Finite Size Scaling in Quantum Mechanics

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The finite size scaling ansatz is combined with the variational method to extract information about critical behavior of quantum Hamiltonians. This approach is based on taking the number of elements in a complete basis set as the size of the system. As in statistical mechanics, the finite size scaling can then be used directly in the Schrödinger equation. This approach is general and gives very accurate results for the critical parameters, for which the bound-state energy becomes absorbed or degenerate with a continuum. To illustrate the applications in quantum calculations, we present detailed calculations for both short- and long-range potentials.

I. Introduction

In statistical mechanics, the singularities in thermodynamic functions associated with a critical point occur only in the thermodynamic limit, when all the dimensions of the system under consideration tend to infinity. Strictly speaking, there are no phase transitions in a finite system at nonzero temperature, and yet, experiments as well as numerical calculations all use finite systems.[1] To address this problem, the finite size scaling method was formulated by Fisher[2] and others[3] to extrapolate information obtained from a finite system to the thermodynamic limit.

In quantum mechanics, when using variation methods, one encounters the same finite size problem in studying the critical behavior of a quantum Hamiltonian $H(\lambda_1,...,\lambda_k)$ as a function of its set of parameters $\{\lambda_i\}$. In this context, critical means the values of $\{\lambda_i\}$ for which a bound-state energy is nonanalytic. In many cases, as in this study, this critical point is the point where a bound-state energy becomes absorbed or degenerate with a continuum. In this case, 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 wave function of a given Hamiltonian.

Recently, we used the finite size scaling and phenomenological renormalization equations for calculations of the critical charges for two-[4,5] and three-electron systems.[6] This approach is based on taking the lowest eigenvalues of a quantum Hamiltonian as the leading eigenvalues of a transfer matrix of a classical pseudosystem.

In this paper we will assume that there exists a scaling function for the truncated mean value of a given operator, and with the help of the Hellmann−Feynman theorem we can obtain a direct finite size scaling approach to the Schrödinger equation.[7] This approach is general and can be used to study critical behavior of a quantum Hamiltonian as a function of its parameters. To illustrate this approach, we include detailed calculations for the critical parameters for two cases with qualitatively different behavior: one with short-range interaction, the Yukawa potential, and one with a long-range interaction, the inverse power law potential.

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II. Finite Size Scaling

In statistical mechanics, the finite size scaling method (FSS) allows a systematic way to extract the critical behavior of infinite systems from studies done on finite systems.[2,3] If in the thermodynamic limit, $N \rightarrow \infty$, a quantity K develops a singularity as a function of the temperature T in the form

$$K(T) = \lim_{N\to\infty} K_N(T) \approx |T - T_c|^{-\rho} \tag{1}$$

and in particular for the correlation length

$$\xi(T) = \lim_{N\to\infty} \xi_N(T) \approx |T - T_c|^{-\nu} \tag{2}$$

then the FSS ansatz assumes the existence of scaling function F_K such that

$$K_N(T) \approx K(T) F_K\left(\frac{N}{\xi(T)}\right) \tag{3}$$

where $F_K(y)$ is an analytical function. Since the FSS ansatz, eq 3, should be valid for any quantity that exhibits an algebraic singularity in the bulk, we can apply it to the correlation length ξ itself. Thus, the correlation length in a finite system should have the form[8]

$$\xi_N(T) \approx N\phi_\xi(N^{1/\nu}|T - T_c|) \tag{4}$$

The special significance of this result was first realized by Nightingale,[9] who showed how it could be reinterpreted as a renormalization group transformation of the infinite system. The phenomenological renormalization (PR) equation for finite systems of sizes N and N' is given by

$$\frac{\xi_N(T)}{N} = \frac{\xi_{N'}(T')}{N'} \tag{5}$$

and has a fixed point at $T^{(N,N')}$. It is expected that the succession of points $\{T^{(N,N')}\}$ will converge to the true T_c in the infinite size limit.

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In order to apply the FSS to quantum mechanics problems, let us consider the following Hamiltonian of the form

$$H = H_0 + V_\lambda \tag{6}$$

where H_0 is λ-independent and V_λ is the λ-dependent term. We are interested in the study of how the different properties of the system change when the value of λ varies. In this study a critical point λ_c will be defined as a point for which a bound state becomes absorbed or degenerate with a continuum.

Without loss of generality, we will assume that the Hamiltonian, eq 6, has a bound state E_λ for $\lambda > \lambda_c$, which becomes equal to zero at $\lambda = \lambda_c$. As in statistical mechanics, we can define some critical exponents related to the asymptotic behavior of different quantities near the critical point. In particular, for the energy we can define the critical exponent α as

$$E_\lambda \approx (\lambda - \lambda_c)^\alpha \quad \text{for} \quad \lambda \rightarrow \lambda_c^{+} \tag{7}$$

For general potentials of the form $V_\lambda = \lambda \bar{V}$, Simon[10] showed that the critical exponent α is equal to 1 if and only if $H(\lambda_c)$ has a normalizable eigenfunction with eigenvalue equal to zero. The existence or absence of a bound state at the critical point is related to the type of singularity in the energy. Using statistical mechanics terminology, we can associate "first-order phase transitions" with the existence of a normalizable eigenfunction at the critical point. The absence of such a function could be related to "continuous phase transitions".

In quantum calculations, the variation method is widely used to approximate the solution of the Schrödinger equation. To obtain exact results, one should expand the exact wave function in a complete basis set and take the number of basis functions to infinity. In practice, one truncates this expansion at some order N. In the present approach, the finite size corresponds not to the spatial dimension, as in statistical mechanics, 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

$$\Psi_\lambda = \sum_n a_n(\lambda)\Phi_n \tag{8}$$

where n represents the set of quantum numbers. In order to approximate the different quantities, we have to truncate the series, eq 8, at order N. Then the Hamiltonian is replaced by $M(N) \times M(N)$ matrix $H^{(N)}$, with $M(N)$ being the number of elements in the truncated basis set at order N. By use of the standard linear variation method, the Nth-order approximation for the energies are given by the eigenvalues $\{\Lambda_i^{(N)}\}$ of the matrix $H^{(N)}$,

$$E_\lambda^{(N)} = \min_{\{i\}}\{\Lambda_i^{(N)}\} \tag{9}$$

The corresponding eigenfunctions are given by

$$\Psi_\lambda^{(N)} = \sum_n^{M(N)} a_n^{(N)}(\lambda)\Phi_n \tag{10}$$

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

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

where $O_{n,m}$ are the matrix elements of O in the basis set $\{\Phi_n\}$. In general, the mean value $\langle O\rangle$ is not analytical at $\lambda = \lambda_c$, and we can define a critical exponent, μ_O, by the relation

$$\langle O\rangle_\lambda \approx (\lambda - \lambda_c)^{\mu_O} \quad \text{for} \quad \lambda \rightarrow \lambda_c^{+} \tag{12}$$

In statistical mechanics, the singularities in thermodynamic functions associated with a critical point occur only in the thermodynamic limit. In the variation approach singularities in the different mean values will occur only in the limit of infinite basis functions.

As in the FSS ansatz in statistical mechanics,[11] we will assume that there exists a scaling function for the truncated magnitudes such that

$$\langle O\rangle_\lambda^{(N)} \approx \langle O\rangle_\lambda F_O(N|\lambda - \lambda_c|^\nu) \tag{13}$$

with a different scaling function F_O for each different operator but with a unique scaling exponent ν.

Now we are in a position to obtain the critical parameters by defining the following function

$$\Delta_O(\lambda;N,N') = \frac{\ln(\langle O\rangle_\lambda^{(N)}/\langle O\rangle_\lambda^{(N')})}{\ln(N'/N)} \tag{14}$$

At the critical point, the mean value depends on N as a power law, $\langle O\rangle \approx N^{-\mu_O/\nu}$; thus, one obtains an equation for the ratio of the critical exponents

$$\Delta_O(\lambda_c;N,N') = \frac{\mu_O}{\nu} \tag{15}$$

which is independent of the values of N and N'. Thus, for three different values N,N' and N'' the curves defined by eq 14 intersect at the critical point

$$\Delta_O(\lambda_c;N,N') = \Delta_O(\lambda_c;N'',N) \tag{16}$$

In order to obtain the critical exponent α, which is associated with the energy, we can take $O = H$ in eq 15 with $\mu_O = \alpha$,

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

and by using the Hellmann−Feynman theorem,[12] we obtain

$$\frac{\partial E_\lambda}{\partial \lambda} = \left\langle \frac{\partial H}{\partial \lambda} \right\rangle_\lambda = \left\langle \frac{\partial V_\lambda}{\partial \lambda} \right\rangle_\lambda \tag{18}$$

Taking $O = \partial V_\lambda/\partial\lambda$ in eq 15 gives an equation for $(\alpha - 1)/\nu$ that, together with eq 17, gives the exponents α and ν.

The FSS equations are valid only as asymptotic expressions, $N \rightarrow \infty$, but with a finite basis set, unique values of λ_c, α, and ν can be obtained as a succession of values as a function of N, N' and N''. The relation between N, N' and N'' was extensively studied in FSS in statistical mechanics,[3] and it is known that the fastest convergence is obtained when the difference between these numbers is as small as possible. In this study we took $\Delta N = 1$, and when there are parity effects, we used $\Delta N = 2$. In order to obtain the extrapolated values for $\lambda^{(N)}$, $\alpha^{(N)}$, and $\nu^{(N)}$ at

$N \rightarrow \infty$, we used the algorithm of Bulirsch and Stoer[13] with $N' = N + \Delta N$ and $N'' = N - \Delta N$. This algorithm was also studied in detail and gives very accurate results for both statistical mechanics problems[14] as well as electronic structure critical parameters.[4−6]

III. Numerical Calculations

To illustrate the applications of the FSS method in quantum mechanics, two cases with qualitatively different behavior near the critical point have been studied: one with short-range interaction, the Yukawa potential, and one with a long-range interaction, the inverse power law potential. In both cases the potential is spherically symmetric, and therefore, the critical behavior can be studied for zero and nonzero angular momentum.

A convenient orthonormal basis set that can be used in both cases is of the form

$$\Phi_{n,l,m}(r,\Omega) = \frac{1}{\sqrt{(n+1)(n+2)}} e^{-r/2} L_n^{(2)}(r) Y_{l,m}(\Omega) \quad (19)$$

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 solid angle Ω.[15]

In this basis set, one has to calculate the lowest eigenvalue and eigenvector of the finite Hamiltonian matrix. The matrix elements of the kinetic energy operator can be calculated analytically, and therefore, the problem reduces to calculation of the matrix elements of the particular potential. Now, in order to obtain the numerical values for λ_c, α, and υ, we can use eqs 16−18 or we can simply define the following function

$$\Gamma_\alpha(\lambda;N,N') = \frac{\Delta_H(\lambda;N,N')}{\Delta_H(\lambda;N,N') - \Delta_{\partial V_\lambda/\partial\lambda}(\lambda;N,N')} \quad (20)$$

which is also independent of the values of N and N' at the critical point $\lambda = \lambda_c$. Plotting $\Gamma_\alpha(\lambda;N,N')$ as a function of λ gives a family of curves with an intersection at λ_c. At the point $\lambda = \lambda_c$ one can read the critical exponent α,

$$\alpha = \Gamma_\alpha(\lambda_c;N,N') \quad (21)$$

and from eq 17 the critical exponent υ is readily given by

$$\upsilon = \frac{\alpha}{\Delta_H(\lambda_c;N,N')} \quad (22)$$

A. Short-Range Potentials. There are many rigorous results known about the critical behavior of short-range one-body potentials. Klaus and Simon[16] consider a family of Schrödinger operators, $-\nabla^2 + \lambda V$, with coupling constant λ and short-range potential V. Their results address two general questions. (i) Is the eigenvalue $E(\lambda)$ analytic at $\lambda = \lambda_c$? (ii) What is the leading order of the expansion in $(\lambda - \lambda_c)^\alpha$?

In this section we will analyze these two questions for the Hamiltonian of the screened Coulomb potential. In atomic units the Hamiltonian can be written as

$$H = -\frac{1}{2}\nabla^2 - \frac{e^{-\sigma r}}{r} \quad (23)$$

It is well-known that the perturbation expansion in σ around the Coulombic limit, $\sigma = 0$, is asymptotic with zero radius of convergence.[17]

TABLE 1: Comparison of the Critical Parameters λ_c, α, and υ for the Short-Range Yukawa Potential for $l = 0$ and $l = 1$

	even N	odd N	ref
		$l = 0$	
λ_c	0.8399039(1)	0.8399039(1)	0.839908
α	2.00000(2)	1.999995(5)	2 (exact[b])
υ	0.9999(2)	0.9999(5)	
		$l = 1$	
λ_c	4.540980(3)	4.540979(1)	4.541[a]
α	0.9999(3)	0.9998(2)	1 (exact[b])
υ	0.501(1)	0.501(1)	

[a] From ref 26. [b] From ref 16.

In order to linearize the Hamiltonian in the external parameter, we perform the following scaling transformation

$$r \rightarrow \sigma r; \quad H \rightarrow \frac{H}{\sigma^2} \quad (24)$$

With $\lambda = 1/\sigma$ the Hamiltonian takes the final form

$$H(\lambda) = -\frac{1}{2}\nabla^2 - \lambda\frac{e^{-r}}{r} \quad (25)$$

This Hamiltonian has bound states for large values of λ, and the exact value of the critical exponent α is $\alpha = 2$ for states with zero angular momentum and $\alpha = 1$ for states with nonzero angular momentum.[16]

We used the finite size scaling equations, eqs 20−22, in order to obtain the pseudocritical $\lambda^{(N)}$, $\alpha^{(N)}$, and $\upsilon^{(N)}$. Owing to parity effects, we have to take $\Delta N = 2$. The extrapolated results for both states with angular momentum $l = 0$ and $l = 1$ are summarized in Table 1. The behavior of the ground-state energy, $E_0^{(N)}$, as a function of λ for different values of N is shown in Figure 1a. For $l = 0$, the energy curve goes smoothly to zero as a function of λ but the second derivative function develops a discontinuity in the neighborhood of the critical point, $\lambda_c \simeq 0.8399$. This behavior is different from that of $l = 1$ results, where the energy curve bends sharply to zero at the critical point, $\lambda_c \simeq 4.5409$, as shown in Figure 1b. As one should expect, there is a discontinuity in the first derivative as a function of λ.

For the case $l = 0$, the eigenfunction is not normalizable at $\lambda = \lambda_c$. It is interesting to note that for the Hülten Hamiltonian, another potential with an exponential decay and exact solution for the ground state,[18] the expansion coefficients of the wave function have the asymptotic form

$$a_n(\lambda) \approx (\lambda - \lambda_c)^{1/2} \quad \text{for} \quad \lambda \rightarrow \lambda_c^+ \quad (26)$$

independent of the basis set and the value of n. It seems that this result is general and suggests that there is a unique critical exponent for the expansion coefficients. We assume that, with $\alpha \neq 1$, there is a unique critical exponent μ_a defined by

$$a_n(\lambda) \approx_{\lambda\rightarrow\lambda_c^+} (\lambda - \lambda_c)^{\mu_a} \quad \text{for} \quad \lambda \rightarrow \lambda_c^+ \quad (27)$$

Assuming this is a universal behavior for the coefficients $\{a_n\}$ it is possible to show, by use of the expansion, eq 8, in the Hellmann−Feynman theorem, that $\mu_a = (\alpha - 1)/2$.

To verify these results, parts a and b of Figure 2 show the behavior of the leading coefficients $a_0^{(N)}$ and $a_1^{(N)}$ as a function of λ. The curves bend to zero at λ_c, and in the limit of $N \rightarrow \infty$ both a_0 and a_1 take the value zero for all λ below λ_c. Figure 3 show the extrapolated value for the critical exponent μ as a

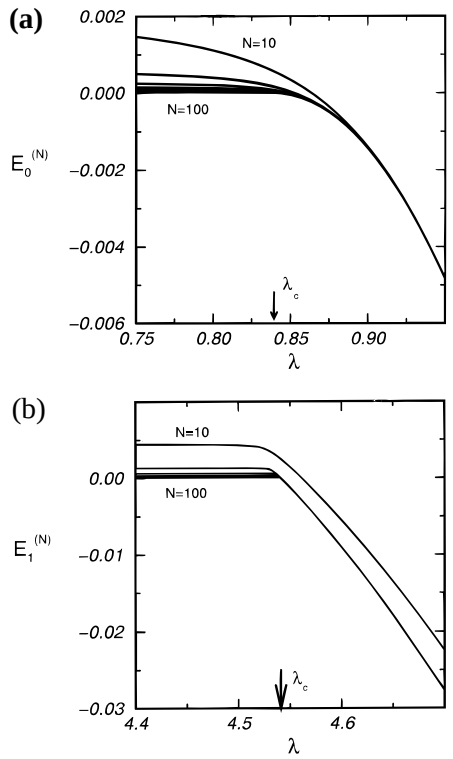

Figure 1. Variational energy for the Yukawa potential as a function of λ for $N = 10, 20, 30, ..., 100$: (a) for the ground-state energy with $l = 0$; (b) for the state with angular momentum $l = 1$. The value of the extrapolated λ_c is also shown by an arrow.

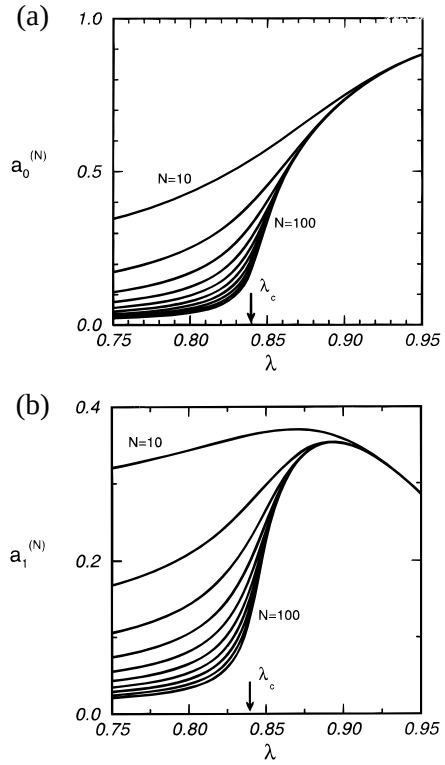

Figure 2. Expansion coefficients for the ground-state wave function of the Yukawa potential as a function of λ for $N = 10, 20, 30, ..., 100$: (a) leading coefficient $a_0^{(N)}$; (b) second coefficient $a_1^{(N)}$.

function of $1/N$ for the first four expansion coefficients $n = 0$, 1, 2, 3. The extrapolated values are 0.4865, 0.4865, 0.4477, and 0.4233, respectively. The larger the value of n, the larger is the numerical error, so we expect the most accurate result is

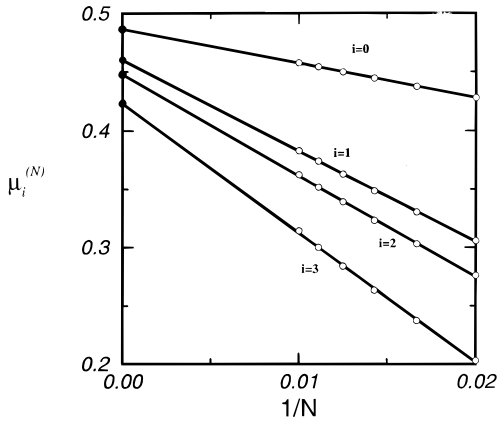

Figure 3. Critical exponent $\mu_n^{(N)}$ as a function of $1/N$ for $n = 0$, 1, 2, 3. Open circles represent $N = 50$, 60, 70, 80, 90, 100, and the extrapolated value of the critical exponent is shown by a dot.

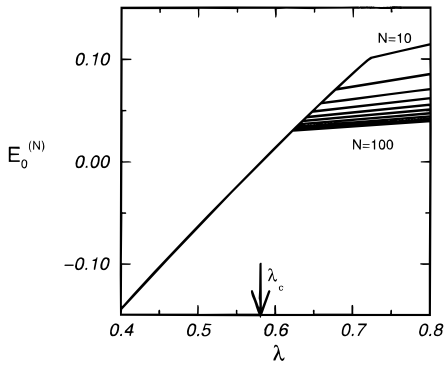

Figure 4. Variational energy for the ground state of the long-range potential (eq 29 in the text) as a function of λ for $N = 10, 20, 30, ..., 100$. The value of the extrapolated λ_c is also shown by an arrow.

for the case $n = 0$. Our conjecture is that the exact value of μ_n is equal to $^1/_2$ for all n; that is, μ is a "universal exponent" for the coefficients independent of the value of n or the basis set.

B. Long-Range Potentials. For the two-electron Coulomb problem, a long-range two-body potential, the ground state is degenerate with the continuum with a critical exponent $\alpha = 1$ and has a normalizable eigenfunction at the critical point.[19] The critical point is the minimum value of the nuclear charge necessary to bind two electrons and is about 0.911 16. Stillinger discussed another family of long-range potentials that can be solved exactly.[20] For the ground state of the potential $V(r) = -3/32r^2 + b/(8\sqrt{r}) - c/(8r)$, he showed that there exists a normalizable eigenfunction at the critical point and that the critical exponent is $\alpha = 1$.

To illustrate the applications of the finite size scaling method for long-range potentials, we investigated the following potential

$$V_\lambda(r) = -\frac{1}{r} + \frac{\lambda}{r^{1/2}} \tag{28}$$

For this potential there is no parity effect, and we choose $\Delta N = 1$. The finite size scaling results are qualitatively very similar to the results of the two-electron atoms.[5] We have found that the energy curves as a function of λ bends over sharply at λ_c to become degenerate with the continuum. This behavior of the ground state for different values of N is shown in Figure 4. In virtue of this behavior, we expect that the first derivative of the energy with respect to λ will develop a steplike discontinuity at λ_c. The first derivative is shown in Figure 5. The extrapolated values of λ_c and α are listed in Table 2.

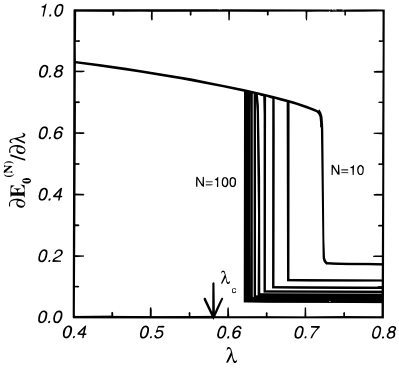

Figure 5. First derivative of the ground-state energy of the long-range potential (eq 29 in the text) as a function of λ for $N = 10, 20, 30, ..., 100$. The value of the extrapolated λ_c is also shown by an arrow.

TABLE 2: Comparison of the Critical Parameter λ_c and α of the Long-Range Potential Eq 29 for $l = 0$ and $l = 1$

	$l = 0$	$l = 1$
λ_c	0.581093706(3)	0.2813341273714(7)
α	1.0000000(4)[a]	1.000000000(3)[a]

[a] Exact $\alpha = 1$ (ref 16).

IV. Conclusions

In the field of atomic and molecular physics, it has been suggested for some time that there are possible analogies between critical phenomena and singularities of the energy.[21−23] In particular, it has been noted that the energy curves of the two-electron atoms as a function of the inverse of the nuclear charge resemble the free energy curves as a function of the temperature for the van der Waals gas.[21] Using the large dimension limit model for electronic structure problems, we showed that symmetry breaking of the electronic structure configurations for the many-electron atoms and simple molecular systems can be studied as mean-field problems in statistical mechanics.[24,25]

Recently, we have shown that the FSS method can be used indirectly to obtain critical parameters for quantum Hamiltonians by taking the lowest eigenvalues of a quantum Hamiltonian as leading eigenvalues of a transfer matrix of a classical pseudo-system. This approach was successfully used to obtain the critical charges for two- and three-electron atoms.[4−6] In this study we present a direct FSS approach for studying the critical behavior of quantum Hamiltonians without the need to make any explicit analogy to classical statistical mechanics. The critical parameters can be calculated by a systematic expansion in a finite basis set.

In this paper we have found that there are fundamental differences between short-range and long-range potentials. For the ground state of the Yukawa potential, the critical exponent $\alpha = 2$, the wave function is not normalizable at $\lambda = \lambda_c$, the energy curves go smoothly to zero as a function of λ, and the second derivative develops a discontinuity in the neighborhood of the critical point. This type of behavior resembles a "continuous phase transition". For the ground state of the inverse power law potential, the critical exponent $\alpha = 1$, the wave function is normalizable at $\lambda = \lambda_c$, the energy curves bend over sharply at λ_c to become degenerate with the continuum, and the first derivative develops a steplike discontinuity at λ_c, which resembles a "first-order phase transition".

It is worth noting that we assumed that for the expansion coefficients of the wave function there is a unique "universal" critical exponent. For the Yukawa and the Hülten potentials $\mu = {}^1/_2$ and in general $\mu = (\alpha - 1)/2$, which is related to the critical exponent on the energy α. This assumption needs further verification, but numerical results in this study indicate that this assumption is general and correct.

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