6, 3), \quad (3.7) \]

while (2.40)\textsubscript{1} gives

\[ E = \lambda \cdot \hat{x} \quad \text{with} \quad \lambda = (1, 1, 1). \quad (3.8) \]

(v) **Example 3.5** (The generalized harmonic oscillator).

\[ \hat{x} = (x_1, x_2, x_3, x_4, x_5) \in \mathbb{R}^5, \quad (m = 5). \]

Here (2.43)\textsubscript{2} gives

\[ \nu \cdot \hat{x} = 0, \quad \text{with} \quad \nu = \frac{1}{\sqrt{34}}(-2, 1, 2, 3, 4), \quad (3.9) \]

while (2.43)\textsubscript{1} gives

\[ E = \lambda \cdot \hat{x}, \quad \text{with} \quad \lambda = (1, 1, 1, 1, 1). \quad (3.10) \]

(vi) **Example 3.6** (ODE).

\[ \hat{x} = (KE_{N_1}, KE_{N_1-1}, \ldots, KE_1, PE_1, PE_2, \ldots, PE_{2N_2}) \in \mathbb{R}^m; \quad m = N_1+2N_2. \]

Here (2.49)\textsubscript{2} gives

\[ \nu \cdot \hat{x} = 0 \quad (3.11) \]

with

\[ \nu = \left( \sum_{j=1}^{N_1} (-2j)^2 + \sum_{j=1}^{2N_2} j^2 \right)^{-1/2} (-2N_1, -2(N_1 - 1), -2(N_1 - 2), \ldots, -2, 1, 2, 3, \ldots, 2N_2), \]
while
\[ E = \lambda \cdot \hat{x}; \quad \lambda = (1, 1, \ldots, 1) \in \mathbb{R}^{N_1+2N_2}. \] (3.12)

Example 2.7 with the Morse potential cannot be synthesized into a finite-dimensional framework. See its infinite-dimensional formulation in Subsection 3.5.

### 3.2 Linear Transformations of the Virial and Eigenvalue Equations in the Finite-Dimensional Framework

In the various examples shown in the preceding subsection, the virial equation and the eigenvalue equation have been synthesized, respectively, into the form
\[ \nu \cdot \hat{x} = 0, \quad E = \lambda \cdot \hat{x}; \quad \nu, \lambda, \hat{x} \in \mathbb{R}^m, \quad |\nu| = 1. \] (3.13)

Obviously, these two equations can be represented in many different equivalent forms. Let \( A \) be any real invertible \( m \times m \) matrix. Define
\[
\begin{aligned}
\hat{x}' &= A\hat{x}, \\
\lambda' &= (A^T)^{-1}\lambda, \quad (A^T: \text{the transpose of } A) \\
\nu' &= (A^T)^{-1}\nu/|(A^T)^{-1}\nu|.
\end{aligned}
\] (3.14)

Then the two equations in (3.13) give
\[ \nu' \cdot \hat{x}' = 0, \quad E = \lambda' \cdot \hat{x}', \] (3.15)
as the transformed virial and eigenvalue equations.

We will need the following property for our future use.

**Proposition 3.1.** (i) Let two given vectors \( \lambda, \nu \in \mathbb{R}^m \) be linearly independent. Then there exists a positive-definite matrix \( P \) such that
\[ \nu \cdot (P\lambda) = 0. \] (3.16)
(ii) If two nonzero vectors $\lambda, \nu \in \mathbb{R}^m$ satisfy $\lambda \cdot \nu = 0$, then there exists a positive-definite matrix $P$ such that

$$\nu \cdot (P\lambda) \neq 0.$$ (3.17)

Proof. Here we regard each vector $u \in \mathbb{R}^m$ as a column vector; $u^T$, its transpose, is then a row vector. Note that

(a) for each $u \in \mathbb{R}^m$, $u \neq 0$, $uu^T$ is a positive semidefinite $m \times m$ matrix;

(b) if $\{u_1, u_2, \ldots, u_n\}$ is a linearly independent set, then the matrix $\sum_{j=1}^n u_j u_j^T$ is positive semidefinite with rank $n$;

(c) if $P = uu^T$ satisfies $\nu^T P \lambda = 0$, then either $\nu \cdot u = 0$ or $u \cdot \lambda = 0$, or both.

Now, consider (i). If $\nu \cdot \lambda = 0$, then we can just choose $P$ to be the identity matrix so that (3.16) is satisfied. Therefore, we may assume that $\nu \cdot \lambda \neq 0$.

In span $\{\nu, \lambda\}$, choose two vectors $u_1, u_2$ by

$$u_1 = \nu - \frac{|\nu|^2}{\nu \cdot \lambda} \lambda, \quad u_2 = -\frac{|\lambda|^2}{\nu \cdot \lambda} \nu + \lambda.$$ (3.18)

Then $u_1 \cdot \nu = 0$ and $u_2 \cdot \lambda = 0$. Note that $u_1$ and $u_2$ are linearly independent, as the determinant of the coefficients is equal to $1 - (|\nu|^2|\lambda|^2/(\nu \cdot \lambda)^2) < 0$ (equal to 0 only when $\nu$ and $\lambda$ are linearly dependent).

Now, choose a basis $\{u_3, u_4, \ldots, u_m\}$ for the orthogonal complement of span $\{\nu, \lambda\}$. Then it is easily seen that

$$P \equiv \sum_{j=1}^m u_j u_j^T$$

satisfies (3.16). So (i) has been proved.

To prove (ii), choose

$$u_1 = \nu + \lambda, \quad u_2 = \frac{1}{2}(\nu - \lambda).$$

Then $u_1$ and $u_2$ are linearly independent. Let $\{u_3, u_4, \ldots, u_m\}$ again be a basis for the orthogonal complement of span $\{\nu, \lambda\}$. Then $P \equiv \sum_{j=1}^m u_j u_j^T$ is
positive definite such that
\[ \nu \cdot (P\lambda) = \nu^T \left( \sum_{j=1}^{m} u_j u_j^T \right) \lambda = |\nu|^2 |\lambda|^2 - \frac{1}{4} |\nu|^2 |\lambda|^2 \]
\[ = \frac{3}{4} |\nu|^2 |\lambda|^2 \neq 0. \]
So (3.17) has been established. □

3.3 Finite-Element Discretization

In any finite element computation of eigenvalues for the examples cited in Subsection 3.1 above, we use a family of nested finite-dimensional spaces \( V_h \) to approximate \( V \), such that
\[ V_{h_1} \subseteq V_{h_2} \subset V, \text{ if } h_1 > h_2 > 0. \] (3.19)
The eigenvalue problem \( H\Psi = E\Psi \) is replaced by its weak formulation \( a(\Psi, v) = E\langle \Psi, v \rangle_{L^2} \), for all \( v \in V \). Let \( \{\varphi_{h_j}^{(k)} | 1 \leq k \leq n_j \} \) be a basis for \( V_{h_j} \), for \( j = 1, 2, \ldots \). Then we have the following discretized problem:

“Find \( \Psi_{h_j}(r) = \sum_{k=1}^{n_j} \alpha_{h_j}^{(k)} \varphi_{h_j}^{(k)}(r) \in \mathcal{V}_{h_j} \) and \( E \in \mathbb{R} \) such that
\[ a(\Psi_{h_j}, \varphi_{h_j}^{(\ell)}) = E\langle \Psi_{h_j}, \varphi_{h_j}^{(\ell)} \rangle, \quad \forall \ell = 1, 2, \ldots, n_j. \]” (3.20)
The above then becomes a matrix eigenvalue problem
\[ (M_{h_j}^{(1)} - EM_{h_j}^{(2)})\alpha_{h_j} = 0, \] (3.21)
where \( M_{h_j}^{(1)} \) and \( M_{h_j}^{(2)} \) are \( n_j \times n_j \) matrices, with respective \( (p, q) \) entries
\[ M_{h_j}^{(1)}(p, q) = a(\varphi_{h_j}^{(p)}, \varphi_{h_j}^{(q)}), \quad M_{h_j}^{(2)}(p, q) = \langle \varphi_{h_j}^{(p)}, \varphi_{h_j}^{(q)} \rangle_{L^2(\mathbb{R}^N)}, \quad 1 \leq p, q \leq n_j, \] (3.22)
and
\[ \alpha_{h_j} = [\alpha_{h_j}^{(1)}, \alpha_{h_j}^{(2)}, \ldots, \alpha_{h_j}^{(n_j)}]^T \in \mathbb{R}^{n_j}, \text{ ("T": transpose).} \] (3.23)
Since the matrix $M_{h_j}^{(2)}$ is invertible, (3.21) can be converted to a standard matrix eigenvalue problem

$$[(M_{h_j}^{(2)})^{-1}M_{h_j}^{(1)} - E_{n_j}]\alpha_{h_j} = 0, \quad (I_{n_j}: \text{the } n_j \times n_j \text{ identity matrix}). \quad (3.24)$$

From (3.24) we obtain $n_j$ eigenvalues $E_{h_j}^{(k)}$, $1 \leq k \leq n_j$, satisfying

$$\det[(M_{h_j}^{(2)})^{-1}M_{h_j}^{(1)} - E_{h_j}^{(k)}I_{n_j}] = 0, \quad \text{("det": the determinant).} \quad (3.25)$$

Each eigenvector $\alpha_{h_j}$ is unique up to a constant factor, which can be determined by the normalization condition

$$\alpha_{h_j}^T M_{h_j}^{(2)} \alpha_{h_j} = 1. \quad (3.26)$$

Note that the ground state $\Psi_1$, the eigenstate corresponding to the smallest eigenvalue $E_1$, satisfies

$$E_1 = \langle H\Psi_1, \Psi_1 \rangle_{L^2} = \min_{\|\Psi\|_{L^2}=1} a(\Psi, \Psi). \quad (3.27)$$

Therefore, if we denote the smallest eigenvalue computed by (3.26) as $E_{h_j,1}$, we have

$$E_{h_j,1} \geq E_1. \quad (3.28)$$

Let the distinct eigenvalues of $H$ be arranged as

$$E_1 < E_2 < E_3 < \cdots < E_j < \cdots$$

such that the eigen-manifold of each $E_j$ is denoted as $W_j$, i.e., $\psi \in W_j$ satisfies

$$H\psi = E_j\psi$$

in the sense of distributions. Then the minimax principle holds:

$$E_{j+1} = \min_{\|\psi\|_{L^2}=1, \Psi \perp W_{k}, k=1,2,\ldots,j} a(\psi, \psi). \quad (3.29)$$
3.4 A Projection Method for Extrapolation

The vector $\hat{x}$ defined for the various examples in (3.4)–(3.12) can be obtained from the bilinear form $a$, with components such as $x_1 = a_K(\Psi, \Psi)$, $x_2 = a_P(\Psi, \Psi)$ in (3.4), for example, for each eigenvalue $E$ corresponding to the eigenstate $\Psi$. Through the finite element calculations given in Subsection 3.3, one obtains a sequence of approximate vectors $\hat{x}_{h_j}$, for $j = 1, 2, \ldots$ to $\hat{x}$. Since $\mathcal{V}_{h_\ell}$ constitutes a better approximation for $\mathcal{V}$ than $\mathcal{V}_{h_k}$ if $h_\ell < h_k$, we see that, in principle, $\hat{x}_{h_\ell}$ should also constitute a better approximation to $\hat{x}$ than $\hat{x}_{h_k}$ does, otherwise the validity of numerical consistency and convergence of $\mathcal{V}_h$ to $\mathcal{V}$ is put into question. Thus, it is reasonable to assume that

$$|x_\ell - \hat{x}| \leq |x_k - \hat{x}|, \quad \text{if } \ell > k,$$

(3.30)

where for brevity, we write $x_j$ for $\hat{x}_{h_j}$ for $j = k$ and $\ell$ in (3.30).

A cherished wish of a numerical analyst is to have $x_\ell$’s such that $|x_\ell - \hat{x}|$ can be made as small as possible by taking $\ell$ as large as possible so as to obtain the computed eigenvalues $E_{h_\ell}^{(k)}$ from

$$E_{h_\ell}^{(k)} = \lambda \cdot x_\ell$$

(3.31)

as accurately as possible, where $E_{h_\ell}^{(k)}$ (satisfying (3.25)) (is the computed eigenvalue that) corresponds to the computed eigenstate $\Psi_{h_\ell}$. As $\ell$ becomes larger and larger, however, the dimensionality of $\mathcal{V}_{h_\ell}$ increases rapidly, eventually overwhelming the available memory of the computer. Therefore, $\ell$ cannot increase indefinitely; it stops at some $L$. At this point, if we still wish to improve the accuracy, of $E$, e.g., then we can extrapolate, by utilizing the theory in the subsequent parts of the section.

First, we note that the accuracy of $x_\ell$ can always be improved by making a projection.

**Theorem 3.2** (Projection by using the virial equation). Let $\tilde{x}, \hat{x} \in \mathbb{R}^m$ be such that

$$\nu \cdot \tilde{x} = 0 \quad \text{for a given} \quad \nu \in \mathbb{R}^m, \ |\nu| = 1.$$  

(3.32)
Define
\[ \tilde{x}_E = \tilde{x} - (\nu \cdot \tilde{x}) \nu, \quad (\text{subscript } E \text{ signifies “extrapolation”).} \tag{3.33} \]

Then
\[ |\tilde{x}_E - \hat{x}| \leq |\tilde{x} - \hat{x}|, \tag{3.34} \]
and
\[ |\tilde{x}_E - \hat{x}| < |\tilde{x} - \hat{x}|, \quad \text{if and only if } \nu \cdot \tilde{x} \neq 0. \tag{3.35} \]

Proof. We have
\[
|\tilde{x} - \hat{x}|^2 = \left| \{ [\tilde{x} - (\nu \cdot \tilde{x}) \nu] - \hat{x} \} + (\nu \cdot \tilde{x}) \nu \right|^2
= |\tilde{x}_E - \hat{x}|^2 + (\nu \cdot \tilde{x})^2,
\]
by an application of the Pythagorean theorem, because \( \nu \cdot \hat{x} = 0 \). So (3.34) and (3.35) follow. \( \square \)

In other words, what we did in Theorem 3.2 is to construct an \( \tilde{x}_E \) that satisfies the virial equation \( \nu \cdot \tilde{x}_E = 0 \). In general, \( \tilde{x} \) per se, as obtained from numerical computations by whatever convergent methods, does not satisfy the virial equation \( \nu \cdot \tilde{x} = 0 \). Therefore, there is a strict improvement of accuracy as indicated by (3.35). On the other hand, if \( \tilde{x} \) itself satisfies the virial equation, then \( \tilde{x}_E = \tilde{x} \) and no improvement of accuracy occurs.

Corollary 3.3. If \( \mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_L, \hat{\mathbf{x}} \in \mathbb{R}^m \) satisfy
\[ |\mathbf{x}_{j+1} - \hat{\mathbf{x}}| < |\mathbf{x}_j - \hat{\mathbf{x}}|, \quad j = 1, 2, \ldots, L - 1, \tag{3.36} \]
then \( \mathbf{x}_{L+1} \equiv (\mathbf{x}_L)_E \) given by (3.33) satisfies
\[ |\mathbf{x}_{L+1} - \hat{\mathbf{x}}| < |\mathbf{x}_j - \hat{\mathbf{x}}|, \quad j = 1, 2, \ldots, L, \text{ if } \nu \cdot \mathbf{x}_L \neq 0. \quad \square \]

The improved accuracy of \( \mathbf{x}_{L+1} \) for \( \hat{\mathbf{x}} \) is of strong interest in its own right, as the various components of the vector \( \hat{\mathbf{x}} \) are of physical interest such as the kinetic energy, moments, etc. Nevertheless, we also need to ask if the improved accuracy of \( \mathbf{x}_{L+1} \) also helps the accuracy for the corresponding eigenvalue \( E \) through (3.31). This is answered in the following.
**Theorem 3.4** (Accuracy of eigenvalues). Let \( \tilde{x}_E, \tilde{x}, \hat{x}, \nu, \lambda \in \mathbb{R}^m \) be as given in Theorem 3.2. Let the respective corresponding eigenvalues be

\[
\tilde{E} \equiv \lambda \cdot \tilde{x}, \quad \tilde{E}_E \equiv \lambda \cdot \tilde{x}_E \quad \text{and} \quad E = \lambda \cdot \hat{x},
\]

where \( E \) corresponds to the “exact eigenvalue.” If

\[
(\lambda \cdot \nu)(\nu \cdot \tilde{x})(\tilde{E} - E) > 0 \quad \text{and} \quad |(\nu \cdot \tilde{x})(\lambda \cdot \nu)| < |\tilde{E} - E|,
\]

then

\[
|\tilde{E}_E - E| < |\tilde{E} - E|,
\]

thus, there is an improvement of computed accuracy for the eigenvalue \( E \) by \( \tilde{E}_E \).

**Proof.** From (3.33) we have

\[
\lambda \cdot (\tilde{x}_E - \tilde{x}) = \lambda \cdot [(\tilde{x} - \hat{x}) - (\nu \cdot \tilde{x})\nu],
\]

i.e.,

\[
\tilde{E}_E - E = [\tilde{E} - E] - [(\nu \cdot \tilde{x})(\lambda \cdot \nu)].
\]

Thus

\[
|\tilde{E}_E - E| < |\tilde{E} - E|
\]

if the two brackets in (3.39) are of the same sign, and \( |(\nu \cdot \tilde{x})(\lambda \cdot \nu)| < |\tilde{E} - E| \).

\[\Box\]

**Remark 2.** In (3.38), the vectors \( \lambda \) and \( \nu \) are known, and the vector \( \tilde{x} \) is obtained through calculations and so \( \tilde{E} \) is also known. But \( E \), the exact eigenvalue, is generally unknown. Therefore, the two conditions in (3.37) cannot be tested in general. It turns out that from concrete numerical data in Tables 1, 2 and 3 in Subsection 4.1, (3.38) often fails, implying that the improved \( \tilde{x}_E \) for \( \tilde{x} \) does not necessarily offer improved accuracy of \( \tilde{E}_E \) for \( E \), in view of the general variational nature that eigenvalues are being approximated from the above because \( \mathcal{V}_h \subseteq \mathcal{V} \). For if \( (\nu \cdot \tilde{x})(\lambda \cdot \nu) < 0 \) in (3.39), then \( \tilde{E}_E > \tilde{E} > E \), causing \( \tilde{E}_E \) to lose accuracy.

\[\Box\]
Remark 3. When \( \lambda \cdot \nu = 0 \), then Theorem 3.4 indicates that \( \tilde{E}_\xi = \tilde{E} \), so there is no improvement of accuracy for the computed eigenvalue \( \tilde{E} \) based on the extrapolation scheme here (even though \( \tilde{E}_\xi \) itself offers improvement of accuracy over that of \( \tilde{x} \)).

The case when \( \lambda \cdot \nu = 0 \) happens for the standard harmonic oscillator (2.41), as we have
\[
\lambda = (1, 1), \quad \nu = \frac{1}{\sqrt{2}}(-1, 1),
\]
and for its PDE version
\[
-\frac{\hbar^2}{2m} \nabla^2 \Psi + \frac{1}{2}(m_1 \omega_1^2 x_1^2 + m_2 \omega_2^2 x_2^2 + m_3 \omega_3^2 x_3^2) \Psi = E \Psi, \quad \text{on } \mathbb{R}^3. \quad \square
\]

**Corollary 3.5.** In Theorem 3.4, if \( \lambda \cdot \nu = 0 \) and \( \nu \cdot \tilde{x} \neq 0 \), then
\[
|\xi - \tilde{\xi}| < |\tilde{x} - \hat{\xi}| \quad \text{and} \quad E_\xi = \tilde{E},
\]
i.e., the accuracy of \( \tilde{\xi} \) improves over that of \( \tilde{x} \) while \( E_\xi \) maintains the same accuracy as \( \tilde{E} \)'s. \( \square \)

**Example 3.7.** Here is an application of Corollary 3.5. Consider the case of the hydrogen atom discussed in Examples 2.2, 3.1 and 3.2. Note that the ground state \( \Psi_1 \) as given by (2.32) corresponds to the eigenvalue \(-1/2\). Then from Examples 3.1 and 3.2, we know that
\[
E = -0.5, \quad KE = 0.5, \quad PE = -1, \quad \nu = \frac{1}{\sqrt{5}}(2, 1), \quad \lambda = (1, 1), \quad \hat{x} = \begin{bmatrix} 0.5 \\ -1.0 \end{bmatrix}.
\]
Consider in a numerical computation, some kind of fluke happens such that one obtains (computed values) for the ground state:
\[
\tilde{E} = -0.5, \quad \tilde{KE} = 0.2, \quad \tilde{PE} = -0.7, \quad (\tilde{E} = 0.2 + (-0.7) = -0.5 = E),
\]
i.e., the computed eigenvalue \( \tilde{E} \) is exact, while \( \tilde{KE} \) and \( \tilde{PE} \) have gross inaccuracy. Then Corollary 3.5 can help us obtain the correct \( KE \) and \( PE \) by using Proposition 3.1.
Choose a positive definite matrix $P$:

$$P = \begin{bmatrix} 2 & -3 \\ -3 & 5 \end{bmatrix}.$$ 

Then $P$ satisfies (3.16): $\nu \cdot P\lambda = 0$. Also, $P$ has a square root $P^{1/2} = \begin{bmatrix} 1 & -1 \\ -1 & 2 \end{bmatrix} \equiv A^{-1}$, where $A = \begin{bmatrix} 2 & 1 \\ 1 & 1 \end{bmatrix} = A^T$.

Here

$$\tilde{x} = \begin{bmatrix} \tilde{KE} \\ \tilde{PE} \end{bmatrix} = \begin{bmatrix} 0.2 \\ -0.7 \end{bmatrix}.$$ 

Define $\tilde{x}' = A\tilde{x}$, $\tilde{x}' = A\tilde{x}$, $\nu' = A^{-1}\nu / |A^{-1}\nu|$, $\lambda' = A^{-1}\lambda$, according to (3.14). Then $\nu' \cdot \lambda' = 0$, and Corollary 3.5 is applicable, with $\tilde{x}_\epsilon$ and $\tilde{x}$ therein being replaced by $\tilde{x}'_\epsilon$ and $\tilde{x}'$. We have

$$\tilde{x}'_\epsilon = \tilde{x}' - (\tilde{x}' \cdot \nu')\nu' = \tilde{x}' - (\tilde{x} \cdot \nu) \frac{\nu'}{|A^{-1}\nu|} = \begin{bmatrix} -0.3 \\ -0.5 \end{bmatrix} - \left( \begin{bmatrix} -0.3 \\ -0.5 \end{bmatrix} \cdot \begin{bmatrix} 1 \\ 0 \end{bmatrix} \right) \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ -0.5 \end{bmatrix}.$$ 

By transforming $\tilde{x}'_\epsilon$ back:

$$\tilde{x}_\epsilon \equiv A^{-1}\tilde{x}'_\epsilon = \begin{bmatrix} 1 & -1 \\ -1 & 2 \end{bmatrix} \begin{bmatrix} 0 \\ 0.5 \end{bmatrix} = \begin{bmatrix} 0.5 \\ -1.0 \end{bmatrix} = \begin{bmatrix} KE \\ PE \end{bmatrix},$$

we obtain the exact $KE$ and $PE$.

In contrast, had we applied Theorem 3.2 directly instead, then we would obtain

$$\tilde{x}_\epsilon = \begin{bmatrix} 0.32 \\ -0.64 \end{bmatrix} \text{ and } \tilde{E}_\epsilon = -0.32$$

and we see that $\tilde{E}_\epsilon$ (versus the exact $E = -0.50$) loses an accuracy of 36%, even though this $\tilde{x}_\epsilon$ satisfies the virial equation $\tilde{x}_\epsilon \cdot \nu = 0$.  

□
Example 3.8. The preceding Example 3.7 gives an extreme case that in a fictitious computation, the computed numerical data of $KE_h$ and $PE_h$ are terribly wrong, and still the resulting eigenvalue $E_h = KE_h + PE_h$ is exact. Here is yet another extreme example: in an (again fictitious) computation, the numerical data of $KE_h$ and $PE_h$ satisfies the virial equation, but the resulting eigenvalue $E_h = KE_h + PE_h$ is terribly wrong.

We return to Example 3.7. Suppose in the calculation of the ground state $\Psi_1$ of the hydrogen atom, we have obtained

$$\tilde{KE} = 0.9, \quad \tilde{PE} = -1.8.$$ 

Thus

$$\tilde{E} = \tilde{KE} + \tilde{PE} = -0.9.$$ 

We see that the virial equation

$$\frac{\tilde{PE}}{\tilde{KE}} = -2$$

is satisfied exactly, but the eigenvalue $E_h = -0.9$ differs from the exact $E = -0.5$ by an 80% error.

In this case, the extrapolation schemes in this paper cannot help at all due to their very nature.

However, in practical computations, extreme situations such as those in Example 3.7 and here almost never happen. Thus, our extrapolation schemes may help.

3.5 The Case of the Morse Potential

Examples 2.7 and 2.8 in Subsection 2.2 cannot be cast into a finite-dimensional setting such that the theorems in Subsection 3.3 becomes applicable. Nevertheless, the special character of the Morse potential $V_M(\cdot)$ in (2.53) of Example 2.7 has a pleasant exponential decay property that can help us establish an extrapolation by projection method in an infinite-dimensional Hilbert space based on this additional summability condition of $V_M(\cdot)$. 

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Consider (2.52)–(2.54). Define the Hilbert space
\[ \mathcal{H} \equiv \mathbb{R} \times L^2(\mathbb{R}^3), \] (3.40)
with the usual direct sum inner product
\[ \langle (r_1, f_1), (r_2, f_2) \rangle_{\mathcal{H}} = r_1 r_2 + \int_{\mathbb{R}^3} f_1 f_2 \, dr, \quad \text{for} \quad (r_j, f_j) \in \mathcal{H}, j = 1, 2. \] (3.41)
Assume that (2.52) has an eigenfunction \( \Psi(\cdot) \) such that
\[ \| \Psi \|_{L^2(\mathbb{R}^3)} = 1. \] (3.42)
Then it is easy to verify that \( \Psi \in H^2(\mathbb{R}^3) \). By the Sobolev imbedding theorem [1, Theorem 5.4, p. 97], we have \( \Psi \in L^4(\mathbb{R}^3) \) and
\[ \| \Psi \|_{L^4(\mathbb{R}^3)} \leq C \| \Psi \|_{H^1(\mathbb{R}^3)}. \] (3.43)
Define
\[ \hat{X} = (KE, |\Psi(\cdot)|^2), \quad \nu = c_\nu (1, \alpha Dr(e^{-2\alpha r} - e^{-\alpha r})), \] (3.44)
where \( c_\nu > 0 \) is a normalization constant such that \( \| \nu \|^2_{\mathcal{H}} = 1 \). Then \( \hat{X}, \nu \in \mathcal{H} \), and (2.54)2 can be written as
\[ \langle \nu, \hat{X} \rangle_{\mathcal{H}} = 0. \] (3.45)

**Theorem 3.6.** Given \( X_h = (r_h, |\Psi_h(\cdot)|^2) \in \mathcal{H} \), define \( X_h \)'s “extrapolation” by
\[ X_{h,\mathcal{E}} = X_h - \langle X_h, \nu \rangle_{\mathcal{H}} \nu. \] (3.46)
Then
\[ \| X_{h,\mathcal{E}} - \hat{X} \|_{\mathcal{H}} \leq \| X_h - \hat{X} \|_{\mathcal{H}}. \] (3.47)
Furthermore,
\[ \| X_{h,\mathcal{E}} - \hat{X} \|_{\mathcal{H}} < \| X_h - \hat{x} \|_{\mathcal{H}} \quad \text{if and only if} \quad \langle X_h, \nu \rangle_{\mathcal{H}} \neq 0. \] (3.48)

**Proof.** Same as that for Theorem 3.2. \[ \square \]
The eigenvalue $E$ corresponding to the eigenstate $\Psi(\cdot)$ satisfying (2.52) can be written as
\[
E = \langle \lambda, \hat{X} \rangle_{\mathcal{H}},
\] (3.49)
where
\[
\lambda \equiv (1, D(e^{-2\alpha \hat{r}} - 2e^{-\alpha \hat{r}})) \in \mathcal{H}.
\] (3.50)
Does the extrapolation $X_{h,E}$ of $X_h$ offer a more accurate approximation to the eigenvalue $E$ than $X_h$ does? This is answered in the following.

**Theorem 3.7.** Let $\nu$ and $\lambda$ be as given in (3.44) and (3.50). Also, let $X_h, X_{h,E}$ and $\hat{X}$ be as given in Theorem 3.6. Define
\[
E_h = \langle \lambda, X_h \rangle, \quad \tilde{E}_h = \langle \lambda, \tilde{X}_h \rangle.
\]
Then for $E$ given by (3.49),
\[
|\tilde{E}_h - E| < |E_h - E|
\]
if
\[
\langle \lambda, \nu \rangle \cdot \langle \nu, X_h \rangle \cdot (E_h - E) > 0, \quad \text{and} \quad |\langle \lambda, \nu \rangle \cdot \langle \nu, X_h \rangle| < |E_h - E|.
\]

**Proof.** Same as that for Theorem 3.4. \qed

The study on the Morse potential in this subsection has utilized the property that $\Psi \in L^4(\mathbb{R}^3)$. The space $L^4(\mathbb{R}^3)$ itself is not an inner product space, but all we need is the $L^4$-summability and nothing else from $L^4(\mathbb{R}^3)$. It seems quite viable to reformulate the virial equation (2.54) into different settings than (3.44) and (3.45), without having to use $L^4(\mathbb{R}^3)$ or other types of non-inner product spaces. This work will be presented elsewhere.

So far, we have covered all the Examples in Subsection 2.2 except Example 2.8, the logarithmic potential case. This case has a virial equation (2.57) not resembling any other cases treated so far in this section. It is not totally clear if simply by setting
\[
K E = \gamma^2/2, \quad \text{cf. (2.57)},
\]
is all we need to do.
3.6 Linear Extrapolation by Two Successive Approximate Solutions using the Virial Equation

Examples 3.7, 3.8 and Corollary 3.5 pretty much tell us the story of the limitation of extrapolation by using the virial equation with a single data point \( \tilde{x} \): we can improve the accuracy of \( \tilde{x} \), but can at best preserve (i.e., not improve) the accuracy of \( \tilde{E} \). By using the virial equation, we propose a two-point linear extrapolation scheme to improve the accuracy of \( \tilde{E} \).

Let \((\hat{x}, E)\) be the exact data for the eigenvalue problem in \( \mathbb{R}^N \) in the finite-dimensional framework of Subsection 3.1 with \( \nu, \lambda \in \mathbb{R}^m \), where \( E = \lambda \cdot \hat{x}, \nu \cdot \hat{x} = 0 \) (the virial equation) and \( |\nu| = 1 \). Assume \( \nu \cdot \lambda > 0 \), which is always guaranteed by Proposition 3.1, after a suitable transformation.

Let \( n \) be a given positive integer. Let \((x_n, E_n)\) and \((x_{n+1}, E_{n+1})\) be two successive numerical approximations of \((\hat{x}, E)\) with mesh size \( h_n \) and \( h_{n+1} \), where \( E_n = \lambda \cdot x_n \) and \( E_{n+1} = \lambda \cdot x_{n+1} \). Note that the notations \( E_1, E_2, \cdots, E_n \) used here are not to be confused with those discussed earlier in (3.27)-(3.29).

We wish to obtain a better numerical approximation \((x_{n+1}, E_{n+1})\) of \((\hat{x}, E)\) from the given two numerical data by utilizing the virial equation. We make the following assumptions on \((x_n, E_n)\) and \((x_{n+1}, E_{n+1})\):

\[
\nu \cdot x_n \neq 0 \quad \text{and} \quad \nu \cdot x_{n+1} \neq 0; \quad (3.51)
\]

\[
\frac{|\nu \cdot x_{n+1}|}{|\nu \cdot x_n|} < \frac{h_{n+1}}{h_n} < 1; \quad (3.52)
\]

\[
E_n > E_{n+1}. \quad (3.53)
\]

Remark 4. (i) Condition (3.51) is the starting point where the virial equation can be used to help improve the accuracy of \( E_{n+1} \).

(ii) Condition on mesh sizes \( h_n \) and \( h_{n+1} \) in (3.52) is a natural requirement for the finite element approximation. We wish to pointed out that both \( h_n \) and \( h_{n+1} \) are not necessarily required for the two-point linear extrapolation scheme to be proposed below.
(iii) Condition (3.53) is motivated by the finite-element approximation that for the ground state, e.g., 

\[
E = \inf_{\|\psi\|_{L^2} = 1} a(\psi, \psi) < E_{n+1} \equiv \inf_{\|\psi\|_{L^2} = 1} a(\psi, \psi)
\]

\[
< E_n \equiv \inf_{\|\psi\|_{L^2} = 1} a(\psi, \psi),
\]

where

\[H^1(\mathbb{R}^N) \supset V_{n+1} \supset V_n,\]

in view of Subsection 3.3.

Let \(\lambda^\perp \in \mathbb{R}^m\) be a unit vector orthogonal to \(\lambda\) such that \(\lambda^\perp \cdot \nu > 0\). Note that the choice of \(\lambda^\perp\) is unique when \(m = 2\). If \(m > 2\), then the choice of \(\lambda^\perp\) is not unique. But this poses no problem in any way. We propose the following two-point linear extrapolation scheme.

(a) If \(\nu \cdot x_n\) and \(\nu \cdot x_{n+1}\) are of same signs, then

\[
\begin{aligned}
x_\varepsilon &\equiv x_{n+1} - \frac{\nu \cdot x_{n+1}}{\nu \cdot x_{n+1} - \nu \cdot x_n} (x_{n+1} - x_n), \\
E_{n+1,\varepsilon} &\equiv \lambda \cdot x_\varepsilon;
\end{aligned}
\]

(b) If \(\nu \cdot x_n\) and \(\nu \cdot x_{n+1}\) are of different signs, then

\[
\begin{aligned}
\tilde{x}_n &\equiv x_n - 2 \frac{\nu \cdot x_n}{\lambda^\perp \cdot \nu} \lambda^\perp, \\
\tilde{x}_\varepsilon &\equiv x_{n+1} - \frac{\nu \cdot x_{n+1}}{\nu \cdot x_{n+1} - \nu \cdot \tilde{x}_n} (x_{n+1} - \tilde{x}_n), \\
\tilde{E}_{n+1,\varepsilon} &\equiv \lambda \cdot \tilde{x}_\varepsilon.
\end{aligned}
\]

We consider first the two-point linear extrapolation scheme (3.54)–(3.55) for the case that \(\nu \cdot x_n\) and \(\nu \cdot x_{n+1}\) are of same signs. Note that (3.54) is derived from the linear extrapolation

\[
X(h) = x_{n+1} + \frac{h - h_{n+1}}{h_{n+1} - h_n} (x_{n+1} - x_n)
\]

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with
\[ h \equiv \tilde{h}_{n+1} = \frac{(\nu \cdot x_{n+1})h_n - (\nu \cdot x_n)h_{n+1}}{\nu \cdot x_{n+1} - \nu \cdot x_n}. \] (3.60)

**Lemma 3.8.** Assume that \( \nu \cdot x_n \) and \( \nu \cdot x_{n+1} \) are of same signs, and (3.51)–(3.53) hold. Then

(i) \( X(h_n) = x_n, \ X(h_{n+1}) = x_{n+1}, \ x_\varepsilon = X(\tilde{h}_{n+1}) = \text{RHS of } (3.54) \),

(ii) \( 0 < \tilde{h}_{n+1} < h_{n+1} \),

(iii) \( \nu \cdot x_\varepsilon = 0 \),

(iv) \( E_{n+1,\varepsilon} \equiv \lambda \cdot x_\varepsilon \) satisfies \( E_{n+1,\varepsilon} < E_{n+1} \).

**Proof.** The verification of (i) is straightforward.

Consider the case that both \( \nu \cdot x_n \) and \( \nu \cdot x_{n+1} \) are positive. By (3.52), we have
\[ \frac{\nu \cdot x_{n+1}}{\nu \cdot x_n} < \frac{h_{n+1}}{h_n} < 1, \] (3.61)
\[ (\nu \cdot x_{n+1})h_n - (\nu \cdot x_n)h_{n+1} < 0. \] (3.62)

(3.61) also gives
\[ 0 < \nu \cdot x_{n+1} < \nu \cdot x_n. \] (3.63)

From (3.62) and (3.63), we obtain \( \tilde{h}_{n+1} > 0 \), and
\[ \tilde{h}_{n+1} = h_{n+1} + \frac{(\nu \cdot x_{n+1})(h_n - h_{n+1})}{\nu \cdot x_{n+1} - \nu \cdot x_n} < h_{n+1}. \] (3.64)

Thus, (ii) has been established when \( \nu \cdot x_n \) and \( \nu \cdot x_{n+1} \) are both positive. The case when \( \nu \cdot x_n \) and \( \nu \cdot x_{n+1} \) are both negative can be similarly established.

The verification of (iii) is straightforward from (3.54).

Finally, it follows from (3.59) and (3.60) that
\[ E_{n+1,\varepsilon} = \lambda \cdot x_\varepsilon = E_{n+1} + \frac{\tilde{h}_{n+1} - h_{n+1}}{h_{n+1} - h_n}(E_{n+1} - E_n) < E_{n+1} \] by (3.64) and (3.53).

So (iv) is proved. \( \Box \)
To answer the question whether $E_{n+1,\varepsilon}$ improves the accuracy of $E_{n+1}$, we replace assumption (3.53) by the condition
\[ E_n > E_{n+1} > E, \] (3.65)
which is a natural condition as explained in (iii) of Remark 4. We need also the following assumption
\[ \frac{E_n - E_{n+1}}{|\nu \cdot x_n| - |\nu \cdot x_{n+1}|} < \frac{2|E_{n+1} - E|}{|\nu \cdot x_{n+1}|}. \] (3.66)

**Theorem 3.9.** Let $\nu \cdot x_n$ and $\nu \cdot x_{n+1}$ be of same signs, and (3.51)–(3.53) hold. Assume (3.65) is true. Then $E_{n+1,\varepsilon}$ improves the accuracy of $E_{n+1}$, that is,
\[ |E_{n+1,\varepsilon} - E| < |E_{n+1} - E|, \] (3.67)
if and only if condition (3.66) holds.

**Proof.** Let $\nu \cdot x_n$ and $\nu \cdot x_{n+1}$ be of same signs. It follows from (3.54) that
\[ E_{n+1,\varepsilon} = E_{n+1} - \frac{\nu \cdot x_{n+1}}{\nu \cdot x_n - \nu \cdot x_{n+1}}(E_n - E_{n+1}). \] (3.68)

By condition (3.52), we have either $\nu \cdot x_n > \nu \cdot x_{n+1}$ if both $\nu \cdot x_n$ and $\nu \cdot x_{n+1}$ are positive, or $\nu \cdot x_n < \nu \cdot x_{n+1}$ if both $\nu \cdot x_n$ and $\nu \cdot x_{n+1}$ are negative. Thus it is always true that
\[ \frac{\nu \cdot x_{n+1}}{\nu \cdot x_n - \nu \cdot x_{n+1}} = \frac{|\nu \cdot x_{n+1}|}{|\nu \cdot x_n| - |\nu \cdot x_{n+1}|} > 0. \]

Then
\[ E_{n+1,\varepsilon} = E_{n+1} - \frac{|\nu \cdot x_{n+1}|}{|\nu \cdot x_n| - |\nu \cdot x_{n+1}|}(E_n - E_{n+1}). \] (3.69)

By condition (3.53), we have
\[ E_{n+1,\varepsilon} - E < E_{n+1} - E. \] (3.70)

If condition (3.66) holds, then it follows from (3.69) that
\[ E_{n+1,\varepsilon} - E > (E_{n+1} - E) - 2|E_{n+1} - E| = -(E_{n+1} - E). \] (3.71)
From (3.70) and (3.71), we have
\[ |E_{n+1,\xi} - E| < |E_{n+1} - E|, \]
which implies that \( E_{n+1,\xi} \) offers an improvement of accuracy for \( E_{n+1} \).

On the other hand, if condition (3.66) is not true, that is,
\[ \frac{E_n - E_{n+1}}{|\mathbf{v} \cdot x_n| - |\mathbf{v} \cdot x_{n+1}|} \geq \frac{2|E_{n+1} - E|}{|\mathbf{v} \cdot x_{n+1}|}, \]
then it follows from (3.69) that
\[ E_{n+1,\xi} - E \leq E_{n+1} - E - 2|E_{n+1} - E| = -(E_{n+1} - E) < 0. \]
Hence
\[ |E_{n+1,\xi} - E| \geq |E_{n+1} - E|, \]
which implies \( E_{n+1,\xi} \) does not offer an improvement of accuracy for \( E_{n+1} \). 

Next, we consider the two-point linear extrapolation scheme (3.56)-(3.58) for the case that \( \mathbf{v} \cdot x_n \) and \( \mathbf{v} \cdot x_{n+1} \) are of different signs. Note that \( \tilde{x}_n \) in (3.56) is the geometrical reflection of \( x_n \) along the direction of \( \lambda^\perp \) with respect to the hyperplane \( \mathbf{v} \cdot x = 0 \). It is straightforward to verify that
\[ \mathbf{v} \cdot \tilde{x}_n = -\mathbf{v} \cdot x_n \quad \text{and} \quad \tilde{E}_n = \lambda \cdot \tilde{x}_n = \lambda \cdot x_n = E_n. \] (3.72)
Note now that \( \mathbf{v} \cdot \tilde{x}_n \) and \( \mathbf{v} \cdot x_{n+1} \) are of the same sign.

**Theorem 3.10.** Let \( \mathbf{v} \cdot x_n \) and \( \mathbf{v} \cdot x_{n+1} \) be of different signs, and (3.51)-(3.53) hold. Let (3.56)-(3.58) be prescribed. Then
\[ \tilde{E}_{n+1,\xi} < E_{n+1} < E_n. \] (3.73)
Furthermore, if (3.65) is true, then \( E_{n+1,\xi} \) improves the accuracy of \( E_{n+1} \), that is,
\[ |E_{n+1,\xi} - E| < |E_{n+1} - E|, \] (3.74)
if and only if condition (3.66) holds.
Proof. By (3.72), conditions (3.51)–(3.53) and (3.65)–(3.66) remain if $\mathbf{x}_n$ is replaced by $\tilde{\mathbf{x}}_n$ and $E_n$ is replaced by $\tilde{E}_n$. Thus (3.73) and (3.74) follow from the direct application of Lemma 3.8 and Theorem 3.9.

Remark 5. As indicated in Theorems 3.9 and 3.10, condition (3.66) plays a key role in improving the accuracy of $(\mathbf{x}_{n+1}, E_{n+1})$. However, the verification of this condition requires the knowledge of the exact eigenvalue $E$, which is unknown and to be computed in most applications. In the numerical example of hydrogen atom to be presented in the next section, we are able to verify this condition due to our knowledge of energy levels of hydrogen atom. The two-point linear extrapolation scheme proposed here provides an excellent improvement of the accuracy of numerical data.

4 Applications and Numerical Data Analysis

In this section, we present a few concrete examples as illustrations.

4.1 Finite Element Computation of the Hydrogen Atom Model (3D)

We compute eigenfunctions and eigenvalues of equation (2.31). Since it is posed on the entire $\mathbb{R}^3$, we need to first truncate the domain to a ball:

$$\Omega \equiv B(0; R),$$

an open ball centered at the origin with radius $R = 60$.

We choose $\mathcal{V}_h(\Omega)$ to be a space of Lagrangian finite elements of degree two polynomials on $\Omega$. Equation (2.31) contains a weak singularity at $r = 0$, where the quadrature needs some special treatment but is otherwise unproblematic. As we know from atomic physics (cf. (2.32)) that the eigenfunctions decay exponentially away from the origin, finer meshes are chosen near the origin but sparser away from there. See Fig. 1 for an illustration of discretization.
Figure 1: A ball with radius 60 is discretized, where it can be seen that grid points are denser near the origin than elsewhere in order to provide a finer resolution there.

A solution’s cross-sectional profile for the ground state $\Psi$ (corresponding to eigenvalue $-1/2$) is illustrated in Fig. 2.

The spectral data are computed on PC by the MEFISTO software [10], for a certain discretization parameter $h$, with $h = 1, 1/2$ and $1/4$. Only the first 14 computed eigenvalues are tabulated, in Tables 1, 2 and 3. The computation is not viable for $h = 1/8$, as the memory of our PC has been exceeded.

In Tables 1, 2 and 3, $m$ denotes the eigenvalue multiplicity, the listing of various vectors $\nu$, $\lambda$ and $\hat{x}$ here are taken from (3.4)–(3.6). Exact values of the eigenvalues, kinetic and potential energies ($KE$ and $PE$) are listed alongside the computed values for easy comparisons. The rightmost columns in the tables contain the extrapolated eigenvalues obtained by Theorem 3.4. Note that all computed eigenvalues (by (3.31)) listed here approximate the exact eigenvalues from above.
Figure 2: Profile of the ground state $\Psi(x_1, x_2, 0)$ on the plane $x_3 = 0$. This ground state corresponds to eigenvalue $-1/2$ and has rotational symmetry. The "cusp" of $\Psi$ is clearly visible, due to the weak singularity of the coefficient $-1/r$ at $r = 0$. (For the cusp condition, and some other atoms and molecules, see [5].) The profiles of $\Psi(0, x_2, x_3)$ and $\Psi(x_1, 0, x_3)$ look identical.

Table 1. Hydrogen energy levels and computation

\[
h = 1, \text{ the normalized maximum edge length}
\]

<table>
<thead>
<tr>
<th>$m$</th>
<th>$x_h$</th>
<th>$PE_h/KE_h$</th>
<th>$E_{exact}$</th>
<th>$E_h$</th>
<th>$E_{h,E}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>(0.5000, 0.5000)</td>
<td>(0.4785, 0.4669)</td>
<td>-1.97103 (0.4741, -0.4929)</td>
<td>-0.5000</td>
<td>-0.4755</td>
</tr>
<tr>
<td>4</td>
<td>(0.1250, 0.2500)</td>
<td>(0.1145, -0.2367)</td>
<td>-2.06744 (0.1176, -0.2352)</td>
<td>-0.1250</td>
<td>-0.12225 -0.11761</td>
</tr>
<tr>
<td>1</td>
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<td>-0.12225 -0.11761</td>
</tr>
</tbody>
</table>

Length of sphere kernel = 2
Number of edges in a direction of kernel = 2
Number of homothetic layers = 3
Number of vertices = 131
Number of nodes = 481
Number of hexahedra = 104
$\nu = \frac{1}{\sqrt{n}} (2, 1)$, $\lambda = (1, 1)$
$\mathbf{x}_h = (KE_h, PE_h)$, $\mathbf{E} = (KE, PE)$
$\mathbf{x}_{h,E} = \mathbf{x}_h - (\nu \cdot \mathbf{x}_h)\nu$, $E_{h,E} = \lambda \cdot \nu$
Table 2. Hydrogen energy levels and computation

\( h = 1/2 \), division of each edge length by 2

length of the spline kernel=2

Number of edges in a direction of kernel=4

Number of homothetic layers=6

Number of vertices=713

Number of nodes=2753

Number of hexahedra=640

\( \nu = \frac{1}{\sqrt{5}}(2, 1), \; \lambda = (1, 1) \)

\( x_h = (KE_h, PE_h), \; \bar{x} = (KE, PE) \)

\( x_{h,\varepsilon} = x_h - (\nu \cdot x_h)\nu, \; E_{h,\varepsilon} = \lambda \cdot \nu \)

<table>
<thead>
<tr>
<th>m</th>
<th>( \bar{x} )</th>
<th>( x_h )</th>
<th>( PE_h / KE_h )</th>
<th>( x_{h,\varepsilon} )</th>
<th>( E_{exact} )</th>
<th>( E_h )</th>
<th>( E_{h,\varepsilon} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>(0.00000, -1.00000)</td>
<td>(0.500000, -1.00000)</td>
<td>-1.99875</td>
<td>(0.500000, -1.00125)</td>
<td>-0.500000</td>
<td>-0.50026</td>
<td>-0.50063</td>
</tr>
<tr>
<td>4</td>
<td>(0.12500, -0.25000)</td>
<td>(0.124950, -0.24990)</td>
<td>-2.000018</td>
<td>(0.124950, -0.24990)</td>
<td>-0.12500</td>
<td>-0.12496</td>
<td>-0.12495</td>
</tr>
<tr>
<td>9</td>
<td>(0.05556, -0.11111)</td>
<td>(0.05554, -0.11108)</td>
<td>-1.99998</td>
<td>(0.05554, -0.11108)</td>
<td>-0.05556</td>
<td>-0.05554</td>
<td>-0.05554</td>
</tr>
<tr>
<td>9</td>
<td>(0.05556, -0.11111)</td>
<td>(0.05554, -0.11108)</td>
<td>-2.000000</td>
<td>(0.05554, -0.11108)</td>
<td>-0.05556</td>
<td>-0.05554</td>
<td>-0.05554</td>
</tr>
<tr>
<td>9</td>
<td>(0.05556, -0.11111)</td>
<td>(0.05554, -0.11108)</td>
<td>-0.000000</td>
<td>(0.05554, -0.11108)</td>
<td>-0.05556</td>
<td>-0.05554</td>
<td>-0.05554</td>
</tr>
</tbody>
</table>

Table 3. Hydrogen energy levels and computation

\( h = 1/4 \), division of each edge length by 4

length of the sphere kernel=2

Number of edges in a direction of kernel=8

Number of homothetic layers=12

Number of vertices=5361

Number of hexahedra=5120

\( \nu = \frac{1}{\sqrt{5}}(2, 1), \; \lambda = (1, 1) \)

\( x_h = (KE_h, PE_h), \; \bar{x} = (KE, PE) \)

\( x_{h,\varepsilon} = x_h - (\nu \cdot x_h)\nu, \; E_{h,\varepsilon} = \lambda \cdot \nu \)

<table>
<thead>
<tr>
<th>m</th>
<th>( \bar{x} )</th>
<th>( x_h )</th>
<th>( PE_h / KE_h )</th>
<th>( x_{h,\varepsilon} )</th>
<th>( E_{exact} )</th>
<th>( E_h )</th>
<th>( E_{h,\varepsilon} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>(0.00000, -1.00000)</td>
<td>(0.500000, -1.00000)</td>
<td>-1.99875</td>
<td>(0.500000, -1.00125)</td>
<td>-0.500000</td>
<td>-0.50026</td>
<td>-0.50063</td>
</tr>
<tr>
<td>4</td>
<td>(0.12500, -0.25000)</td>
<td>(0.124950, -0.24990)</td>
<td>-2.000018</td>
<td>(0.124950, -0.24990)</td>
<td>-0.12500</td>
<td>-0.12496</td>
<td>-0.12495</td>
</tr>
<tr>
<td>9</td>
<td>(0.05556, -0.11111)</td>
<td>(0.05554, -0.11108)</td>
<td>-1.99998</td>
<td>(0.05554, -0.11108)</td>
<td>-0.05556</td>
<td>-0.05554</td>
<td>-0.05554</td>
</tr>
<tr>
<td>9</td>
<td>(0.05556, -0.11111)</td>
<td>(0.05554, -0.11108)</td>
<td>-2.000000</td>
<td>(0.05554, -0.11108)</td>
<td>-0.05556</td>
<td>-0.05554</td>
<td>-0.05554</td>
</tr>
<tr>
<td>9</td>
<td>(0.05556, -0.11111)</td>
<td>(0.05554, -0.11108)</td>
<td>-0.000000</td>
<td>(0.05554, -0.11108)</td>
<td>-0.05556</td>
<td>-0.05554</td>
<td>-0.05554</td>
</tr>
</tbody>
</table>

In Table 1, except for the first entry on the rightmost column, all the other entries show deterioration of accuracy. In Table 2, all entries in the column corresponding to \( PE_h / KE_h \) are very close to \(-2\), showing improvement over the same column in Table 1. However, all entries on the rightmost column in
Table 2 show again deterioration of accuracy in $E_{h,\varepsilon}$. In Table 3, the entries in the column of $PE_h/KE_h$ show further improvement of accuracy in general. However, $E_{h,\varepsilon}$ shows no improvement over $E_h$ in Table 3.

Tables 1, 2 and 3 indicate that the extrapolation by one-point projection (Subsection 3.4) does not work well.

4.2 Linear Extrapolation of the Hydrogen Atom Spectra by Two Successive Approximate Data

Tables 1, 2 and 3 in Subsection 4.1 show that using Theorems 3.2 and 3.4, the extrapolated eigenvalues $E_{h,\varepsilon}$ usually lose accuracy. In this subsection, we perform the extrapolation based on the two-point extrapolation scheme (3.54)–(3.58), using the pairs $h_1 = 1$, $h_2 = 1/2$ and $h_1 = 1/2$, $h_2 = 1/4$. The outcomes are tabulated in Tables 4 and 5.

As can be seen, the extrapolated eigenvalues $E_{\varepsilon}$ in Table 4 show a favorable improvement of accuracy, while those $E_{\varepsilon}$ values in Table 5 show somewhat mixed outcomes. Nevertheless, sources of deterioration of accuracy of $E$ can all be pinpointed as indicated above for Tables 4 and 5.

Additional reasons are possible. For example,

(i) the accumulation of round-off errors (which has caused, e.g., $E_{h_2} = 0.50026$, for $h = 1/4$, to go below the ground-state energy level $-0.50000$, truly an error);
We use the two-point extrapolation scheme (3.54)–(3.58). Note that the entries given in the rightmost column for $E_x$, except those marked with "$\ast$", show improvement of accuracy over those in the column of $E_{h_2}$. The entries for $E_x$ marked with "$\ddagger$" fail to improve the accuracy of $E_{h_{n+1}}$ due to the violation of condition (3.66). Only two rows, marked with "$\ddagger$", have different signs for $\boldsymbol{v} \cdot \mathbf{x}_{h_1}$ and $\boldsymbol{v} \cdot \mathbf{x}_{h_2}$.

<table>
<thead>
<tr>
<th>$m$</th>
<th>$\mathbf{x}$</th>
<th>$\mathbf{x}_{h_1}$</th>
<th>$\mathbf{x}_{h_2}$</th>
<th>$E_{\text{exact}}$</th>
<th>$E_{h_1}$</th>
<th>$E_{h_2}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1$^\ddagger$</td>
<td>(0.50000, 0.00000)</td>
<td>(0.47854, -0.94600)</td>
<td>(0.49720, -0.99479)</td>
<td>(0.49870, -0.99741)</td>
<td>-0.50000</td>
<td>-0.46755</td>
</tr>
<tr>
<td>4</td>
<td>(0.12500, -0.25000)</td>
<td>(0.11452, -0.23677)</td>
<td>(0.12415, -0.24852)</td>
<td>(0.12443, -0.24886)</td>
<td>-0.12500</td>
<td>-0.12225</td>
</tr>
<tr>
<td>9</td>
<td>(0.5556, -0.11111)</td>
<td>(0.03995, -0.08991)</td>
<td>(0.05501, -0.11021)</td>
<td>(0.05530, -0.11060)</td>
<td>-0.05556</td>
<td>-0.04996</td>
</tr>
<tr>
<td>12</td>
<td>(0.12500, -0.25000)</td>
<td>(0.11452, -0.23677)</td>
<td>(0.12403, -0.24840)</td>
<td>(0.12447, -0.24893)</td>
<td>-0.12500</td>
<td>-0.12225</td>
</tr>
</tbody>
</table>

Again we use the two-point extrapolation scheme (3.54)–(3.58). In the column for $E_x$, those entries marked with "$\ddagger$" have lost accuracy over the corresponding entries for $E_{h_2}$ due to the violations of condition (3.52) or (3.66). Those entries marked with "$\ddagger$" have maintained exactly the same accuracy due to the fact $\boldsymbol{v} \cdot \mathbf{x}_{h_{n+1}} = 0$, a violation of (3.51). Those entries unmarked have shown improvement of accuracy. The columns with the "$\ddagger$" sign have different signs for $\boldsymbol{v} \cdot \mathbf{x}_{h_1}$ and $\boldsymbol{v} \cdot \mathbf{x}_{h_2}$.

<table>
<thead>
<tr>
<th>$m$</th>
<th>$\mathbf{x}$</th>
<th>$\mathbf{x}_{h_1}$</th>
<th>$\mathbf{x}_{h_2}$</th>
<th>$E_{\text{exact}}$</th>
<th>$E_{h_1}$</th>
<th>$E_{h_2}$</th>
<th>$E_{x}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1$^\ddagger$</td>
<td>(0.50000, 0.00000)</td>
<td>(0.47920, -0.99479)</td>
<td>(0.50808, -1.00113)</td>
<td>(0.49863, -0.99727)</td>
<td>-0.50000</td>
<td>-0.49759</td>
<td>-0.49863$^*$</td>
</tr>
<tr>
<td>4</td>
<td>(0.12500, -0.25000)</td>
<td>(0.12415, -0.24852)</td>
<td>(0.12494, -0.24890)</td>
<td>(0.12503, -0.25006)</td>
<td>-0.12500</td>
<td>-0.12437</td>
<td>-0.12496</td>
</tr>
<tr>
<td>9</td>
<td>(0.5556, -0.11111)</td>
<td>(0.05501, -0.11021)</td>
<td>(0.05554, -0.11108)</td>
<td>(0.05554, -0.11108)</td>
<td>-0.05556</td>
<td>-0.05554</td>
<td>-0.05554$^\dagger$</td>
</tr>
<tr>
<td>12</td>
<td>(0.12500, -0.25000)</td>
<td>(0.12403, -0.24840)</td>
<td>(0.12442, -0.24890)</td>
<td>(0.12509, -0.25019)</td>
<td>-0.12500</td>
<td>-0.12437</td>
<td>-0.12496</td>
</tr>
</tbody>
</table>

(ii) the effect of the truncation of the domain;
(iii) distribution pattern of the density of meshes.

These require further investigation. However, we feel that extrapolation by the virial theorem seems to bring more benefits when the directly computed data are farther from the exact solutions, such as Table 4. When the directly computed data are already very close the exact data, such as those in Table 5, the virial equations are already nearly satisfied. (As we have learned from
Example 3.8, no scheme developed in this paper can help improve accuracy once the virial equation is satisfied by the data.) Thus, any other post-processing is hardly necessary and possible gains offered by extrapolation using the virial theorem seem to diminish.

4.3 Assessing the Proper Radius for Domain Truncation—A Direct Application of the Virial Theorem

Consider a quartic harmonic oscillator

\[-\frac{1}{2} \nabla^2 \psi(r) + 10^{-6} r^4 \psi(r) = E \psi(r), \quad r \in \mathbb{R}^3.\]  

(4.1)

This is a special case of Examples 2.5 (cf. (2.44)) and 3.5 discussed in Sections 2 and 3. For any eigenfunction \( \psi \) satisfying (4.1), if we define

\[ KE = \frac{1}{2} \int |\nabla \psi|^2 \, dr, \quad PE = \int 10^{-6} r^4 |\psi|^2 \, dr, \]

then by Theorem 2.1,

\[ PE/KE = 1/2. \]  

(4.2)

It is our understanding that for (4.1), no exact data of \( E \) are available. By truncating the domain \( \mathbb{R}^3 \) into balls with radii \( R = 20, 40, 60, \) and by imposing the homogeneous Dirichlet condition \( \psi = 0 \) on the bounding sphere, we obtain the first few spectral data as given in Tables 6, 7 and 8.

<table>
<thead>
<tr>
<th>( j )</th>
<th>Eigenvalue ( E_j )</th>
<th>( KE )</th>
<th>( PE )</th>
<th>( PE/KE )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>( 2.4079 \times 10^{-2} )</td>
<td>( 0.163 \times 10^{-1} )</td>
<td>( 0.777 \times 10^{-2} )</td>
<td>( 0.477 )</td>
</tr>
<tr>
<td>2</td>
<td>( 4.5184 \times 10^{-2} )</td>
<td>( 0.310 \times 10^{-1} )</td>
<td>( 0.142 \times 10^{-1} )</td>
<td>( 0.457 )</td>
</tr>
<tr>
<td>3</td>
<td>( 4.5211 \times 10^{-2} )</td>
<td>( 0.310 \times 10^{-1} )</td>
<td>( 0.142 \times 10^{-1} )</td>
<td>( 0.458 )</td>
</tr>
<tr>
<td>4</td>
<td>( 4.5220 \times 10^{-2} )</td>
<td>( 0.310 \times 10^{-1} )</td>
<td>( 0.142 \times 10^{-1} )</td>
<td>( 0.459 )</td>
</tr>
</tbody>
</table>

Table 6. \( R = 20, \) and 2401 tetrahedra are used.
Table 7. $R = 40$, and 12929 tetrahedra are used.

<table>
<thead>
<tr>
<th>$j$</th>
<th>Eigenvalue $E_j$</th>
<th>$KE$</th>
<th>$PE$</th>
<th>$PE/KE$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$2.3951 \times 10^{-2}$</td>
<td>$0.1596 \times 10^{-1}$</td>
<td>$0.7995 \times 10^{-2}$</td>
<td>0.501</td>
</tr>
<tr>
<td>2</td>
<td>$4.4360 \times 10^{-2}$</td>
<td>$0.2978 \times 10^{-1}$</td>
<td>$0.1505 \times 10^{-1}$</td>
<td>0.505</td>
</tr>
<tr>
<td>3</td>
<td>$4.4844 \times 10^{-2}$</td>
<td>$0.2978 \times 10^{-1}$</td>
<td>$0.1506 \times 10^{-1}$</td>
<td>0.506</td>
</tr>
<tr>
<td>4</td>
<td>$4.4848 \times 10^{-2}$</td>
<td>$0.2978 \times 10^{-1}$</td>
<td>$0.1507 \times 10^{-1}$</td>
<td>0.506</td>
</tr>
</tbody>
</table>

Table 8. $R = 60$, and 15788 tetrahedra are used.

<table>
<thead>
<tr>
<th>$j$</th>
<th>Eigenvalue $E_j$</th>
<th>$KE$</th>
<th>$PE$</th>
<th>$PE/KE$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$2.3950 \times 10^{-2}$</td>
<td>$0.1597 \times 10^{-1}$</td>
<td>$0.7985 \times 10^{-2}$</td>
<td>0.500</td>
</tr>
<tr>
<td>2</td>
<td>$4.4825 \times 10^{-2}$</td>
<td>$0.2985 \times 10^{-1}$</td>
<td>$0.1497 \times 10^{-1}$</td>
<td>0.502</td>
</tr>
<tr>
<td>3</td>
<td>$4.4831 \times 10^{-2}$</td>
<td>$0.2985 \times 10^{-1}$</td>
<td>$0.1499 \times 10^{-1}$</td>
<td>0.502</td>
</tr>
<tr>
<td>4</td>
<td>$4.4833 \times 10^{-2}$</td>
<td>$0.2987 \times 10^{-1}$</td>
<td>$0.1497 \times 10^{-1}$</td>
<td>0.501</td>
</tr>
</tbody>
</table>

Figure 3: Profile of the ground state of the quartic harmonic oscillator (4.1): $\psi(x_1, x_2, 0)$, computed by truncating $\mathbb{R}^3$ to a ball with radius 20, with the zero Dirichlet condition.
Figure 4: Profile of the ground state of the quartic harmonic oscillator (4.1): \( \psi(x_1, x_2, 0) \), computed by truncating \( \mathbb{R}^3 \) to a ball with radius 60, with the zero Dirichlet condition. In comparison with Fig. 3, we see that the solution “is allowed more room to decay”.

Figure 5: Profile of \( \Psi_2(x_1, x_2, 0) \) of the excited state for \( j = 2 \) in Table 8.
Figure 6: Profile of $\Psi_3(x_1, x_2, 0)$ of the excited state for $j = 3$ in Table 8.
We have also included the graphics of the ground state of (4.1), corresponding to, respectively, $R = 20$ and $R = 60$, in Figs. 3 and 4. Graphics of three additional excited states are given in Figs. 5–7 with $R = 60$.

![Figure 7: Profile of $\Psi_4(x_1, x_2, 0)$ of the excited state for $j = 4$ in Table 8.](image)

From the rightmost columns of Tables 6, 7 and 8, we see that the ratios $PE/KE$ show a trend of convergence toward the satisfaction of (4.2). The assessment here is that $R = 60$ would be a good choice for the truncation of the domain $\mathbb{R}^3$ (to a ball of radius 60) as far as the calculation of the first four eigenvalues are concerned, while the choice of $R = 20$ would not because the rightmost column of Table 6 deviates from 0.500 with $5 \sim 8\%$ of error.

**Summary.** Projection and extrapolation methods are developed in this paper based on the virial equation for the Schrödinger operator on the whole space with various type of quantum-mechanical potentials $V$. The setting of such a projection is a finite-dimensional space $\mathbb{R}^m$ equipped with the usual dot product if the potential $V$ consists of finitely many terms with varying
degrees of homogeneity. But otherwise the setting must be cast in an infinite-dimensional Hilbert space when the potential $V$ is a transcendental function in order for the projection method to work. Theoretical and numerical results using the finite element method has demonstrated some limitation and effectiveness for improving the accuracy of computed eigenvalues of our approach here. Other schemes utilizing the virial equation are possible and remain to be investigated.

References


