PHYSICAL REVIEW A VOLUME 57, NUMBER 3 MARCH 1998

Finite-size scaling approach for the Schrödinger equation

Pablo Serra, Juan Pablo Neirotti, and Sabre Kais
Department of Chemistry, Purdue University, West Lafayette, Indiana 47907
(Received 18 September 1997)

We present a finite-size scaling approach for the calculations of the critical parameters of the few-body Schrödinger equation. This approach gives very accurate results for the critical parameters by using a systematic expansion in a finite basis set. To illustrate this approach we added detailed calculations for the critical screening length and the critical exponents for the Yukawa potential. [S1050-2947(98)50103-5]

PACS number(s): 31.15.−p, 05.70.Jk

A finite-size scaling approach [1] has been used to study problems of critical behavior in statistical mechanics in order to extrapolate the information available from a finite system to the thermodynamic limit. This approach has been used increasingly as a method of analyzing numerical data, especially from two-dimensional lattice systems and Monte Carlo calculations [2–5].

Recently [6] we presented a method to calculate the critical parameters of a few-body quantum Hamiltonian. In that method we assumed that the two lowest eigenvalues of the quantum Hamiltonian could be taken as the leading eigenvalues of a transfer matrix of a classical pseudosystem. Using finite-size scaling arguments [1,5], the phenomenological renormalization equation [7] was used to obtain the critical properties of the classical pseudosystem and therefore of the quantum system.

In this paper we present a direct finite-size scaling (FSS) approach to study the critical behavior of the quantum Hamiltonian without the need to make any explicit analogy to classical statistical mechanics. This approach assumes an explicit form for the asymptotic behavior of the quantum mean values near the critical point. The critical parameters can be calculated by a systematic expansion in a finite (truncated) basis set.

In order to present this approach, let us consider a general Hamiltonian of the form

$$\mathcal{H}=\mathcal{H}_0+\mathcal{V}_\lambda, \tag{1}$$

where $\mathcal{H}_0$ is λ-independent and $\mathcal{V}_\lambda$ is the λ-dependent term. We are interested in the study of the critical behavior of the Hamiltonian, Eq. (1), as a function of the parameter λ. A critical point λ_c is defined as a point for which a bound state becomes absorbed or degenerate with the continuum. Without loss of generality, we will assume that the threshold energy or the bottom of the continuum is equal to zero.

As in statistical mechanics, we can define some critical exponents related to the asymptotic behavior of different magnitudes near the critical point. We will assume that the Hamiltonian, Eq. (1), has a bound state E_λ for $\lambda>\lambda_c$ that becomes equal to zero at $\lambda=\lambda_c$. In particular, this energy defines the critical exponent α

$$E_\lambda \underset{\lambda\to\lambda_c^+}{\sim} (\lambda-\lambda_c)^\alpha. \tag{2}$$

The existence or absence of a bound state at the critical point is related to this kind of singularity. For general potentials of the form $\mathcal{V}_\lambda=\lambda\bar{\mathcal{V}}$, Simon [8] has proven that the critical exponent α is equal to 1 if and only if $\mathcal{H}(\lambda_c)$ has a normalizable eigenfunction with eigenvalue equal to zero. Using statistical-mechanics terminology, we can associate ''first-order phase transitions'' with the existence of a normalizable bound state at the critical point.

In statistical mechanics, the finite-size scaling method provides a way of extrapolating information obtained from a finite (or partially infinite) system to the thermodynamic limit. In the present 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. For a given complete orthonormal λ-independent basis set $\{\Phi_n\}$, the ground-state eigenfunction has the following expansion:

$$\Psi_\lambda=\sum_n a_n(\lambda)\Phi_n, \tag{3}$$

where n represents the adequate set of quantum numbers. In order to approximate the different quantities, we have to truncate the series, Eq. (3) at order N. Then the Hamiltonian is replaced by the $M(N)\times M(N)$ matrix $\mathcal{H}^{(N)}$, 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 $\mathcal{H}^{(N)}$.

The Nth-order approximation for the energy is given by

$$E_\lambda^{(N)}=\min_{\{i\}}\{\Lambda_i^{(N)}\}, \tag{4}$$

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

$$\Psi_\lambda^{(N)}=\sum_n^{M(N)} a_n^{(N)}(\lambda)\Phi_n, \tag{5}$$

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

$$\langle\mathcal{O}\rangle_\lambda^{(N)}=\sum_{n,m}^{N} a_n^{(N)}(\lambda)a_m^{(N)}(\lambda)\mathcal{O}_{n,m}, \tag{6}$$

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

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

$$\langle\mathcal{O}\rangle_\lambda \underset{\lambda\to\lambda_c^+}{\sim} (\lambda-\lambda_c)^{\mu_{\mathcal{O}}}. \tag{7}$$

As in the FSS *Ansätze* in statistical mechanics [9], we will assume that there exists a scaling function for the truncated magnitudes such that

$$\langle\mathcal{O}\rangle_\lambda^{(N)} \sim \langle\mathcal{O}\rangle_\lambda F_{\mathcal{O}}(N|\lambda-\lambda_c|^\nu), \tag{8}$$

with a different scaling function $F_{\mathcal{O}}$ for each different operator but with a unique scaling exponent ν. In statistical mechanics, the exponent ν is defined by the singularity of the correlation length at the critical point. In the framework of the Schrödinger equation we do not have yet a clear interpretation for this exponent. Since the $\langle\mathcal{O}\rangle_\lambda^{(N)}$ is analytical in λ [10], then from Eqs. (7) and (8) the asymptotic behavior of the scaling function must have the form

$$F_{\mathcal{O}}(x)\sim x^{-\mu_{\mathcal{O}}/\nu}. \tag{9}$$

Now, to obtain the critical parameters, we define the function

$$\Delta_{\mathcal{O}}(\lambda;N,N')=\frac{\ln(\langle\mathcal{O}\rangle_\lambda^{(N)}/\langle\mathcal{O}\rangle_\lambda^{(N')})}{\ln(N'/N)}. \tag{10}$$

At the critical point, this function $\Delta_{\mathcal{O}}$ along with Eqs. (8) and (9) gives an equation for the ratio of the critical exponents,

$$\Delta_{\mathcal{O}}(\lambda_c;N,N')=\frac{\mu_{\mathcal{O}}}{\nu}, \tag{11}$$

which is independent of the values of N and N'. Thus, for three different values N, N', and N'' the curves defined by Eq. (10) intersect at the critical point

$$\Delta_{\mathcal{O}}(\lambda_c;N,N')=\Delta_{\mathcal{O}}(\lambda_c;N'',N). \tag{12}$$

In order to obtain the critical exponents, we need two independent equations for the same quotient of exponents. These two equations can be obtained for the exponent α, which is associated with the energy [see Eq. (2)]. If we take $\mathcal{O}=\mathcal{H}$, we obtain from Eq. (11) with $\mu_{\mathcal{O}}=\alpha$

$$\frac{\alpha}{\nu}=\Delta_{\mathcal{H}}(\lambda_c;N,N'). \tag{13}$$

From Eq. (2) we know that

$$\frac{\partial E_\lambda}{\partial\lambda} \underset{\lambda\to\lambda_c^+}{\sim} (\lambda-\lambda_c)^{\alpha-1}, \tag{14}$$

and by using the Hellmann-Feynman theorem [11] we obtain

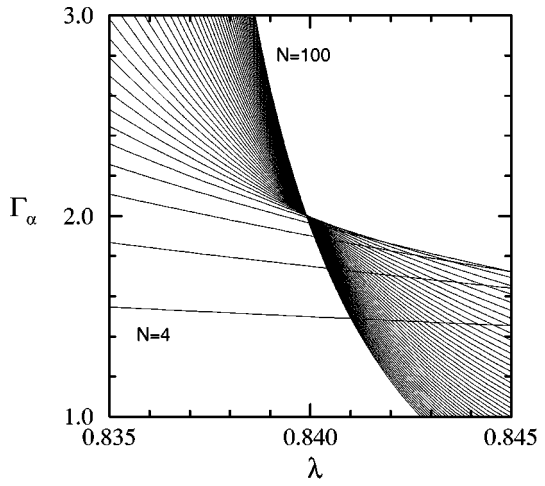

FIG. 1. $\Gamma_\alpha(\lambda;N,N-2)$ as a function of λ for the ground state of the Yukawa potential for even values of $4\leqslant N\leqslant 100$.

$$\frac{\partial E_\lambda}{\partial\lambda}=\left\langle\frac{\partial\mathcal{H}}{\partial\lambda}\right\rangle_\lambda=\left\langle\frac{\partial\mathcal{V}_\lambda}{\partial\lambda}\right\rangle_\lambda. \tag{15}$$

Taking $\mathcal{O}=\partial\mathcal{V}_\lambda/\partial\lambda$ in Eq. (11) gives an equation for $(\alpha-1)/\nu$ that together with Eq. (13) give the exponents α and ν. Now, we can define the function

$$\Gamma_\alpha(\lambda;N,N')=\frac{\Delta_{\mathcal{H}}(\lambda;N,N')}{\Delta_{\mathcal{H}}(\lambda;N,N')-\Delta_{\partial\mathcal{V}_\lambda/\partial\lambda}(\lambda;N,N')}, \tag{16}$$

which is also independent of the values of N and N' at the critical point $\lambda=\lambda_c$ and gives the critical exponent α,

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

From Eq. (13) the critical exponent ν is readily given by

$$\nu=\frac{\alpha}{\Delta_{\mathcal{H}}(\lambda_c;N,N')}. \tag{18}$$

The FSS equations are valid only as symptotic expressions, but unique values of λ_c, α, and ν (or any other quantity of interest) can be obtained as a succession of values as a function of N, N', and N''. The relation among N, N', and N'' was extensively studied in FSS in statistical mechanics [5], and it is known that the faster convergence is obtained when the difference among these numbers is as small as possible. This condition means $\Delta N=1$, except when there are parity effects; then one has to take $\Delta N=2$.

Then for $N'=N+\Delta N$, $N''=N-\Delta N$, we can obtain from Eqs. (16) and (18) successions of values for $\lambda^{(N)}$, $\alpha^{(N)}$, and $\nu^{(N)}$. The problem of the extrapolation of these data to $N\to\infty$ was also studied in detail [12], and in that study we used the algorithm of Bulirsch and Stoer [13] to obtain the extrapolated values of all the magnitudes.

At this point, as an example, let us illustrate how to use this approach to calculate the critical parameters for the Yukawa potential $(\exp[-\sigma r]/r)$. The scaled Hamiltonian for the Yukawa potential in atomic units $(r\to\sigma r;\ \mathcal{H}\to\mathcal{H}/\sigma^2)$ can be written as

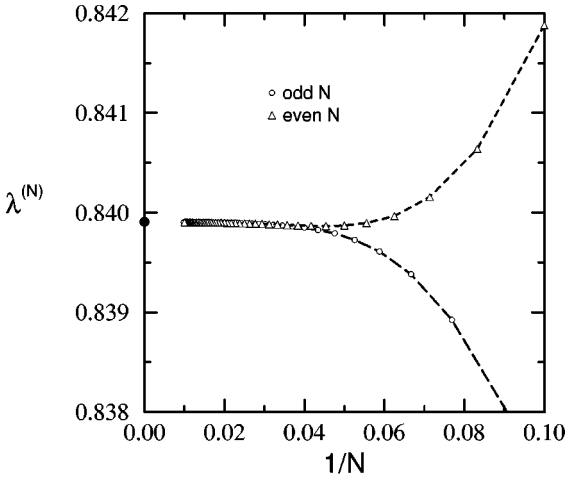

FIG. 2. $\lambda^{(N)}$ vs $1/N$ for the ground state of the Yukawa potential. The value of the extrapolated λ_c is also shown by a dot.

$$\mathcal{H}(\lambda) = -\frac{1}{2}\nabla^2 - \lambda\frac{e^{-r}}{r}, \tag{19}$$

where $\lambda = 1/\sigma$. It is known that perturbation expansion around the Coulombic limit $\sigma = 0$ is asymptotic with zero radius of convergence [14]. This Hamiltonian has bound states for large values of λ, and the exact value of the critical exponent is $\alpha = 2$ for states with zero angular momentum and $\alpha = 1$ for states with nonzero angular momentum [15].

To carry out the calculations for the critical parameters one should proceed with the following scheme. First, choose a convenient orthonormal basis set; for the Yukawa potential this is given by

$$\Phi_n(r,\Omega) = \frac{1}{\sqrt{(n+1)(n+2)}} e^{-r/2} L_{n-1}^{(2)}(r) Y_{l,m}(\Omega), \tag{20}$$

where $L_n^{(2)}(r)$ is the Laguerre polynomial of degree n and order 2 and $Y_{l,m}(\Omega)$ are the spherical harmonic functions of the solid angle Ω [16]. In this basis set one has to calculate the lowest eigenvalue and eigenvector of the finite Hamiltonian matrix. Second, use Eqs. (16), (17), and (18) in order to obtain $\lambda^{(N)}$, $\alpha^{(N)}$, and $\nu^{(N)}$. Due to parity effects we have to choose $\Delta N = 2$.

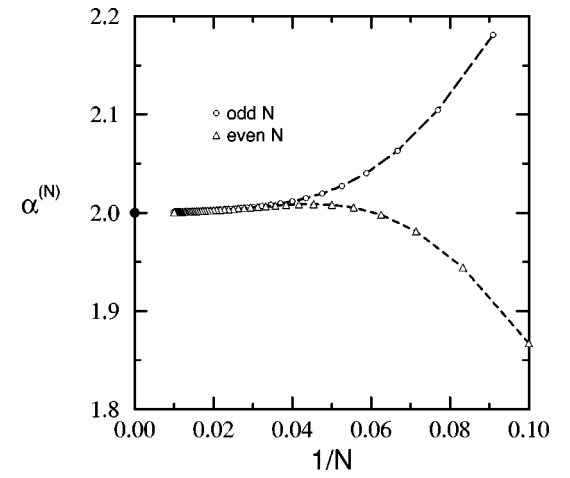

FIG. 3. $\alpha^{(N)}$ vs $1/N$ for the ground state of the Yukawa potential. The exact value of α is also shown by a dot.

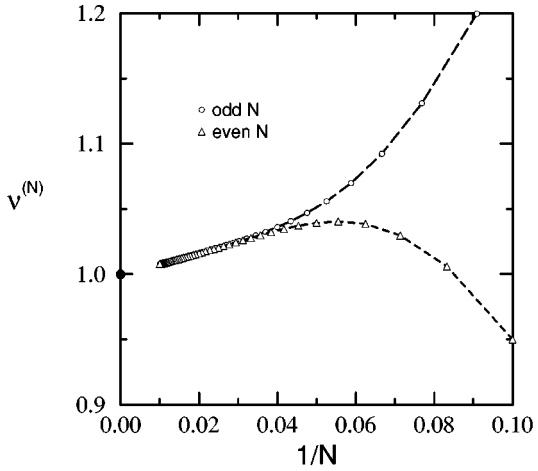

FIG. 4. $\nu^{(N)}$ vs $1/N$ for the ground state of the Yukawa potential. The value of the extrapolated ν is also shown by a dot.

For the ground state, the curves of $\Gamma_\alpha(\lambda;N,N-2)$ as a function $1/N$ for even values of N are shown in Fig. 1 for $4 \leqslant N \leqslant 100$. The curves of $\lambda^{(N)}$, $\alpha^{(N)}$, and $\nu^{(N)}$ against $1/N$ for $10 \leqslant N \leqslant 100$ are shown in Figs. 2, 3, and 4, respectively. It seems that a reasonable, large-N regime was obtained when $N > 20$. Finally, obtain the extrapolated values as $N \to \infty$ by using the algorithm of Bulirsch and Stoer [13]. The extrapolated values calculated with the points corresponding to $20 \leqslant N \leqslant 100$ for $l = 0$ are given in Table I and are in excellent agreement with the numerical value of λ_c [17] and the exact value for α [15].

In summary, we have presented an FSS approach to study directly the critical behavior of the different quantities in the Schrödinger equation. Results show that the method is very accurate for estimating the critical parameters. As far as we know these results are the most accurate estimates reported using an FSS approach for systems with no exact solutions. The method can be used to obtain the critical parameters for excited states. This can be achieved if the Hamiltonian com mutes with a given operator $\mathcal{A}$. Then, if we choose the basis set $\{\Phi_n\}$ as eigenfunctions of $\mathcal{A}$, the Hamiltonian becomes

TABLE I. Comparison of the critical parameters for the Yukawa potential for $l = 0$ and $l = 1$.

	Even N	Odd N	Ref.
		$l = 0$	
λ_c	0.839 903 9(1)	0.839 903 9(1)	0.839 908
α	2.000 00(2)	1.999 995(5)	2 (exact [a])
ν	0.999 9(2)	0.999 9(5)	
		$l = 1$	
λ_c	4.540 980(3)	4.540 979(1)	4.541 [a]
α	0.999 9(3)	0.999 8(2)	1 (exact [b])
ν	0.501(1)	0.501(1)	

[a]From Ref. [17].
[b]From Ref. [15].

block-diagonal, and therefore the method will be useful for the lowest eigenvalue of each block. An important case is when the Hamiltonian commutes with the total angular momentum. In this case we can study the critical behavior of each lowest-energy eigenvalue corresponding to a given value of the angular momentum. Results for estimating the critical parameters for Yukawa with $l=1$ are also given in Table I. The method is general, simple to implement, and can be generalized in a straightforward manner to treat Hamiltonians with many parameters $\{\lambda_i\}$.

We would like to acknowledge the financial support of the Office of Naval Research (Grant No. N00014-97-1-0192).

[1] M.E. Fisher, in *Critical Phenomena*, Proceedings of the 51st Enrico Fermi Summer School, Varenna, Italy, edited by M.S. Green (Academic Press, New York, 1971); M.E. Fisher and M.N. Barber, Phys. Rev. Lett. **28**, 1516 (1972).

[2] P.J. Reynolds, H.E. Stanley, and W. Klein, Phys. Rev. B **21**, 1223 (1980).

[3] J.P. Neirotti and M.J. de Oliveira, Phys. Rev. B **53**, 668 (1996); **54**, 6351 (1996).

[4] J.L. Cardy, *Finite-Size Scaling* (Elsevier Science Publishers, New York, 1988).

[5] *Finite Size Scaling and Numerical Simulations of Statistical Systems*, edited by V. Privman (World Scientific, Singapore, 1990).

[6] J.P. Neirotti, P. Serra, and S. Kais, Phys. Rev. Lett. **79**, 3142 (1997).

[7] M.P. Nightingale, Physica A **83**, 561 (1976).

[8] B. Simon, J. Funct. Anal. **25**, 338 (1977).

[9] B. Derrida and L. De Seze, J. Phys. (France) **43**, 475 (1982).

[10] T. Kato, *Perturbation Theory for Linear Operators*, 2nd ed. (Springer, New York, 1976).

[11] See, for example, E. Merzbacher, *Quantum Mechanics*, 2nd ed. (John Wiley, New York, 1970).

[12] M. Henkel, in *Finite Size Scaling and Numerical Simulations of Statistical Systems* (Ref. [5]), Chap. VIII.

[13] R. Bulirsch and J. Stoer, Numer. Math. **6**, 413 (1964).

[14] V.M. Vainberg, V.L. Eletskii, and V.S. Popov, Sov. Phys. JETP **54**, 833 (1981).

[15] M. Klaus and B. Simon, Ann. Phys. (Paris) **130**, 251 (1980).

[16] *Handbook of Mathematical Functions*, edited by M. Abramowitz and I. Stegun (Dover, New York, 1972).

[17] F.J. Rogers, H.C. Graboske, and D.J. Harwood, Phys. Rev. A **1**, 1577 (1970).