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Data collapse for the Schrödinger equation

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Abstract

We present a data-collapse study for quantum few-body problems. Our data strongly support a recent hypothesis for the application of the finite-size scaling approach for the calculation of the critical parameters for the few-body Schrödinger equation. We test the data collapse using very accurate calculations of the one-body Yukawa potential. This powerful tool is used to obtain an estimation of the critical exponents for the lithium-like atoms. © 2000 Elsevier Science B.V. All rights reserved.

1. Introduction

The finite-size scaling (FSS) theory is widely used in statistical mechanics to study lattice systems, for analysis of Monte Carlo data, etc. [1,2]. In phase transition theory, finite size means that a system is finite in one or more spatial dimensions, and then the thermodynamic quantities are analytical functions of the temperature and the microscopic parameters. FSS tells us how the singularities in the thermodynamic functions develop at a critical point when the size of the system goes to infinity (the thermodynamic limit).

Recently, we have shown that this theory is very useful in studying critical points in quantum few-body problems (for a recent review, see Ref. [3]). In particular, we used a phenomenological renormalization equation to obtain the critical nuclear charges for two- and three-electron atoms [4,5]. This equation was introduced in a phenomenological way in statistical mechanics and we show that the same form can be used to study critical behavior of quantum systems [3]. In this approach one assumes that the two lowest eigenvalues of the quantum Hamiltonian could be taken as the leading eigenvalues of a transfer matrix of a classical pseudosystem. Moreover, in a subsequent study we developed a direct finite size scaling approach to study critical parameters in quantum systems without the need to make any explicit analogy to classical statistical mechanics [6].

In this Letter, we present for the first time results which strongly support the hypothesis, or the ansätze we used to obtain critical parameters. This study is very important in order to complete the analogy between finite size scaling in classical statistical mechanics and quantum systems. Using this data collapse we were able to estimate the critical exponent, ν, for the lithium-like atoms.

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2. Finite size scaling and data collapse

In order to show the data collapse for quantum few-body problems, let us first briefly present the general form of scaling [6] for different quantities of a given Hamiltonian of the form

$$\mathscr{H} = \mathscr{H}_0 + \mathscr{V}_\lambda \ . \tag{1}$$

where $\mathscr{H}_0$ is λ-independent and $\mathscr{V}_\lambda$ is the λ-dependent term. A critical point, λ_c, is defined as a point for which a bound state becomes absorbed or degenerate with a continuum.

For a given complete orthonormal λ-independent basis set $\{\Phi_n\}$, the ground-state eigenfunction has the following expansion

$$\Psi_\lambda = \sum_n a_n(\lambda)\Phi_n \ , \tag{2}$$

where n represents the adequate set of quantum indices. As usual, in order to approximate the different quantities, we have to truncate the series Eq. (2) at order N. Then the Hamiltonian is replaced by a $M(N)\times M(N)$ matrix $\mathscr{H}^{(N)}$, with $M(N)$ being the number of elements in the truncated basis set at order N. Using the standard linear variational method, the Nth-order approximation for the energies is given by the eigenvalues of the matrix $\mathscr{H}^{(N)}$. In particular, the ground state is given by

$$E_\lambda^{(N)} = \min_{\{i\}} \left\{ \Lambda_i^{(N)} \right\} , \tag{3}$$

where $\{\Lambda_i^{(N)}\}$ are the eigenvalues of the matrix $\mathscr{H}^{(N)}$. The corresponding eigenfunction are given by

$$\Psi_\lambda^{(N)} = \sum_n^{M(N)} a_n^{(N)}(\lambda)\Phi_n \ , \tag{4}$$

where the coefficients, $a_n^{(N)}$, are the components of the ground-state eigenvector. In this representation, the expectation value of any operator $\mathscr{O}$ at order N is given by

$$\langle \mathscr{O} \rangle^{(N)}(\lambda) = \sum_{n,m}^{N} a_n^{(N)}(\lambda)\, a_m^{(N)}(\lambda)\, \mathscr{O}_{n,m} \ , \tag{5}$$

where $\mathscr{O}_{n,m}$ are the matrix elements of $\mathscr{O}$ in the basis set $\{\Phi_n\}$.

In general, the mean value $\langle \mathscr{O} \rangle$ is not analytical at $\lambda = \lambda_c$, and we can define a critical exponent, $\mu_\mathscr{O}$, by the relation

$$\langle \mathscr{O} \rangle(\lambda) \underset{\lambda \to \lambda_c^+}{\sim} (\lambda - \lambda_c)^{\mu_\mathscr{O}} . \tag{6}$$

The main assumption we have made in Ref. [6] is the existence of a scaling function for each truncated magnitude such that

$$\langle \mathscr{O} \rangle^{(N)}(\lambda) \sim \langle \mathscr{O} \rangle(\lambda)\, F_\mathscr{O}\left(N|\lambda - \lambda_c|^\nu\right) \tag{7}$$

with a unique scaling exponent ν.

Since the $\langle \mathscr{O} \rangle_\lambda^{(N)}$ is analytical in λ, then from Eqs. (6) and (7) the asymptotic behavior of the scaling function must have the form

$$F_\mathscr{O}(x) \sim x^{-\mu_\mathscr{O}/\nu} . \tag{8}$$

Eqs. (7) and (8) have the scaling form as presented in Ref. [6]. For our purposes, it is convenient to write this in a slightly different form. From Eqs. (7) and (8)

$$\langle \mathscr{O} \rangle^{(N)}(\lambda_c) \sim N^{-\mu_\mathscr{O}/\nu} \tag{9}$$

for large values of N.

Because the same argument of regularity holds for the derivatives of the truncated expectation values, we have that

$$\left. \frac{\partial^m \langle \mathscr{O} \rangle^{(N)}}{\partial \lambda^m} \right|_{\lambda = \lambda_c} \sim N^{-(\mu_\mathscr{O} - m)/\nu} . \tag{10}$$

$\langle \mathscr{O} \rangle^{(N)}$ is analytical in λ, so using Eq. (10), the Taylor expansion could be written as

$$\langle \mathscr{O} \rangle^{(N)}(\lambda) \sim N^{-\mu_\mathscr{O}/\nu} G_\mathscr{O}\left(N^{1/\nu}(\lambda - \lambda_c)\right) , \tag{11}$$

where $G_\mathscr{O}$ is an analytical function of its argument.

This equivalent expression for the scaling of a given expectation value has the correct form for studying the data collapse in order to test the FSS hypothesis in quantum few-body Hamiltonians. If the scaling Eq. (7) or Eq. (11) holds, then, near the critical point, the physical quantities will collapse to a single universal curve when plotted in the appropriate form $\langle \mathscr{O} \rangle^{(N)} N^{\mu_\mathscr{O}/\nu}$ against $N^{1/\nu}(\lambda - \lambda_c)$.

As we have shown in previous works (see Ref. [3]), if the Hamiltonian commutes with the total angular momentum, then we can choose a basis set which block-diagonalize, $\mathscr{H}^{(N)}$, and FSS arguments are valid for the lowest eigenvalue of each block of the finite Hamiltonian matrix. It is also shown in Ref. [7] that the coefficients, $a_n^{(N)}$, of the ground-state wavefunction expansion in Eq. (2) obey the same scaling law with a unique exponent μ_{a} $\forall n$.

3. Results and discussions

At this point, in order to check FSS assumptions, let us show the data collapse for the one-body Yukawa potential.

$$\mathscr{H}(\lambda) = -\tfrac{1}{2}\nabla^2 - \lambda \frac{e^{-r}}{r}. \tag{12}$$

The advantage of studying this simple model is that there exist rigorous theorems which give the exact values for energy-critical α-exponents [8] and accurate values for the critical screening length and the universal exponent ν [6] for both zero and non-zero angular momenta. The values of the critical lengths λ_c, the energy exponents $\alpha \equiv \mu_{\mathscr{H}}$ and the exponents μ_{a} for the wavefunction expansions are listed in Table 1 for angular momenta $l=0$ and $l=1$.

As a complete basis set we have used the Laguerre polynomials and the spherical harmonics, details are given in Refs. [6,7]. We applied the data-collapse method to the ground-state energy and the lowest $l=1$ energy. Results are shown in Fig. 1a for $l=0$, and in Fig. 1b for $l=1$. Data collapse of the wavefunction coefficients for $l=0$ are shown in Fig. 2a for $n=0$ and in Fig. 2b for $n=1$. In order to make the plots clear, we show in all figures curves for only some values of $N = 20, 40, 60, 80, 100$.

We note that in analogy with statistical mechanics, each block ($l=0$ and $l=1$) of the Hamiltonian

Table 1
Critical parameters for the Yukawa potential for $l=0$ and $l=1$

	λ_c	α	μ_{a}	ν
$l=0$	0.8399039[a]	2[b]	1/2[c]	1[a]
$l=1$	4.54098[a]	1[b]	0[c]	1/2[a]

[a] From Ref. [6].
[b] From Ref. [8].
[c] From Ref. [7].

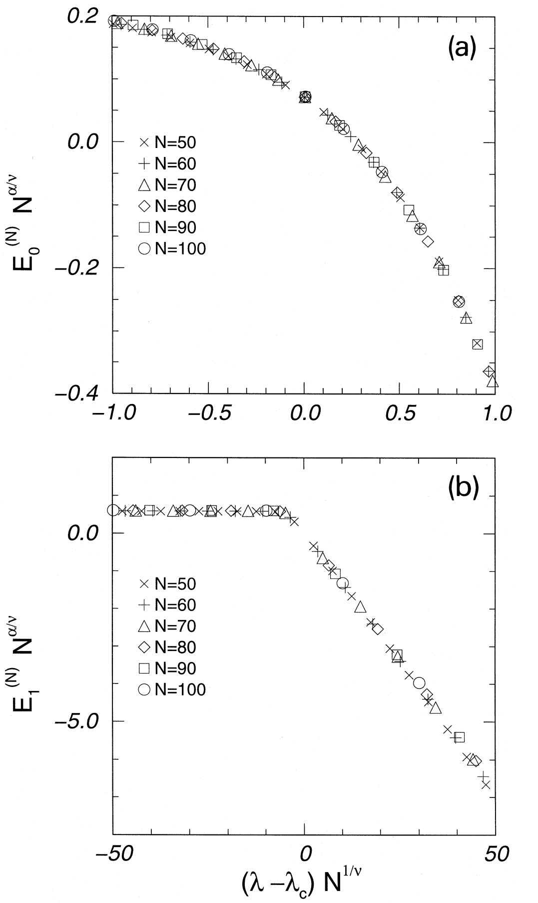

Fig. 1. Data collapse for the energy of the Yukawa potential for: (a) the ground state with $\alpha = 2$ and $\nu = 1$; and (b) the lowest $l=1$ level with $\alpha = 1$ and $\nu = 1/2$

matrix could be interpreted as a transfer matrix of a classical pseudo-system. Within this analogy, the lowest eigenvalue is associated with the free energy and the critical point as a first-order phase transition for $\alpha = 1$ [2] or as a continuous phase transition for $\alpha > 1$. As a result of this analogy, we can use scaling laws from statistical mechanics to be applied to the classical pseudo-system. In particular, for continuous phase transitions we can calculate the spatial dimen-

[2] Note that the α exponent is related to the statistical mechanics α_{sm} exponent for the specific heat by the relation $\alpha_{\mathrm{sm}} = \alpha - 2$.

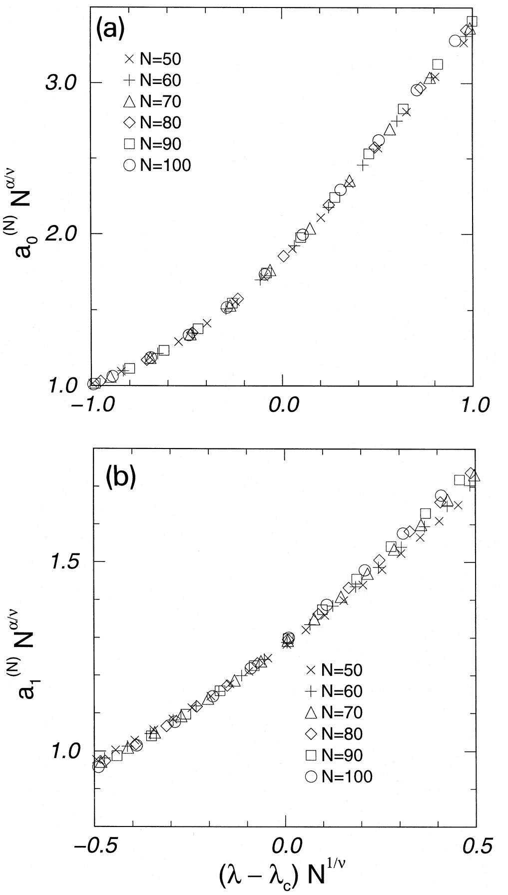

Fig. 2. Data collapse for the coefficients of the ground-state wavefunction expansion of the Yukawa potential with $\mu_a = 1/2$ and $\nu = 1$ for: (a) the first coefficient a_0; and (b) the second coefficient a_1.

sion, d, of the pseudo-system using the hyperscaling relation (see, e.g., Ref. [9])

$$4 - \alpha = d\nu, \tag{13}$$

where d is the spatial dimension of the pseudo-system. Then for $\alpha = 2$ and $\nu = 1$ it gives a spatial dimension $d = 2$. For $l = 1$ there is a first-order phase transition, therefore the relation between the ν exponent and the spatial dimension of the pseudo-system is $d = 1/\nu$ [10], which gives again $d = 2$. The excellent collapse of the curves gives a strong support to the FSS arguments in quantum mechanics.

Now, let us use the data-collapse method to obtain numerical values for critical parameters for the lithium-like atoms. The scaled Hamiltonian has the form [5]

$$\mathscr{H}(\lambda) = \sum_{i=1}^{3}\left[-\tfrac{1}{2}\nabla_i^2 - \frac{1}{r_i}\right] + \lambda \sum_{i<j=1}^{3} \frac{1}{r_{ij}}, \tag{14}$$

where r_{ij} are the interelectron distances, and λ is the inverse of the nuclear charge.

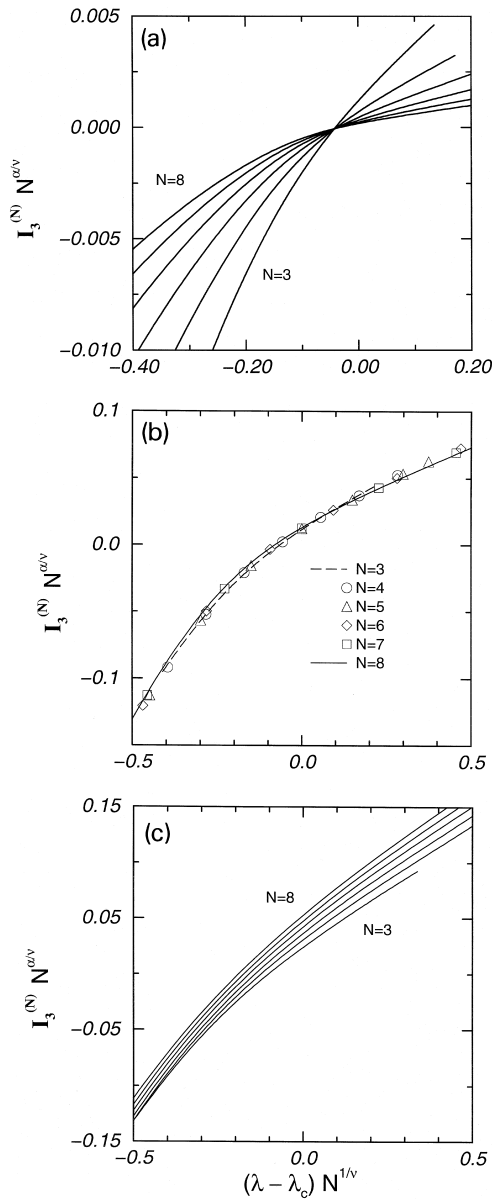

Fig. 3. Data collapse for the ionization energy of the three-electron atom with $\alpha = 1.64$ with: (a) $\nu_2 = 1.2$; (b) $\nu_3 = 0.8$; and $\nu_4 = 0.6$.

Recently, by using a phenomenological renormalization approach [5], we have obtained numerical evidence to support the exact value of the inverse critical charge being $\lambda_c = 0.5$ and the energy exponent having a value $\alpha = 1.64 \pm 0.05$. The basis set and details of the calculations are given in Ref. [5].

For the data collapse we also need the value of the critical exponent ν. In order to test the FSS assumption and to calculate the ν exponent, the value of ν is varied until a good data collapse is obtained. Now we can use the hyperscaling relation (Eq. (13)) to get an estimate of the exponent ν. Using the value of $\alpha = 1.64$, we obtain three different values of ν for $d = 2, 3$ and 4, which are respectively $\nu_2 \approx 1.2$, $\nu_3 \approx 0.8$ and $\nu_4 \approx 0.6$.

We applied data collapse to the ionization energy of the three-electron atom in its ground state

$$I_3(\lambda) = E_0^{\mathrm{Li}}(\lambda) - E_0^{\mathrm{He}}(\lambda), \tag{15}$$

where E_0^{He} is the ground-state energy of the two-electron atom. The calculation was done with the Hylleraas basis set with $N = 3, 4, \cdots, 8$, which means up to 1589 Hylleraas functions. Numerical values of the basis set parameters are given in Ref. [5]. The helium-like atom ground-state energy was calculated with more than ten digits, so it can be considered to be exact for the lithium-like atoms calculation.

The curves for I_3 are shown in Fig. 3a for $\nu_2 = 1.2$, Fig. 3b for $\nu_3 = 0.8$ and Fig. 3c for $\nu_4 = 0.6$. These figures show clearly that the value $\nu_3 = 0.8$ is the only one that gives a unique curve for all N. Our estimate for the lithium exponent is $\nu = 0.8 \pm 0.1$.

In summary, we have presented a data collapse for quantum few-body problems. The results support the hypothesis for the direct application of the finite size scaling approach for the calculation of critical parameters for the Schrödinger equation. Also, the data collapse can be used to obtain numerical values for the critical parameters. Results for the lithium-like atoms show that one can use the data collapse to estimate the ν exponent. The method is general and can be used to obtain critical parameters for other Hamiltonians.

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