Quantum criticality for few-body systems: Path-integral approach

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We present the path-integral approach to treat quantum phase transitions and critical phenomena for few-body quantum systems. Allowing the space and time variables to have discrete values, we turn the quantum problem into an effective classical lattice problem. Imposing the constraint that any change in space time must preserve the scaling invariance of Brownian paths, we show that the mapped classical lattice system has a known scaling behavior when the particle is free, which breaks down when the strength of the interaction potential reaches a certain value. In principle, any quantity with known scaling behavior may be used to determine the transition point. We illustrate the method by numerically evaluating the correlation length and the radial mean distance for a system composed of a single particle in the presence of an attractive Pöschl-Teller potential in one and three dimensions. The method is general and has potential applicability for large systems.

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I. INTRODUCTION

Recently, several analogies have been proposed to describe the ground-state stability of atoms and molecules in terms of phase-transition and critical phenomena [1]. One of the goals of such analogies is to provide a systematic procedure to extrapolate numerical data calculated with truncated basis sets to the infinite limit [2]. The phase-transitions analogies are supported by the fact that a D-dimensional quantum system can be mapped to a $(D+1)$-dimensional classical pseudosystem [3]. For the classical pseudosystem, the statistical mechanics formalism holds. Thus, the idea that a phase transition leads to a divergence in certain quantities at the thermodynamic limit may be mapped in terms of quantities of the original quantum problem [4]. In particular, the size of the classical pseudo-system is mapped as the number of elements of the truncated basis set used to study the quantum system [2,5]. The phase transition of a statistical-mechanics systems that occurs only in the thermodynamic limit is mapped into divergences of quantities of the original quantum problem that emerges as more elements are added to the truncated basis set. With this analogy, we have shown that the finite-size scaling theory is very useful in studying critical points in quantum few-body problems [6]. In particular, we used a phenomenological renormalization equation to obtain the critical nuclear charges for few-electron atoms [2,5] and simple diatomic molecules [7,8].

Recently, we have presented explicitly the $(D+1)$-dimensional classical system using Feynman's path integral formalism [9]. With this formalism, the quantum partition function in D-dimensions looks like a classical partition function of a system in $D+1$ dimensions with the extra dimension being the time. With this mapping, and allowing the space and time variables to have discrete values, we turn the quantum problem into an effective classical lattice problem. This natural choice of Feynman's path integral makes the analogies less abstract and gives a physical meaning to the formulas used to obtain the phase transition in the original quantum problem [9]. In this paper, we show that the mapping to a classical lattice system brings a more fundamental definition of phase transition, and consequently, other tools to find the transition points.

Having a classical pseudosystem connected to the original quantum problem allows us to go further in the phase-transition analogies by realizing that the divergences in thermodynamic quantities are consequences of a more fundamental phenomena. The divergence of the correlation length when the system is critical is due to the fact that the classical lattice shows fractal patterns, or in other words, the classical lattice becomes self similar in all length scales. Thus, it is not necessary to limit the phase-transition analogies to the search for points where the correlation length diverges. Any quantity that changes its scaling behavior in a phase transition can be used. In this paper, we show that the classical lattice mapping using Feynman's path integral has a known scaling behavior when the particle is free, which breaks down when an external potential is made strong enough.

II. PATH-INTEGRAL APPROACH AND QUANTUM CRITICALITY

Using the Feynman's path-integral approach, the fundamental equation to describe a system is the integral kernel of the time evolution operator $\exp(-i(t''-t')/\hbar\mathcal{H})$ from $t=t'$ to $t=t''>t'$. The integral kernel of the operator $\exp(-T\mathcal{H}/\hbar)$, which is the analytic continuation to imaginary time of the evolution operator, is known as the Feynman-Kac formula and reads

$$K(x',x'';T)=\int_{(x',t')}^{(x'',t'')}\mathcal{D}x(t)\times\exp\left[-\frac{1}{\hbar}\int_{t'}^{t''}\left(\frac{m}{2}\dot{x}^2+V(x;\lambda)\right)dt\right], \quad (1)$$

where the imaginary time interval $T=t''-t'$ is assumed to be positive, and $x=x(t)$. The notation $\int\mathcal{D}x(t)$ means an integration over all paths that begins in the space-time point

(x',t') and ends in (x'',t''). The potential function $V(x;\lambda)$ depends on the parameter λ, which sets its strength [10,11].

In practical calculation, it is preferred to use the path-integral lattice definition, where the time t is defined only in the sites of a regular time lattice with lattice-constant $\Delta T = T/N_T$. The initial lattice point is $t_0 = t'$, the last one is $t_{N_T} = t''$, and any intermediate instant is given by $t_j = t' + j\Delta T$, $j = 0,1,\ldots,N_T$. The position in each instant is given by $x_j = x(t_j)$. Using this construction, the Feynman-Kac lattice formula reads [12]

$$K(x',x'';T) = \lim_{N_T\to\infty}\left(\frac{m}{2\pi\hbar\Delta T}\right)^{N_T/2}\prod_{k=1}^{N_T-1}\int dx_k \times\exp\left[-\frac{1}{\hbar}\sum_{j=1}^{N_T}\left(\frac{m}{2\Delta T}(x_j-x_{j-1})^2 + \Delta T V(x_j;\lambda)\right)\right]. \tag{2}$$

The path-integral summation is performed doing a regular integration over the N_T-1 real variables $x_k \in [-\infty,\infty]$. The original definition is recovered in the limit $N_T\to\infty$ and $\Delta T \to 0$ with T finite.

The integral kernel $K(x'',x';T)$ is formally equal to the probability density function of statistical-mechanics $\rho(x'',x',\beta)$, where the imaginary time interval T and the inverse temperature β are related by $T = \beta\hbar$. Thus, the Feynman-Kac formula may be used to evaluate the statistical-mechanics partition function, $Z = \mathrm{Tr}\,\rho$, by summations in the Euclidean space instead of the Hilbert space. The Euclidean space variables may be viewed as state variables of a space-time lattice. Thus, we see that the quantum problem may be mapped into a classical pseudosystem. The imaginary time is the extra dimension that was added in order to overcome the summation in the Hilbert space.

In the absence of the potential, the path-integral summation is a summation over Brownian paths. Given the position x_{j-1} and the time interval ΔT, the increment $y_j = x_j - x_{j-1}$ is a random variable with probability proportional to $e^{-my^2/(2\hbar\Delta T)}$. The Brownian paths have a fractal nature and are self similar as long as one scales the space and time direction with [13]

$$x \to bx, \quad t \to b^2 t, \tag{3}$$

where the scale factor b is any real positive number.

The classical system, whose states are given by the Brownian paths, (the system may be also interpreted as a Gaussian polymer [14]) may be rescaled by the relations given in Eq. (3) to preserve the same structure. This fact makes the time lattice critical in the sense of renormalization-group theory [15,16]. When the strength of the attractive potential $\lambda\to\infty$, the particle must be bound and the contribution to the path integral summation of the Brownian paths are weighted by the factor $\exp[(-1/\hbar)\int_{t'}^{t''}V(x(t);\lambda)dt]$. Thus, the paths in the neighborhood of the origin contribute much more than paths filling uniformly the whole space. The system is not scaling invariant anymore because we can devise two regions in the space, one where the particle is likely to be localized and the other where it is not.

We may classify the system by the Brownian paths that effectively contribute to the evaluation of the Feynman-Kac formula. If the system is scale invariant, the system is in a critical phase. If the scaling invariance is broken by the potential, we have a noncritical phase. The transition between these two phases at a finite value of lambda $\lambda = \lambda_c$ will be properly called a phase transition.

In order to numerically study this problem, we consider a finite and discrete space. The coordinates x_j are defined in a regular lattice with lattice-constant ΔL. The linear system size is given by $L = N_L\Delta L$, where N_L is the number of points along the position coordinate axis. Thus, the Feynman-Kac formula may be written in terms of matrix products $K(x_0,x_{N_T};T) = T(x_0,x_1)T(x_1,x_2)\ldots T(x_{N_T-1},x_{N_T})$ where, the matrix T is called a transfer matrix and is defined as

$$T(x_j,x_{j-1}) = \left(\frac{m\Delta L^2}{2\pi\hbar\Delta T}\right)^{1/2}\exp\left[-\frac{1}{\hbar}\left(\frac{m}{2\Delta T}(x_j-x_{j-1})^2 + \Delta T V(x_j;\lambda)\right)\right]. \tag{4}$$

Notice the transfer matrix is a matrix representation of the short-time evolution operator $\exp(-\Delta T\mathcal{H}/\hbar)$.

The original Euclidean system may be recovered by taking the continuum limit of both $\Delta L\to 0$ and $\Delta T\to 0$. In order to preserve the scaling properties of the Brownian paths given in Eq. (3), the ratio $\Delta L/\Delta T^2$ must remain constant. The number of points of the space-time lattice is given by $N_T N_L$. Thus, the thermodynamic limit is given by $N_T\to\infty$ and $N_L\to\infty$. However, in order to preserve the scaling properties we must also set $N_T = N_L^2$.

The numerical study of the phase transition is made by fixing the grid spacing ΔL and ΔT and the discretization number N_L, which sets the rank of the transfer matrix to be diagonalized. The numerical calculation in a discrete and finite system gives an estimate of the actual values of all observables. The ground-state energy $E_L^{(0)}$ is given by

$$e^{-N_T\Delta T E_L^{(0)}/\hbar} = Z = \mathrm{Tr}[T^{N_T}]. \tag{5}$$

The above expression is valid in the limit of large $T = N_T\Delta T$. The subscript L in Eq. (5) stresses the existence of finite-size effects, and the dependence on the grid spacing is omitted to avoid overcrowding the notation.

For a large N_T, the trace is dominated by the leading eigenvalue of the transfer-matrix $Z \approx (a_L^{(0)})^{N_T}$ and the ground-state energy is given by

$$E_L^{(0)} = -\frac{\hbar}{\Delta T}\ln(a_L^{(0)}), \tag{6}$$

where $a_L^{(0)}$ is the leading eigenvalue of the transfer matrix. Having the leading eigenvector of the transfer matrix, one may evaluate any other ground-state expectation value. Be-

cause all geometric properties of the fractal Brownian paths are preserved in the critical region, the root-mean-square displacement $R_L=\langle x^2\rangle^{1/2}$ must scale with the macroscopic dimension L. If the particle is bound, R_L must achieve a finite value independent of L. Hence, R_L has a different scaling behavior if the particle is free or bound. This, in principle, may be used to determine the phase-transition point.

The correlation length ξ along the imaginary time direction is the other quantity we can use to determine the critical region. The correlation length is defined as the asymptotic behavior of the correlation function

$$C(j\Delta T)=\langle x_0 x_j\rangle-\langle x_0\rangle^2\approx\exp\left(-\frac{j\Delta T}{\xi}\right)\quad j\to\infty. \quad (7)$$

The correlation length may be written in terms of the two leading eigenvalues $a_L^{(0)}$ and $a_L^{(1)}$ of the transfer matrix

$$\xi_L=-\Delta T\frac{1}{\ln(a_L^{(1)}/a_L^{(0)})}. \quad (8)$$

When the system is critical, the quantum states must be correlated in all length scales along the time direction, and thus, the correlation length must scale with $\xi\sim T$. Hence, in the true free-particle case with $T\to\infty$ and $L\to\infty$ the correlation length diverges. Since L is finite, one cannot have a true divergence, but the scaling relations presented in Eq. (3) should still apply if L is finite and sufficiently large. Thus, the correlation length must scale as $\xi\sim L^2$ in the critical region.

For a given value of the critical parameter λ, we perform calculations with different system sizes. If $\xi_L(\lambda)$ scales with L^2 and $R_L(\lambda)$ scales with L, we call the system critical because the particle behaves like a free particle. When the strength of the potential breaks down this scaling behavior, the system is not critical and the particle is bound. The value of $\lambda=\lambda_c$ is the transition point.

The grid spacing ΔT and ΔL do not affect the scaling properties of any quantity. The smaller the grid spacing, the smoother is the representation we get from the actual Euclidean space. Because the potential function is not scaled, the potential function range sets the magnitude of the real-space L, which must be covered. So a small ΔL means a big N_L, and thus, a large transfer matrix to be diagonalized.

III. NUMERICAL EXAMPLE

In order to illustrate this method, we study the case of a single particle in the presence of the Pöschl-Teller [17] potential $V(x;\lambda)=-\lambda(\lambda-1)/\cosh^2(x)$, with $\lambda\geqslant 1$. This problem has an exact solution. In the one-dimensional case, there is always a bound solution unless $\lambda=1$ when the potential vanishes, and the particle is free. In three dimensions, the behavior is much more interesting. Regardless of the presence of an attractive potential in the interval $1<\lambda<2$, there is no bound solution until $\lambda\geqslant 2$. Hence, there is a finite value of the potential strength parameter, $\lambda_c=2$, that defines the stability limit of the bound solution. In the present approach, this point may be obtained by investigating the scaling properties of the correlation length ξ_L and the mean radial distance R_L.

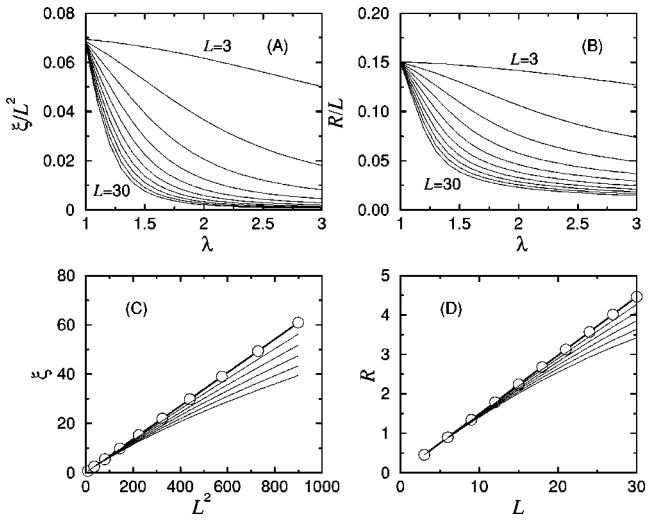

FIG. 1. Upper panels (A) and (B) show the scaled correlation length ξ/L^2 and the scaled radial mean distance R/L as a function of the potential strength λ for different system sizes with $L=3,6,9,\ldots,30$. The grid spacing is kept fixed $\Delta L=0.03$ so the smallest system has $N_L=100$ and the largest has $N_L=1000$ points. Lower panels (C) and (D) illustrate the scaling of ξ and R with the system size L for different values of $\lambda=1(\bigcirc),1.02,1.04,1.06,1.08,1.10$. All numerical values are in atomic units.

The one-dimensional case is a straight forward application of Eq. (4). The lattice in the position space is defined by picking evenly spaced points in the interval $x\in[-L/2,L/2]$. The results are obtained by exact diagonalization of the transfer matrix for every system size defined by $L=N_L\Delta L$. To investigate the trivial transition at $D=1$, it is enough to consider only one grid spacing $\Delta L=0.03$. For the remainder of this paper, we consider that the particle has a mass equal to the electron mass and atomic units ($m=\hbar=1$) are implied for all numerical quantities. Thus, the values of ξ_L and R_L are calculated with ten different system sizes, $L=100,200,\ldots,1000$, where L is measure in units of ΔL. The results are shown in Fig. 1. In Fig. 1(a) we plot ξ_L/L^2 and in Fig. 1(b) R_L/L as a function of λ. The curves correspond to different system sizes $L=100,200,\ldots,1000$. For a given value of λ, it is clear that the only point where $R_L\sim L$ and $\xi_L\sim L^2$ is $\lambda=1$. Thus, the one-dimensional system is critical only when the potential vanishes, and the particle is free. So $\lambda=1$ is regarded as a trivial critical point. In Figs. 1(c) and 1(d), we show ξ_L and R_L as a function of L^2 and L for fixed value of λ. The curve with circles corresponds to $\lambda=1$, the other five correspond to small deviations from the free-particle case with $\lambda=1.02$, 1.04, 1.06, 1.08, and 1.10. The only case that can be adjusted to a straight line is $\lambda=1$. In the presence of a weak potential, the scaling of ξ_L and R_L deviates from the critical scaling represented by the straight lines.

In order to solve the three-dimensional case, we obtained the transfer matrix using the spherical coordinates path integral which reads

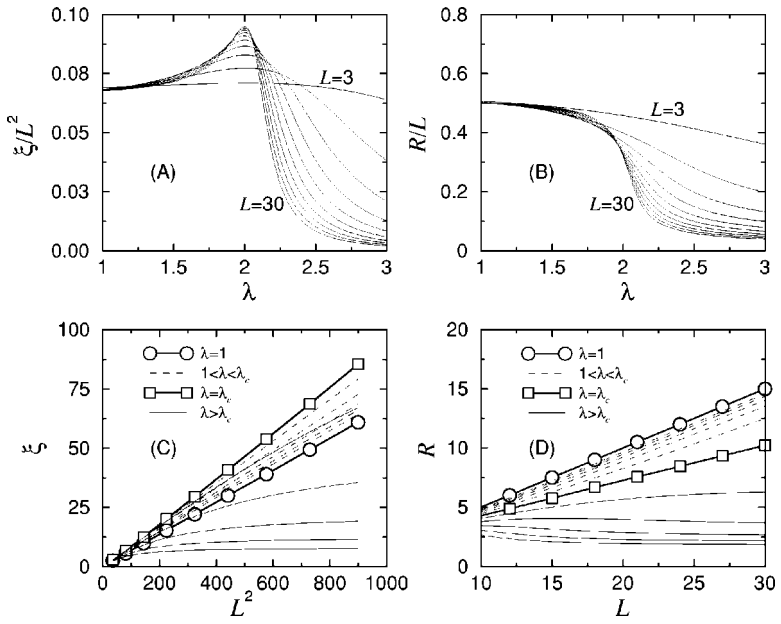

FIG. 2. Upper panels (A) and (B) show the scaled correlation length ξ/L^2 and the scaled radial mean distance R/L as a function of the potential strength λ for different system sizes with $L=3,6,9,\ldots,30$. The grid spacing is kept fixed, $\Delta L=0.03$, so the smallest system has $N_L=100$ and the largest has $N_L=1000$ points. Lower panels (C) and (D) illustrate the scaling of ξ and R with the system size L for different values of λ. The perfect linear fit with $\lambda=1$ ($\bigcirc$) and $\lambda=\lambda_c$ ($\square$). The dashed lines correspond to values of λ that are smaller than the critical value of 5, 10, 15, 20, and 25 %. The continuous lines have values of λ greater than λ_c by the same relative amounts. All numerical values are in atomic units.

$$T_{rad}(r_j,r_{j-1})=M_{l+3/2}(r_j,r_{j-1})T(r_j,r_{j-1}), \tag{9}$$

where r is the particle radial coordinate and $T(r_j,r_{j-1})$ is the same transfer matrix defined in Eq. (4). The factor $M_{l+3/2}(r_j,r_{j-1})$ is introduced by the discrete radial *functional weight*

$$M_{l+3/2}(r_j,r_{j-1})=\sqrt{\frac{2\pi m r_j r_{j-1}}{\hbar\Delta T}}\exp\left[-\frac{m r_j r_{j-1}}{\hbar\Delta T}\right] \times I_{l+3/2}\left(\frac{m r_j r_{j-1}}{\hbar\Delta T}\right), \tag{10}$$

where $I_{l+3/2}$ is the modified Bessel function. The quantum number l sets the angular momentum. Since we are studying the ground state, it is enough to consider only the solutions with $l=0$.

Now, the discretization is done over the radial coordinate, excluding the origin $r_i=i\Delta L$, $i=1,2,\ldots,N_L$, for each instant t_j. The quantity R_L is now the ground-state expectation valu $R_L=\langle r\rangle$. The transfer matrix is obtained using different values of grid spacing ΔL=0.01, 0.02, 0.03, 0.04, 0.05, and 0.06 for ten different system sizes. The system sizes set by discretization numbers starting from $N_L=100,200,300,\ldots$, up to 1000. For each case, the two leading eigenvalues and its leading eigenvector are numerically evaluated and used to compute the correlation length and radial mean distance.

In Fig. 2 we present the results using only the grid spacing $\Delta L=0.03$ of the three dimensional case. In Fig. 2(a), ξ_L/L^2 is shown as a function of the potential parameter λ, each curve corresponds to a different system size. Notice that ξ_L/L^2 curves exhibit a peak around $\lambda=2$, the biggest system ($L=1000$) has the highest and sharpest peak, and the smallest system ($L=100$) has the lowest and widest peak. Comparing the curves for different system sizes we see that the values of ξ_L with λ to the left of the peak tend to a limiting curve where ξ scales with L^2. In the other region, to the right of the peak, the value of ξ_L/L^2 tends to vanish as the system size is increased. Thus, we may consider the value of λ_c determined as the peak of the ξ_L curve for a given system size as a pseudocritical transition point, which must converge to the true transition point in the thermodynamic limit. Moreover, it is important to note that the system is critical not only when $\lambda=\lambda_c$ but is critical in the entire region $1\leqslant\lambda\leqslant\lambda_c$. This is because the scaling of ξ with the system size is the same as the scaling of a free particle. In Fig. 2(b), we turn our attention to the scaling behavior of R as a function of λ for the ten different system sizes. The curves correspond to different system sizes ($L=100$ for the highest curve to $L=1000$ for the lowest curve). As the system size increases, the R_L/L curve tends toward a limiting curve that vanishes as λ increases and goes to a constant when $\lambda=1$. The value of λ where the particle changes its scaling behavior may be identified as the crossing point of the R_L/L curves for different system sizes. The limiting scaling behavior of the R_L/L curves to the left of the limiting crossing point is the same of a free particle where R_L scales with L, hence the system is critical. For values of λ to the right of the limiting crossing point R_L/L tends to vanish and the system is not critical anymore. Looking to the scaling behavior of R_L curves, we define a pseudocritical transition point λ_c as the point where the $R_L(\lambda)$ and $R_{L'}(\lambda)$ curves cross. In this pa-

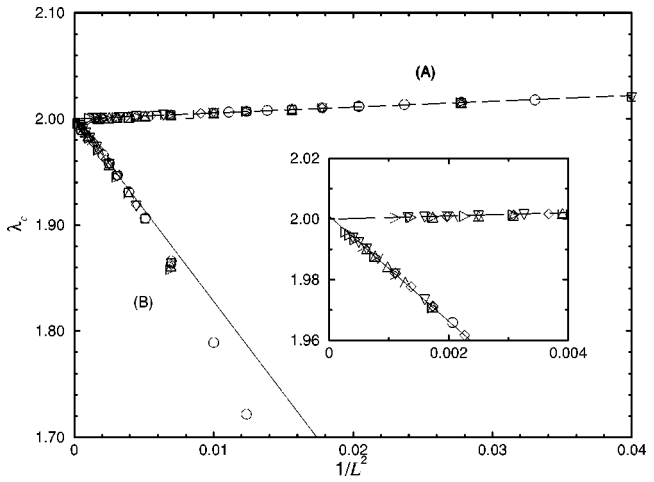

FIG. 3. The value of the pseudocritical λ evaluated at different system sizes and different grid $\Delta L = 0.01$ (○),0.02 (□), 0.03 (◇), 0.04 (△), 0.05 (▽), 0.06 (▷). Note that the extrapolated value is $\lambda_c = 2$. All numerical values are in atomic units.

per, we fixed the value of the grid spacing and consider $N_L' = 1.1N_L$, and the λ_c this way determined is regarded a function of ΔL and N_L.

In Figs. 2(c) and 2(d), we stress the existence of a range of values of λ where the system preserves the same scaling behavior of a free particle and may be called critical. In these two plots we fix the value of λ and present ξ_L as a function of L^2 and R_L as a function of L. The data plotted as circles are for the free-particle case $\lambda = 1$ and the squares for $\lambda = \lambda_c$, where λ_c is the pseudocritical transition point determined as discussed above. By examining the scaling behavior of ξ_L in Fig. 2(c) and R_L in Fig. 2(d), we clearly see that these two sets of data each fit perfectly to straight lines showing that the system is critical. This is illustrated by the dashed lines in Figs. 2(c) and 2(d) which correspond to values of lambda that are smaller than the critical value of 5, 10, 15, 20, and 25 %. Their linear behavior shows that systems with $1 < \lambda < \lambda_c$ are critical. The continuous lines have values of λ greater than λ_c by the same relative amounts, the lines eventually bend from the linear behavior showing that for $\lambda > \lambda_c$ the system critical-scaling behavior is destroyed.

In Fig. 3, we present all the numerical estimates of the critical phase-transition point λ_c for the three-dimensional Pöschl-Teller system. Along the straight line (A) are plotted the values of λ_c determined as the peak of the correlation length curve. Along the straight line (B) are plotted the values of λ_c determined by the crossing points of the curves R_L and $R_{L'}$. As discussed above, the values of λ_c depend on the discretization number N_L and the grid spacing ΔL. However, we plotted the data as a function of $1/L^2$, because $L = N_L \Delta L$ is the relevant scaling dimension. In this plot, each symbol corresponds to a different grid spacing. Despite the fact that they were evaluated with different grid spacing, when plotted against $1/L^2$, the set of data obtained using the scaling of ξ_L are grouped along one curve and the set of data obtained using the R_L scaling are grouped along another curve. Only the linear behavior of this curve for large system is plotted as the straight lines (A) and (B). The linear adjustments for large systems give the following estimates for the infinite system: $\lambda_c = 2.0000(2)$ when using the ξ_L scaling and $\lambda_c = 1.9998(8)$ when using the R_L scaling. The two schemes extrapolate to the the same result and are in very good agreement with the exact result $\lambda_c = 2$. However, one may notice that the convergence of the data obtained using ξ_L is much faster than the data obtained using R_L.

IV. CONCLUSIONS

We have shown that the path-integral approach to quantum mechanics for a system composed of only one particle in the presence of an attractive potential with strength set by a continuous parameter is a natural approach to describe and understand phase-transition phenomena. In this case, the ''collective'' phenomena behind the phase transition is a property of the space-time lattice. The transition is between a critical phase, where the paths that effectively contribute to the Feynman's path integral have the same scaling behavior as the Brownian paths that describe a free quantum particle, and a noncritical phase, where only paths around the attraction center effectively contribute to the Feynman's path integral. Like the wave function, paths in the path integral are not observables. However, one may say that the experimental fact that a particle is bound or not are special averages over these experimentally inaccessible quantities. Consequently, the stability limit of the bound state of a single-quantum particle reflects the phase transition in the paths used to describe it in Feynman's approach. We have illustrated these ideas by a numerical study of a single-quantum particle in the presence of the Pöschl-Teller potential in one and three dimensions.

Furthermore, we showed that the study of the scaling behavior of the space-time lattice may provide other numerical tools to determine the ground-state stability limit of a bound solution. In this numerical example, we saw that besides the correlation length ξ one may look at the scaling behavior of the radial mean distance R. The extrapolated numerical results for the three-dimensional Pöschl-Teller potential for the critical lambda are $\lambda_c = 2.0000(2)$ when estimated using ξ_L and $\lambda_c = 1.9998(8)$ when using R_L, with the exact result $\lambda_c = 2$. Thus, we showed that both quantities may be used to determine the transition point within the same accuracy. However the convergence of the R_L data is much slower, because depending on the grid spacing, it is necessary to go to bigger systems compared to the ξ_L data in order to observe the large system asymptotic behavior. Moreover, one must calculate the the ground-state and first excited-state energies to estimate ξ_L while we need only the ground-state properties to obtain R_L.

This approach is based on the breakdown of the free-particle scaling properties as the strength of the attractive external potential is made strong enough. This general idea can certainly be applied to systems with more than one particle as long as the unbound solution can be well represented by noninteracting free particles. This would be the case of a few particles that interact with each other by repulsive forces that decay with the distance between them. Hence, in the

absence of any external attractive potential, the particles will be far away from each other and consequently will behave like free particles. In particular, we expect that the radii of the closed path of each particle will scale according to the relations given in Eq. (3). Now we consider what will happen when the particles are also under the influence of an external attractive potential. If the potential is made strong enough, it will eventually localize the particles, destroying the scaling behavior of the free-particle paths. The transition from the states where all particles are localized to the states where all particles are free will be qualitatively the same as the transition of the one-particle system presented in this paper. This transition may be studied either by looking at the correlation length or at the radii of the particle paths. However, the phase diagram of the many-body system could be much richer, because not all particles may be localized at the same time. In this case, the correlation length defined in Eq. (7) may not be used to identify these intermediate transitions because it is associated with the correlation function among quantum states of the whole system. However, the particle path radii may still be used to investigate if there are some particles that behave like free particles and others that do not. Naturally, this method is not suitable to study transitions between two kinds of localized states. This approach is general and might be used with other simulation techniques, such as Monte Carlo methods [18], to obtain critical parameters for few-electron atoms and simple molecular systems.

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