A Monte Carlo Study of the Relativistic Harmonic Oscillator [1]

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Abstract

We present a Monte Carlo calculation of the ground-state wave function for the relativistic harmonic oscillator using the classical action in the path integral representation of quantum mechanics. The ground-state wave function has the usual Gaussian shape in the non-relativistic limit, but is not described by a single Gaussian function in the extreme relativistic limit and appears to remain square-integrable for arbitrary values of $mc^2/\hbar\omega$. A comparison is made with the ground state of the Klein-Gordon equation in the presence of the harmonic oscillator potential and the differences are presented. Also we present a realization of the non-relativistic ground-state problem in terms of a first-order auto-regressive time series with an extension for periodicity which can be implemented as a $3n$ computer algorithm.

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1 Introduction

The theory of elementary scalar particles is of central importance for the Standard Model because of the Higgs mechanism. In addition there have been many attempts to calculate relativistic bound states based on the harmonic oscillator potential and other confinement mechanisms [1], [2], [3]. Even though the harmonic oscillator potential is used in the context of the Klein-Gordon equation for the above bound-state calculations we should keep in mind that the propagation and interaction of elementary scalar particles such as the Higgs boson is ultimately an experimental question which may lead to modifications of the current quantum mechanical theory of such particles.

In this paper we take a close look at two different methods to make quantum mechanical calculations and compare their results for scalar particles interacting with a simple harmonic oscillator potential. We show that both methods agree in the non-relativistic limit, but that there are significant differences in the relativistic regime. The usual picture used in these computations is based on the Klein-Gordon equation which makes a definite choice of the representation for momentum and position operators. An alternative viewpoint is to use the Feynman path integral. These two methods usually agree, but the classical relativistic action deviates sufficiently from the polynomial form used in Klein-Gordon case that a direct comparison of the two approaches is worthwhile.

We use the classical action instead of the classical Hamiltonian because we want investigate the implications of using the original Feynman correspondence principle to make the transition from classical to quantum mechanics. According to the Feynman correspondence principle the classical path is the only path to contribute to the path integral involving the classical action as $\hbar \to 0$. The Feynman correspondence principle, therefore, differs somewhat from the Bohr-Dirac correspondence principle which holds $\hbar$ finite and demonstrates that quantum mechanics goes over to classical mechanics in the limit of large quantum numbers.

We make no assumptions about operators or commutation relations and instead use a Monte Carlo method based on the Metropolis Algorithm [4] with a Euclidean metric to investigate the ground state of the relativistic harmonic oscillator. We then present a comparison with the ground state computed from the Klein-Gordon equation. Finally we show the connection between the non-relativistic Euclidean path integral and strongly stationary auto-regressive time series.

2 Path Integral for the Relativistic Harmonic Oscillator

The equilibrium position of the harmonic oscillator defines a natural preferred frame of reference. The classical action for the relativistic harmonic oscillator can be written as

$$S(a,b) = \int_{t_a}^{t_b} \left[-mc^2 \left(\sqrt{1-\beta^2} - 1 \right) - \frac{1}{2} k x^2(t) \right] dt, \tag{1}$$

where $\beta = (1/c)dx/dt$.

The first term in Eq. (1) is the relativistic kinetic energy. In principle the subtraction of 1 from $\sqrt{1-\beta^2}$ does not change the variational problem and does not modify the fluctuations about the extremum [5] since this term is a function only of the end points.

The Feynman path integral for the above action is given by

$$K(a,b) = \int_{t_a}^{t_b} \exp\left[\frac{i}{\hbar}\, S(a,b)\right] \mathcal{D}x(t). \tag{2}$$

Since $K(a,b)$ behaves as a propagator for the quantum mechanical wave function for the relativistic harmonic oscillator, one can extract the square of the ground-state wave function by working in Euclidean spacetime (i.e., $t \to -i\tau$) and taking the large τ limit.

Eq. (1) represents the natural action based on classical relativity. Using Monte Carlo techniques has an advantage over analytical methods because one can directly investigate the numerical properties of the solution. Also, even though the classical action admits reparameterization invariance, we see no need to explore the arc-length parameterization or other action principles. Kleinert [6] advocates moving over to arc length parameterization for the paths and also modifies the action in such a way as to change the fluctuations off the extremum. The modifications proposed by Kleinert are designed to reproduce the results of the Klein-Gordon theory. We see no need to modify the classical action at all and would like to emphasize any differences that can be quantified between the scalar theory based on Eq. (2) and the Klein-Gordon theory. Ultimately the issue of how elementary scalar particles interact is an experimental question to be investigated with data (e.g., Higgs boson events).

3 Description of the Monte Carlo Technique Used

Working in Euclidean spacetime, we measure τ in units of $1/\omega$, where ω represents the ratio $\sqrt{k/m}$ and coincides with the angular frequency for the non-relativistic classical harmonic oscillator. We set up a time slicing in the parameter τ using n time steps and define ϵ as $\epsilon = T/n$, where T is the overall Euclidean time length of the path. The paths are functions of the parameter τ. We label the paths in terms of the dimensionless variable, $z(\tau) = x(\tau)\sqrt{m\omega/\hbar}$, where x is the coordinate designating the displacement from the equilibrium position of the oscillator. Using the above time slicing we have a set of $n+1$ numbers, $z_i = z(\tau_i)$, where $\tau_i = (i-1)\epsilon$ and $\tau_1 = 0, \tau_{n+1} = T$, for $i = 1, 2, ..., n+1$. We also impose the usual periodic boundary conditions on the path

$$z_1 = z_{n+1}. \tag{3}$$

There is a natural dimensionless number, $mc^2/\hbar\omega$, which characterizes the relativistic harmonic oscillator and which we designate as N. The Euclidean version of Eq. (1) then takes the form (after absorbing a factor of $1/\omega$ from τ)

$$S(0,T) \approx \sum_{i=2}^{n+1} \epsilon \left[N \left(\sqrt{1 + (z_i - z_{i-1})^2/(N\epsilon^2)} - 1 \right) + \frac{1}{8}(z_i + z_{i-1})^2 \right]. \tag{4}$$

The non-relativistic limit corresponds to large values of N where the oscillator energy is much smaller than rest-mass energy. The extreme relativistic region is described by very small values of N.

We generate configurations (i.e., paths), $z_i, i = 1, 2, 3, ..., n$, where the configuration length, n was chosen to be 2000 time steps, using a random walk in each z_i with a maximum step size of 1/4. Each configuration is tested using a Boltzmann weighting factor of the form

$$\exp(-\Delta S), \tag{5}$$

where $\Delta S = S_{\text{new}} - S_{\text{previous}}$. If ΔS is a negative number, then the configuration is accepted. Otherwise, if ΔS is positive, the new configuration is accepted with probability given by Eq. (5).

We used a "burn in" time of 1000 complete sweeps of configurations (i.e., 1000 steps in each of the links in a configuration) in order for the Metropolis algorithm to reach reasonable equilibrium conditions.

4 Monte Carlo Simulation Results

According to Ref. [7], the ground-state wave function of the Klein-Gordon equation in the presence of the harmonic oscillator potential can be expressed in terms of the variable $\alpha = \sqrt{1 + z^2/N}$ as follows

$$\psi_0(z) = C \exp(i\phi) \alpha^{-N}, \tag{6}$$

where C is a normalization constant, $N = mc^2/\hbar\omega$, and ϕ is a real-valued phase function. The non-relativistic limit of Eq. (6) corresponds to very large values of N

$$\lim_{N\to\infty} \left[\sqrt{1 + z^2/N} \right]^{-N} = \exp\left(-\frac{1}{2} z^2 \right). \tag{7}$$

Fig. [1] compares the path integral Monte Carlo result for $|\psi_0|$ with the Klein-Gordon result at $N = 100$. We see agreement between both methods in the non-relativistic (i.e., large N) limit. In Fig. [2] we compare the normalized wave function from the Monte Carlo calculation with the wave function of the Klein-Gordon result from Ref. [7] for $N = 1$. We conclude that there are significant differences between the ground state of the path integral Monte Carlo based on the relativistic classical action and the Klein-Gordon equation when the oscillator frequency becomes large.

Fig. [3] continues the Monte Carlo calculation into the relativistic region at $N = 0.01$ which is beyond the region of applicability of the Klein-Gordon equation, i.e., $|\psi_0|$ is not square-integrable in the Klein-Gordon equation when $N < 1/2$ (see Ref. [7]). From Fig. [3] we see no reason to suspect a problem with square-integrability of the ground-state

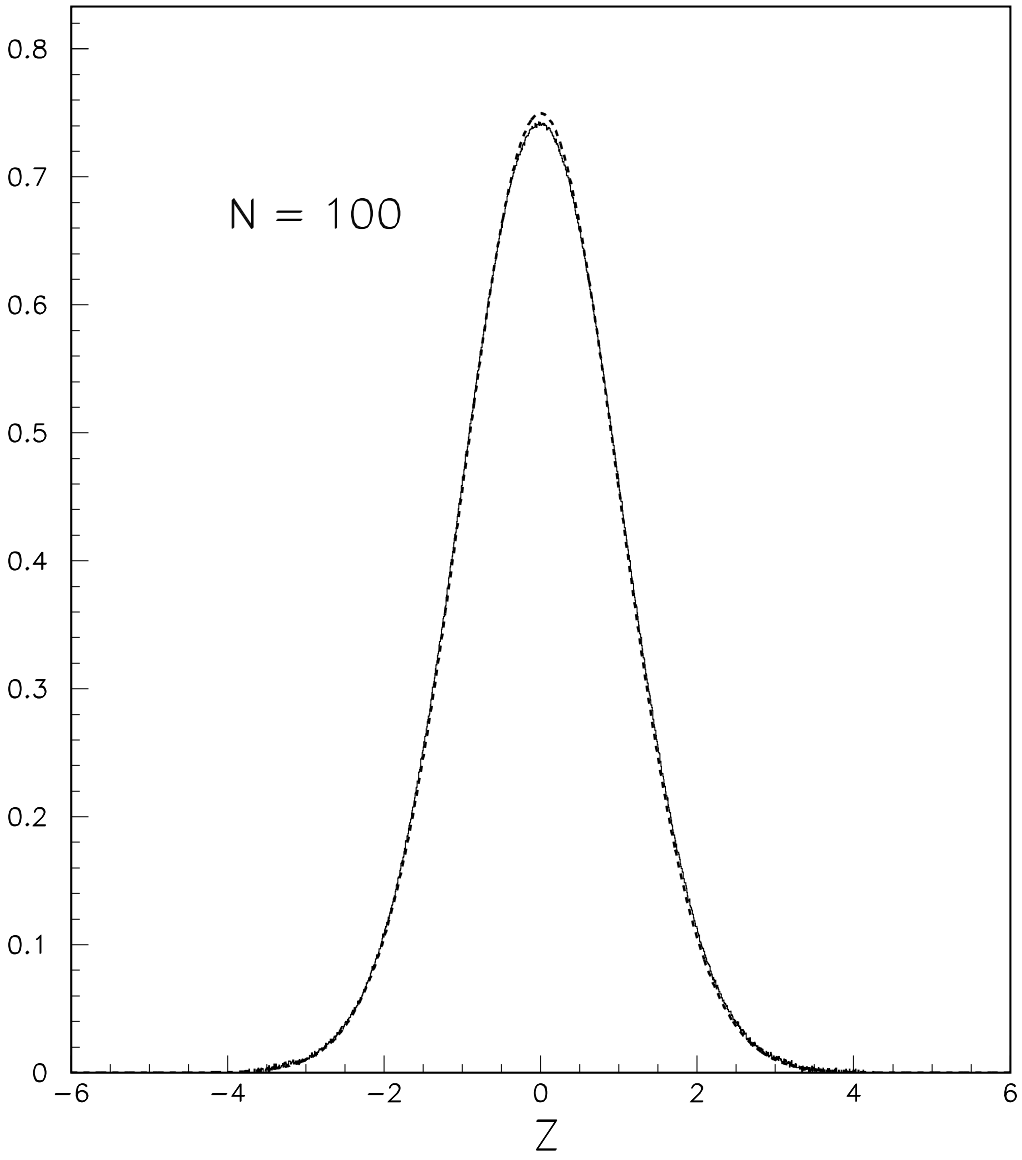

Figure 1: The ground-state wave function for the parameter value $N = mc^2/\hbar\omega = 100$ (the non-relativistic region) as calculated by the path integral method in Euclidean spacetime (solid) and also from the Klein-Gordon Equation (dashed).

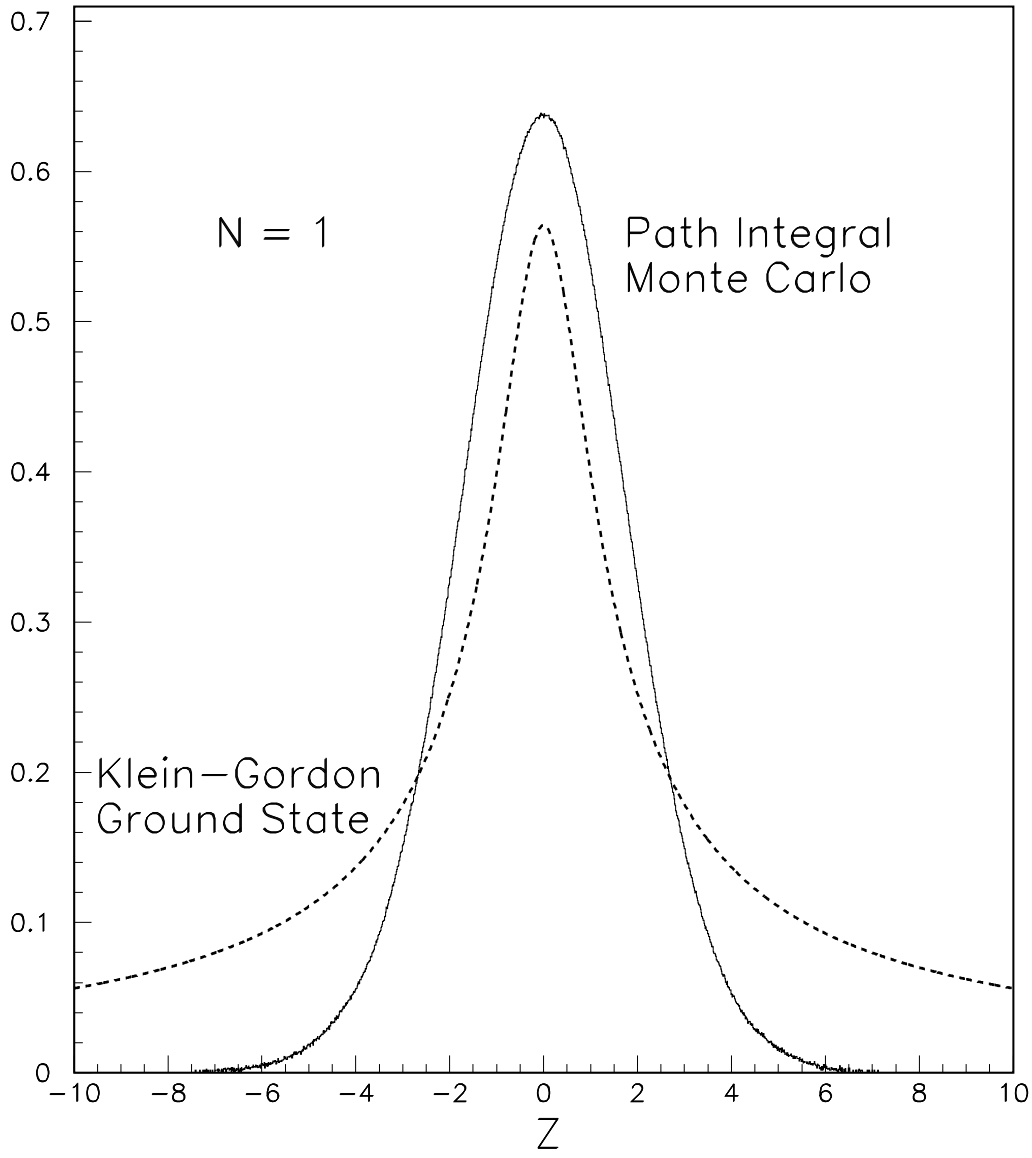

Figure 2: The ground-state wave function for the parameter value $N = mc^2/\hbar\omega = 1$ as calculated by the path integral method in Euclidean spacetime (solid) and also from the Klein-Gordon Equation (dashed).

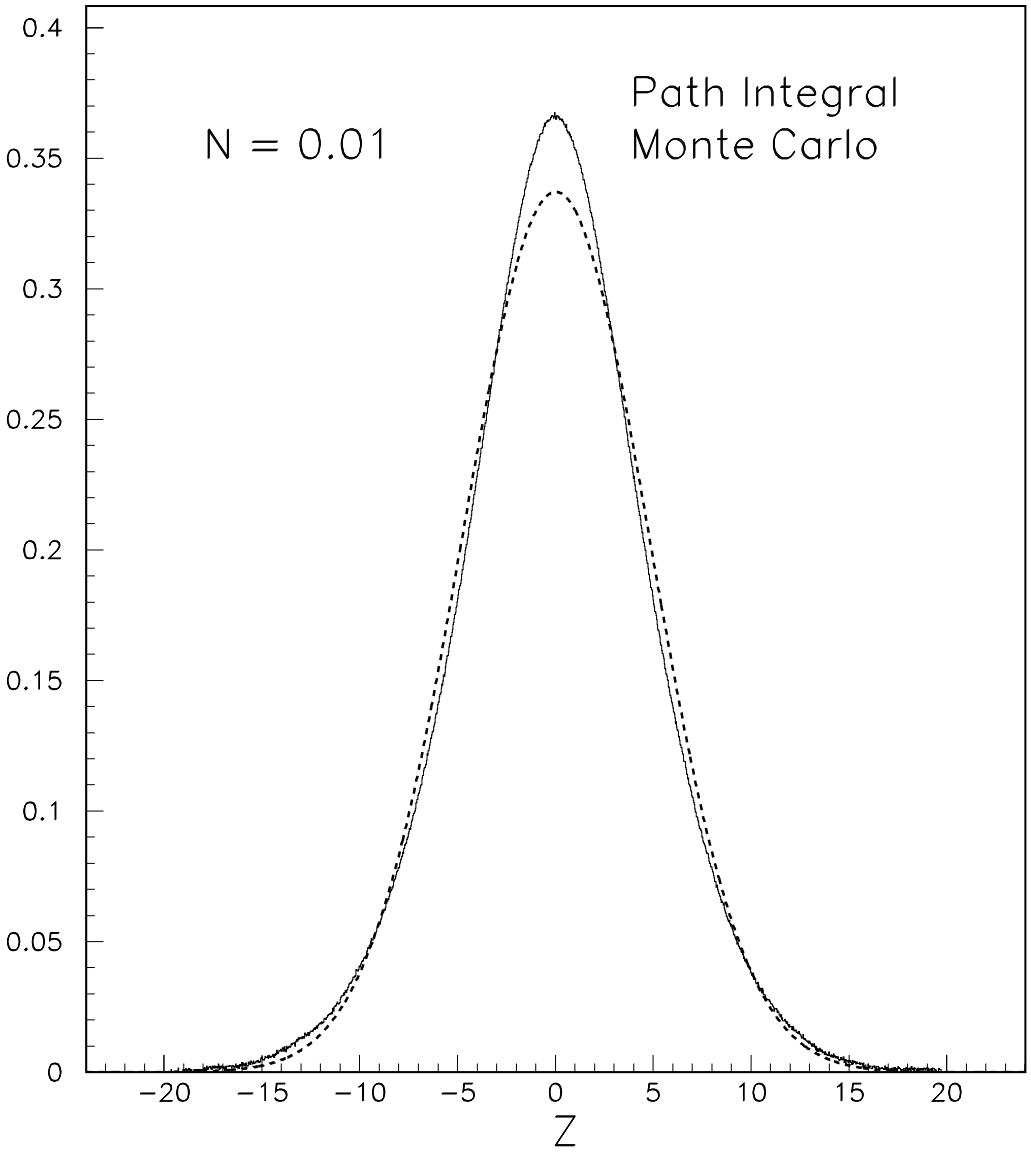

Figure 3: The ground-state wave functions in the relativistic region at $N = 0.01$. The Klein-Gordon theory does not produce a square-integrable ground-state wave function for $N < 1/2$ and is not shown. Instead we present the best fit of the Monte Carlo result (solid) to a single Gaussian function (dashed). Note the non-Gaussian features of the Monte Carlo distribution.

wave function based on the path integral representation. The smooth curve on Fig. [3] represents a fit to a Gaussian function and we conclude that the Monte Carlo result cannot be represented as a single Gaussian function. The function in Fig. [3] fits very well to the sum of two Gaussian functions, but we have no simple interpretation of the physical implications suggested by this fact.

5 A Time-Series View of the Non-Relativistic Limit

In this section we investigate the ground-state properties wave function using Eq. (4) and first principals of time series analysis. The non-relativistic classical action can be viewed as a quadratic form in the n-dimensional column vector Z, where $Z = (z_1, z_1, z_3, ..., z_n)$, together with a positive definite and symmetric matrix Q, as follows

$$Z'QZ = \sum_{i=2}^{n+1} \left[\frac{(z_i - z_{i-1})^2}{\epsilon} + \frac{\epsilon}{4}(z_i + z_{i-1})^2 \right], \tag{8}$$

where z_{n+1} is equivalent to z_1 by periodicity.

The only non-zero elements of the matrix Q can be shown to have the form

$$\begin{aligned} Q_{i,i} &= 2/\epsilon + \epsilon/2 \qquad \text{(diagonal elements)}, \\ Q_{i,i+1} &= \epsilon/4 - 1/\epsilon \qquad \text{(super-diagonal elements)}, \\ Q_{i+1,i} &= Q_{i,i+1} \qquad \text{(sub-diagonal elements)}, \qquad . \\ Q_{1,n} &= \epsilon/4 - 1/\epsilon \qquad \text{(upper right-hand element)}, \\ Q_{n,1} &= Q_{1,n} \qquad \text{(lower left-hand element)}, \end{aligned} \tag{9}$$

By performing a little algebra, we can re-express Q in a form that is related to a first-order Gaussian auto-regressive process [8], i.e., a Gaussian AR(1), with a straightforward extension to treat periodicity

$$Q = \frac{1}{\sigma^2} \begin{pmatrix} 1+\rho^2 & -\rho & 0 & 0 & 0 & ... & -\rho \\ -\rho & 1+\rho^2 & -\rho & 0 & 0 & ... & 0 \\ 0 & -\rho & 1+\rho^2 & -\rho & 0 & ... & 0 \\ 0 & 0 & -\rho & 1+\rho^2 & -\rho & ... & 0 \\ ... & ... & ... & ... & ... & ... & ... \\ -\rho & 0 & 0 & ... & ... & ... & 1+\rho^2 \end{pmatrix}. \tag{10}$$

To see the connection between Eq. (10) and Eq. (9) set

$$c = \frac{2/\epsilon - \epsilon/2}{2/\epsilon + \epsilon/2} \tag{11}$$

and then we have the following relations between Eqs. (9) and (10).

$$\rho = \frac{1 - \sqrt{1-c^2}}{c} \qquad \text{and} \quad \sigma^2 = \frac{1+\rho^2}{2/\epsilon + \epsilon/2} \tag{12}$$

The matrix Q describes a Gaussian multivariate distribution which can be related to a set of n independent and identically distributed N(0,1) Gaussian random numbers using the methods of Gaussian elimination and back-substitution. The associated equations can be trivially solved in this case and one can obtain the z_i variables from the independent N(0,1) Gaussian variables by using the following $3n$ computer algorithm

$$\begin{array}{ll} 1. & z_i \leftarrow \sigma x_i,\ x_i \sim N(0,1),\ i = 1, 2, ..., n. \\ 2. & \text{Evaluate } t = \rho z_1 + \rho^2 z_2 + ... + \rho^{n-1} z_{n-1} \text{ by the recursion:} \\ & \quad t \leftarrow 0,\ t \leftarrow \rho(t + z_i),\ i = n-1, n-2, ..., 1. \\ 3. & \text{Then set } z_n \leftarrow (z_n + t)/(1 - \rho^n). \\ 4. & z_i \leftarrow z_i + \rho z_{i+1},\ i = n-1, n-2, ..., 1. \\ 5. & z_{n+1} \leftarrow z_1. \end{array} \tag{13}$$

The path integral can be worked out explicitly in this case using the normalization for Gaussian distributed variables as follows

$$\int \exp\left[-\frac{1}{2} Z' Q Z\right]\, d^n Z = (1 - \rho^n)^{-1} \left[\sqrt{2\pi}\sigma\right]^n, \tag{14}$$

where ρ and σ are given by Eq. (12). Note that the integral in Eq. (14) is independent of the parameter ρ in the event that $|\rho| < 1$ because ρ^n is negligible for large n values.

The above method illustrates the connection between the non-relativistic harmonic oscillator and Gaussian AR(1) time series. This provides a fast alternative to working in the Fourier space (frequency domain).

6 Conclusion

The quantum mechanical ground state arising from the application of the Metropolis algorithm to the classical relativistic harmonic oscillator does not replicate the results of the Klein-Gordon theory. The Klein-Gordon theory cannot be applied if $N < 1/2$ because the wave function loses the square-integrability property (i.e., the eigenfunctions are not in the usual Hilbert space). This property of the Klein-Gordon equation and the Dirac equation arises in other cases, for example, it arises in the Coulomb bound state problem. One finds that the lowest energy eigenvalues become complex in the Coulomb problem for the Klein-Gordon equation if $Ze^2 > 1/2$ (e^2 is the fine structure constant). For the Dirac Equation the same thing happens at $Ze^2 > 1$. The implication is that the Hamiltonian is not a Hermitian operator if the potential is too strong. This same property is also related to the loss of square-integrability of the ground-state wave function. One can conclude that perhaps the same thing occurs for the Klein-Gordon theory in the presence of the harmonic oscillator potential if the spring constant becomes too large. It is interesting that the ground state of the path integral representation of the classical relativistic action appears to maintain square-integrability in the highly relativistic region.

One might be tempted to attribute an effective wave equation to the path-integral formulation of the harmonic oscillator problem based on the square-root Klein-Gordon equation as follows:

$$\left[\sqrt{m^2c^4 - \hbar^2\nabla^2} - \frac{1}{2}kx^2\right]\psi = E\psi. \tag{15}$$

Such an interpretation suggests itself upon first glance of the classical relativistic Hamiltonian if one also assumes that the correct operator assignment for momentum is $p = -i\hbar\nabla$. We do not advocate such a view and have taken pains not to make operator assumptions beyond what is implied in the path integral formulation. The reason for our caution is that the classical action has the correct symmetry properties of Lorentz invariance and, in the presence of gauge interactions, gauge invariance. Even though we work in the preferred frame of the equilibrium position of the oscillator and have subtracted 1 from $\sqrt{1-\beta^2}$, we have not disturbed the symmetry properties, because subtracting 1 only adds a term that depends on the end points and does not affect variations that vanish on the end points.

The reasons that we do not advocate interpreting the path integral result as a possible representation of Eq. (15) are two-fold. The first reason is that the ground-state wave function for the square-root Klein-Gordon equation loses square-integrability in another bound-state problem, specifically, in the Coulomb problem when Ze^2 is large [9], [10], [11], [12], [13]. This symptom is connected with the fact that the ground-state energy eigenvalue becomes complex for $Ze^2 > \pi/2$ (see Ref. [14]). The second reason that gives us pause to assume that Eq. (15) is a possible wave equation for the relativistic path integral is that it has been shown [15] that the interacting square-root Klein-Gordon equation does not admit Lorentz scalar wave function solutions in the presence of interactions. Since the classical action has good symmetry properties, and also, since we see no evidence of loss of square-integrability from the Monte Carlo results, we infer that Eq. (15) and the quantum mechanics based on Eq. (2) are two different theories.

Hence the path integral formulation produces a result that is new and is unlikely to be explained using the the usual assumptions based on operator approaches to relativistic quantum mechanics such as the Klein-Gordon equation or the (non-Lorentz invariant) interacting square-root Klein-Gordon equation.

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