Comparison study of finite element and basis set methods for finite size scaling

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We compare two methods of obtaining critical parameters for a quantum Hamiltonian using a finite size scaling approach. A finite element and basis set method were used in conjunction with the finite size scaling to obtain the critical parameters for the Hulthen potential. The critical parameters obtained analytically were the coupling constant $\lambda_c=\frac{1}{2}$, the critical exponents for the energy $\alpha=2$ and for the "correlation length" $\nu=1$. The extrapolated results for finite size scaling with the basis set method are $\lambda_c=0.499\,99$, $\alpha=1.9960$, and $\nu=0.999\,10$. The results for the finite element solutions are $\lambda_c=0.501\,84$, $\alpha=1.999\,93$, and $\nu=1.000\,79$ for the linear interpolation and $\lambda_c=0.500\,00$, $\alpha=2.000\,11$, and $\nu=1.000\,32$ for the Hermite interpolation. The results for each method compare very well with the analytical results obtained for the Hulthen potential. However, the finite element method is easier to implement and may be combined with *ab initio* and density functional theory to obtain quantum critical parameters for more complex systems. © *2009 American Institute of Physics*. [doi:10.1063/1.3207909]

I. INTRODUCTION

Phase transitions are associated with singularities of the free energy. These singularities occur only in the thermodynamic limit[1,2] where the dimension of the system approaches infinity. However, calculations are done only on finite systems. A finite size scaling (FSS) approach is needed in order to extrapolate results from finite systems to the thermodynamic limit.[3] FSS is not only a formal way to understand the asymptotic behavior of a system when the size tends to infinity but also a theory that also gives us numerical methods[4–10] capable of obtaining accurate results for infinite systems by studying the corresponding small systems. Recently, we have applied the FSS theory to quantum systems.[11–20] In this approach, the finite size corresponds not to the spatial dimension but to the number of elements in a complete basis set used to expand the exact eigenfunction of a given Hamiltonian.[21–25]

Most of our FSS calculations for atomic and molecular systems were done previously based on expanding the wave function in a Slater-type basis sets. Recently, we were able to apply Gaussian-type basis functions[26] and use the finite element method[27] to achieve the same results.

For this paper, we will be investigating the different methods, finite element, and basis set to obtaining quantum critical parameters for a given Hamiltonian. In the proceeding sections, we outline the use of FSS to obtain the critical parameters for a given potential. For the Hulthen potential, we give the analytical solution, basis set expansion, finite element method, and the renormalization group (RG) solution. We will also discuss the possibility of combining a finite element orbital-free density functional approach for FSS analysis on more complex systems.

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II. ANALYTICAL SOLUTION

The Hulthen potential has the following form:

$$V(r) = -\frac{\lambda}{a^2}\frac{e^{-r/a}}{1-e^{-r/a}}, \tag{1}$$

where λ is the coupling constant and a is the scaling parameter. For small values for r/a the potential $V(r)\rightarrow -(1/a)\lambda/r$, whereas for large values of r/a the potential approaches zero exponentially fast, therefore the *scale a* in the potential regulates the infinite number of levels that would otherwise appear with a large-distance *Coulomb* behavior.

Shrödinger radial differential equation in the dimensionless variable $r=r/a$ becomes

$$\frac{1}{2}\frac{d^2\chi}{dr^2} + \left(-\alpha^2 + \lambda\frac{e^{-r}}{1-e^{-r}}\right)\chi = 0, \tag{2}$$

where we used the abbreviations $\alpha^2=-Ea^2\geqslant 0$ (in atomic units $m=\hbar=1$). The complete solutions for the wavefunctions are written in term of hypergeometric functions[28] as follows:

$$\chi = N_0 e^{-\alpha r}(1-e^{-r})_2F_1(2\alpha+1+n, 1-n, 2\alpha+1; e^{-r}), \tag{3}$$

where the normalization factor is given by $N_0=[\alpha(\alpha+n)\times(2\alpha+n)]^{1/2}[\Gamma(2\alpha+n)/\Gamma(2\alpha+1)\Gamma(n)]$. It follows that the energy levels are given by

$$E_n = -\frac{1}{a^2}\frac{(2\lambda-n^2)^2}{8n^2}, \quad n=1,2,3,\ldots,n_{\max}. \tag{4}$$

We can make the following comments concerning the energy levels obtained for the Hulthen potential: There exists a *critical* value for the coupling λ_c to have the given energy levels, $\lambda_c=n^2/2$. It follows directly from the first observation that number of levels $n_{\max}$ allowed is *finite* and it depends on the size of the coupling constant $n_{\max}^2\leqslant 2\lambda$. As $\lambda\rightarrow\infty$ the

potential is well behaved, which can be seen as follows: In this limit we get the obvious inequality $\alpha^2 \ll 2\lambda \Rightarrow \sqrt{2\lambda} \approx n$. It follow that we can set $\alpha \approx 0$ in Eq. (3) to obtain

$$\chi_{\alpha\to 0} = (1-e^{-r})_2F_1(1+n,1-n,1;e^{-r}), \tag{5}$$

which is the wave function at threshold. This wave function is not normalizable as expected when the energy exponent $\alpha=2$, $E \sim (\lambda-\lambda_c)^{\alpha}$. For the ground state, the asymptotic limit of the probability density for $r \gg 1$ and $\lambda \to \lambda_c$ becomes

$$P(r) \sim e^{-r/\xi}, \quad \xi \sim |\lambda-\lambda_c|^{-\nu}, \tag{6}$$

with a characteristic length ξ and exponent $\nu=1$. The Hulthen potential has a finite capacity determined by the critical coupling λ_c. The potential admits bound states between the range of values for the coupling: $\lambda=[1/2,\infty)$.

III. RG

Physical parameters describing the Hulthen system contain an implicit dependence on the scale a. The physics, however, should not depend on the normalization that is chosen, any scale is as good as any other.[29] RG provides the constraint that the theory should be invariant under transformations that merely change the normalization conditions.

To show this, we ask how the ground state energy $E_1(a,\lambda)$ is to remain independent of a transformation of the unit length $r \to r/a$ (in wave number component $k \to ka$). The RG constrain results in a *running* coupling $\tilde{\lambda}(a)$ depending on a in such a way that when the scale is *dilated* (or *contracted*) the ground state remains independent of a.

We can write the condition for the independence of the ground state energy on the normalization[30] in the form

$$a\frac{dE_1(\lambda,a)}{da}=0.$$

We then obtain the RG *equation* for the ground state energy,[31]

$$\left(a\frac{\partial}{\partial a}+\underbrace{\left(a\frac{d\lambda(a)}{da}\right)}_{-\beta(\lambda)}\frac{\partial}{\partial\lambda}\right)E_1=0, \tag{7}$$

where we have introduced the Callan–Symanzik $\beta(\lambda)$. The $\beta(\lambda)$ relates the *flow* of the coupling constant as a function of the scale a. Of importance are *fixed points* of the $\beta(\lambda)$ when the coupling does not change under the iterative application of the rescaling. For systems with many degrees of freedom the transformation $r \to r/a$ relates *correlation functions* on the different scales. Near a fixed point, the system shows simple behavior under the transformation which allows one to determine critical exponents.[30] For single particle case, the zeroes of the $\beta(\lambda)$ can provide long-distance behavior of the theory (*infrared limit*) or short-distance behavior (*ultraviolet limit*).

For the Hulthen potential we obtain the fixed points given by the zeroes of the $\beta(\lambda)$ in Eq. (7). As noted in Ref. 31 the $\beta(\lambda)$ function is a vector field and the transformation $2\lambda \to 1/w$ can be used to understand the behavior of the beta function $\tilde{\beta}(w)$ in the infinite coupling limit $\lambda \to \infty$, this leads to the following: A *nontrivial* fixed point is obtained at $\lambda=1/2$ from $\beta(\lambda)=-(\lambda-1/2)$. The second fixed point is obtained from $\tilde{\beta}(w)=w(1-w)$, this relation provides additionally the *trivial* fixed point given by $\lambda \to \infty$.

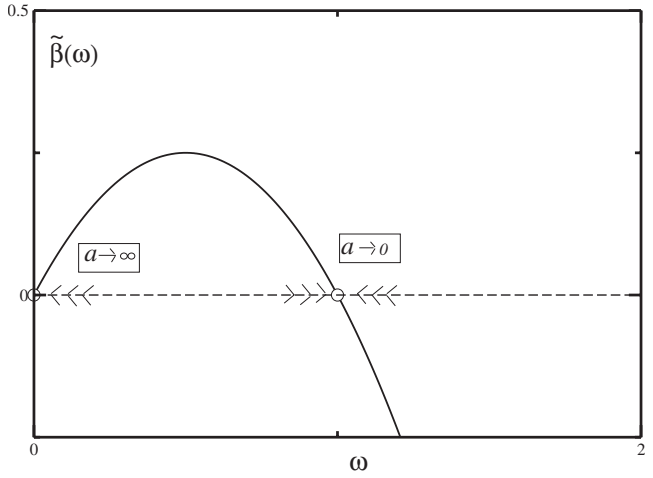

FIG. 1. The function $\tilde{\beta}(w)$, as a function of $w=(2\lambda)^{-1}$. The zeroes of the beta function give the IR-stable fixed point and UV-fixed point

In Fig. 1, we show the $\tilde{\beta}(w)$ as a function of w since it shows both fixed points. Recall that the beta function is defined as $\tilde{\beta}(w) \equiv -d(w)/d\ln a$, with $w \to 1/(2\lambda)$ or equivalently $\tilde{\beta}(w) \equiv d(w)/d\ln(1/a)$. We note the following two points. First, between the two critical points $dw/d\ln(1/a) > 0$. Therefore, w *decreases* as $\ln(1/a)$ decreases. In the limit $\ln(1/a) \to -\infty$ (UV limit), $w \to 0$, and the $\beta(w)$ goes to zero from above. Thus we get the *trivial fixed point* $\lambda \to \infty$.

In the opposite limit as $\ln(1/a) \to \infty$ (IR limit) we have two cases: (1) if w is below $w^*=1$, then w *increases* versus $\ln(1/a)$, and (2) if w is above w^*, then w decreases versus $\ln(1/a)$. Therefore the behavior of the $\tilde{\beta}(w)$ shows an attraction of w toward the fixed point $w^*=1$. The values of the fixed points are summarized in Table I.

IV. FSS

The FSS method is a systematic way to extract the critical behavior of an infinite system from analysis on finite systems. It is efficient and accurate for the calculation of critical parameters of the Schrödinger equation. Let us assume we have the following Hamiltonian:

$$H = H_0 + V_\lambda, \tag{8}$$

where λ is a parameter and there is a critical point λ_c that indicates where the bound state becomes degenerate with the continuum.

TABLE I. Fixed points given by $\beta(\lambda)=0$.

$E_1=-\frac{1}{a^2}\frac{(2\lambda-1)^2}{8}$	$\lambda \to 1/2$	$\lambda \to \infty$
IR $(a\to 0)$	Stable (no levels)	Unstable
UV $(a\to\infty)$	Unstable	Stable (*infinite levels*)

As in statistical mechanics, there are critical exponents related to the asymptotic behavior of different properties near the critical point. The exponent α for the energy can be define as

$$E_\lambda \approx (\lambda - \lambda_c)^\alpha. \tag{9}$$

We will compare the two methods to obtain the matrix elements needed to apply the FSS ansatz. The size of our system for the basis set expansion will correspond to the dimension of the Hilbert space. For a given complete basis set Φ_n, the ground state eigenfunction has the following expansion:

$$\Psi_\lambda = \sum_n a_n(\lambda)\Phi_n, \tag{10}$$

where n is the set of quantum numbers. We have to truncate the series at order N and the expectation value of any general operator O at order N is given by

$$\langle O\rangle^N = \sum_{n,m}^{N} a_n^{(N)} a_m^{(N)} O_{n,m}. \tag{11}$$

For the finite element method (FEM), the wavefunction $\psi_n(r)$ in the nth element is expressed in terms of local shape functions. For our calculations, we use Hermite interpolation polynomials with two nodes and three degrees of freedom. (We have also applied the linear interpolation method for this problem.) This choice ensures the continuity of the wavefunction and its first two derivatives. Then in nth element the wavefunction is (for Hermite interpolation),

$$\psi_n(r) = \sum_{i=1}^{2} [\phi_i(r)\psi_n^i + \bar{\phi}_i(r)\psi_n'^{\alpha} + \bar{\bar{\phi}}_i(r)\psi_n''^{i}], \tag{12}$$

with α indicating the nodal index of the element; $i=1$ for the left and $i=2$ for the right border of the element. The functions $\phi_i(r)$, $\bar{\phi}_i(r)$, and $\bar{\bar{\phi}}_i(r)$ are the (fifth degree) Hermite interpolation polynomials. Then ψ_n^i, $\psi_n'^i$, and $\psi_n''^i$ are the undetermined values of the wavefunction and its first and second derivatives on the nodal points. The size for the case of solving the equation with the FEM will be the number of elements used. The average value for any operator in FEM is

$$\langle O\rangle^N = \sum_{n=1}^{N} \int_{r_n}^{r_{n+1}} r^2 \psi_n^*(r) O \psi_n(r) dr, \tag{13}$$

where N is the number of elements used. We have omitted the angular terms for simplicity.

Since $\langle O\rangle_\lambda$ is not analytical at $\lambda=\lambda_c$, then we define a critical exponent μ_O if the general operator has the following relation:

$$\langle O\rangle_\lambda \approx (\lambda - \lambda_c)^{\mu_O} \quad \text{for } \lambda \to \lambda_c^+, \tag{14}$$

where $\lambda \to \lambda_c^+$ represents taking the limit of λ approaching the critical point from larger values of λ. We assume the existence of a scaling function for the truncated magnitudes, such that

$$\langle O\rangle_\lambda^{(N)} \sim \langle O\rangle_\lambda F_O(N|\lambda - \lambda_c|^\nu), \tag{15}$$

with the scaling function F_O being particular for different operators but all having the same unique scaling exponent ν.

To obtain the critical parameters, we define the following function:

$$\Delta_O(\lambda;N,N') = \frac{\ln(\langle O\rangle_\lambda^N / \langle O\rangle_\lambda^{N'})}{\ln(N'/N)}. \tag{16}$$

At the critical point, the expectation value is related to N as a power law, $\langle O\rangle \sim N^{\mu_O/\nu}$, and Eq. (16) becomes independent of N. For the energy operator $O=H$, and using the customary α Greek letter for the corresponding exponent μ_O we have

$$\Delta_H(\lambda_c;N,N') = \frac{\alpha}{\nu}. \tag{17}$$

In order to obtain the critical exponent α from numerical calculations, it is convenient to define a new function,

$$\Gamma_\alpha(\lambda,N,N') = \frac{\Delta_H(\lambda;N,N')}{\Delta_H(\lambda,N,N') - \Delta_{\partial V_\lambda/\partial\lambda}(\lambda;N,N')}, \tag{18}$$

which at the critical point is independent of N and N' and takes the value of α. Namely, for $\lambda=\lambda_c$ and any values of N and N' we have

$$\Gamma_\alpha(\lambda_c,N,N') = \alpha. \tag{19}$$

V. BASIS SET EXPANSION

For the Hulthen potential, the wavefunction can be expanded in the following Slater basis:

$$\Phi_n(r) = \sqrt{\frac{1/4\pi}{(n+1)(n+2)}} e^{-r/2} L_n^{(2)}(r). \tag{20}$$

$L_n^{(2)}(r)$ is the Laguerre polynomial of degree n and order of 2.

The kinetic term can be written analytically,

$$\left\langle a\left|-\frac{1}{2}\nabla^2\right|b\right\rangle = -\frac{1}{2\sqrt{(a+1)(a+2)(b+1)(b+2)}}\left\{\frac{1}{4}\frac{\Gamma(a+3)}{a!}\delta(a,b) - (b+1)\frac{\Gamma(\min(a,b)+3)}{2\min(a,b)!}\right.$$
$$- b\frac{\Gamma(\min(a,b)+3)}{6\min(a,b)!}\quad (2[a+b-2\min(a,b)+1]+(a+b+1))$$
$$\left. + (b+2)\frac{\Gamma(\min(a,b-1)+3)}{6\min(a,b-1)!}(2[1+b-1-2\min(a,b-1)+1]+(a+b))\right. . \tag{21}$$

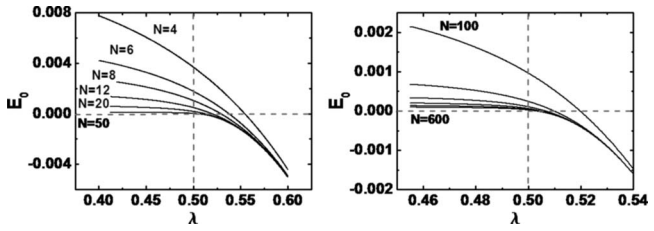

FIG. 2. The ground state energy as a function of λ. The exact λ_c is 0.5. On the left is the basis set method solutions with *N* equal to the number of basis functions used. The right is the FEM solutions with *N* equal to the number of elements.

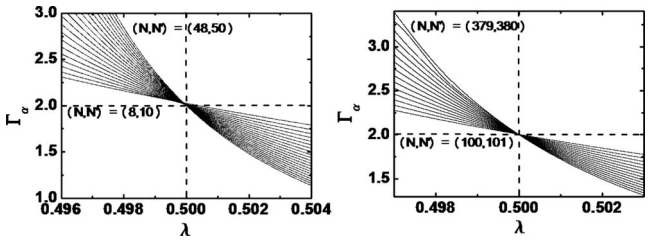

FIG. 3. Plot of Γ_α, obtained by FSS method, as a function of λ. Using the number of basis *N* from 8 to 48 in steps of 2. For FEM the number elements used were from 100 to 380 in steps of 20.

The potential term can be calculated numerically.

When we plot $\Gamma_\alpha(\lambda,N,N')$ as a function of λ with different *N* and *N'*, all the curves will cross exactly at the critical point. Due to the parity effects, we have taken $N'=N+2$.

VI. THE FINITE ELEMENT METHOD

The FEM is a numerical technique that gives approximate solutions to differential equations. In the case of quantum mechanics, the differential equation is formulated as a boundary value problem. For our purposes, we are interested in solving the time-independent Shrödinger equation with finite elements,

$$H\Psi = E\Psi. \tag{22}$$

We will require our boundary conditions to be restricted to the Dirichlet type. The procedure for FEM to solve for differential equations can be found in many textbooks in engineering.[32,33] In our previous paper we successfully applied the FEM to solve for the Yukawa potential and obtained the quantum critical parameters.[27] For this problem, we will use two interpolation methods (linear interpolation and Hermite interpolation polynomials) to solve for this potential. The results will be discussed later in the article.

We once again start by integration by parts and impose the boundary conditions for the kinetic energy and reduce it to the weak form,

$$\frac{1}{2}\int_0^\infty r^2\psi^{*\prime}(r)\psi'(r)dr. \tag{23}$$

We will only consider the case for $l=0$ for the Hulthen potential. For the potential energy,

$$\int_0^\infty r^2\psi^*(r)\psi(r)\lambda\frac{-e^{-r}}{1-e^{-r}}dr. \tag{24}$$

We calculated the local matrix elements of the potential energy by using a four point Gaussian quadrature to evaluate the integral. We set the cutoff for the integration to r_c. To include the integration to infinity, we added an infinite element approximation. To do so, we approximate the solution of the wave function in the region of $[r_c,\infty)$ to be an exponentially decaying function with the form $\psi(r)=\psi(r_c)e^{-r}$.

The local matrices are then assembled to form the complete solution, and by invoking the variational principle on the nodal values ψ_i, we obtain a generalized eigenvalue problem representing the initial Schrödinger equation,

$$H_{ij}|\psi_j\rangle = \epsilon U_{ij}|\psi_j\rangle. \tag{25}$$

Solution of Eq. (25) is achieved using standard numerical packages.

VII. RESULTS AND DISCUSSION

For previous studies of the Yukawa potential, parity effects were observed depending on the basis set used.[15] This was also observed for the Hulthen potential solved with the basis set expansion. However, similar to the case with the previous study of the Yukawa potential solved using the FEM, there were no observed parity effects with the FEM analysis. The FSS equations are valid only as asymptotic expressions, but unique values of λ_c, α, and ν can be obtained as a succession of values as a function of *N*. The lengths of the elements are set $h=0.5$.

In Fig. 2, we show the behavior of the ground state energy as a function of λ. We see that as the size of the basis and number of elements increases, the ground state energy becomes positive at λ closer to λ_c only for the case of the basis set and Hermite interpolation with the infinite element approximation. The linear interpolation has a different behavior as we approach the critical λ. The energy do, in fact, becomes more positive, but the electron never truly becomes unbound. It is still bound (very weakly), while the basis set method and the Hermite interpolation gave similar results.

For each of the values of *N*, we actually solve the problem three times (*N*, *N*+1, and *N*+2 for FEM and *N*,*N*+2, and *N*+4 for the basis set method due to parity effects) in order to obtain two Γ curves. The crossing of these two curves defines the pseudocritical parameters $\lambda_c^{(N)}$ and $\alpha^{(N)}$. The exponent $\nu^{(N)}$ is easily obtained from Eq. (17).

In the plots of Γ_α in Fig. 3 the basis set expansion is giving values very close to the analytical solution of the Hulthen potential. For the plot of Γ_α for the FEM estimation of λ_c is producing results very close to exact values with Hermite interpolation (linear approximation produces slightly higher estimation of λ_c). The intersection of these curves indicates the λ_c on the abscissa. The ordinate gives

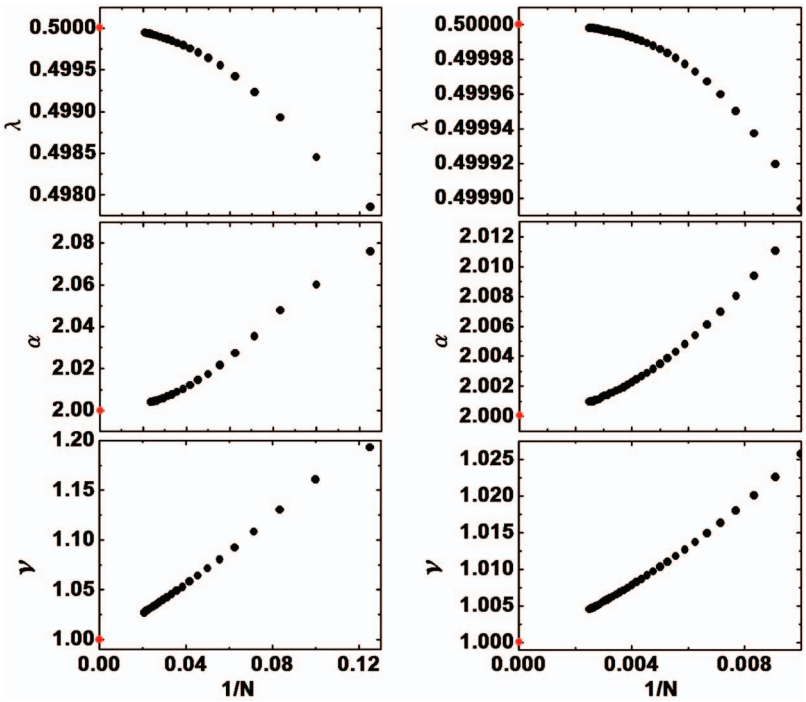

FIG. 4. Extrapolated values for the critical exponents and the critical parameter λ. The solid dots at $1/N=0$ are the extrapolated critical values. The left side is the basis set method while the right is the FEM with Hermite interpolation polynomials.

the critical exponents α (in Γ_α plots). In Fig. 4, we observed the behavior of the pseudocritical parameters as a function of $1/N$. The three curves monotonically converge to limiting values for the Hermite interpolation and the basis set expansion.

To check the validity of our FSS assumptions, we performed a data collapse calculation of the Hulthen potential. In Fig. 5 we plot the results corresponding to the basis set method (right panel) and Hermite interpolation (left panel), which have been calculated with $\lambda_c=0.499\,99$, $\alpha=1.9960$, and $\nu=0.999\,10$ for the basis set method and for the Hermite interpolation we have $\lambda_c=0.500\,00$, $\alpha=2.000\,11$, and $\nu=1.000\,322$. The data collapse study do, in fact, supports our FSS assumptions.

We have conveniently summarized our results for the critical parameters for the analytical, linear interpolation, Hermite interpolation, and the basis set expansion in Table II.

We have studied the critical parameters using the RG. We obtain critical parameters (λ_c) with the RG approach by demanding *invariance* on the normalization on the ground state energies. The critical parameter coincides with analytical result and FSS estimates.

We have successfully obtained the critical exponents and the critical parameter for the Hulthen potential using FSS with the basis set method and the FEM. The results are in excellent agreement with the analytical solution even for the very simplistic linear interpolation used for the FEM calculations. However, the ability of the FEM to describe the wavefunction locally in terms of elements affords a very natural way to extend its use for FSS purposes. In the past the size of the system was related to the number of basis functions used to solve for the system. With FEM the size is now related to the number of elements used.

We conclude that the FEM approach produces results just as well as the basis set method. Even with a simplistic linear approximation the critical parameters obtained were still in excellent agreement with the exact parameters obtained from RG or the analytical approach.

In future studies, we plan to implement an orbital free density functional[34,35] approach and density matrices[36–39] to obtain matrix elements needed to carry out a FSS study for more complex systems. The implementation should be straightforward. We will obtain the matrix elements needed to calculate Γ_α as a function of the number of elements used in solving for the system. The solution region will be discretized into elements composed of tetrahedrons. Then we may implement the FSS equations needed to obtain the critical parameters.

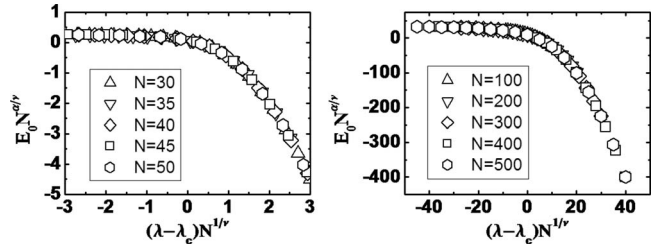

FIG. 5. Data collapse study of the basis set method and FEM. The left is the basis set method and the right being the FEM.

TABLE II. Results for critical parameters.

	Analytical	Linear	Hermite	Basis set
λ	0.5 (exact)	0.501 84	0.500 00	0.499 99
α	2 (exact)	1.999 93	2.000 11	1.996 0
ν	1 (exact)	1.000 79	1.000 32	0.999 10

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