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Relativistic path integral Monte Carlo: Relativistic oscillator problem

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Relativistic generalization of path integral Monte Carlo (PIMC) method has been proposed. The problem of relativistic oscillator has been studied in the framework of this approach. Ultrarelativistic and nonrelativistic limits have been discussed. We show that PIMC method can be effectively used for investigation of relativistic systems.

Keywords: Path integral; Monte Carlo algorithms; relativistic effects; oscillator.

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1. Introduction

Path integral Monte Carlo method (PIMC)[1] is one of the most popular *ab initio* numerical approach to the investigation of quantum systems. This method becomes especially useful in modelling properties of quantum many-body problems. Schrodinger equations become difficult to study in this case, but the number of quantum degrees of freedom is still not so large to use quantum statistics.

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This work is devoted to the generalization of PIMC to the case of relativistic systems. There are many physical problems connected with simulations of relativistic quantum mechanical systems. Relativistic corrections play very essential role in the physics of atomic systems with heavy elements due to the strong interaction potentials.[2] One may find the problems with simulations of relativistic quantum systems in the nuclear physics, physics of hadron structure and quark–gluon plasma.[3,4] Recently, another interesting application of the relativistic quantum mechanics has arisen. These are so-called (pseudo) relativistic condensed matter systems and one of the most famous examples of such systems is graphene.[5]

The remarkable property of graphene is that it's effective charge excitations have very small mass. In case of the ideal graphene without defects and boundary effects, the mass of excitations is equal to zero. On the other hand, the interaction between excitations is very strong. It means that the excitations on the graphene sheet can be treated as some strongly interacted two-dimensional relativistic gas with instantaneous interaction.

The correct formulation of the many-body relativistic quantum mechanical problem has some well-known difficulties. The kinetic and potential part of the Hamiltonian must be invariant at Lorentz transformation. The kinetic part of Hamiltonian can be formulated in Lorentz-invariant form quite easy but relativistic formulation of interaction requires the quantum field theory approach in general case. If we want to work in the framework of the quantum mechanics approach, we are to use some additional assumptions. In this work, we study just kinetic part of Hamiltonian. The interaction part cannot be studied in general case, as the first approximation consider the relativistic quantum systems with instantaneous interaction between particles. This approximation works very well in case of relativistic quantum chemistry and for investigation of the properties of (pseudo) relativistic condensed matter systems like graphene. In these systems, the correction from relativistic nature of the interaction is fortunately very small in comparison with the correction that comes from relativistic nature of the particles. The nuclear and high-energy systems require some special considerations and these tasks will be the key point of our future works.

Relativistic generalization of the path integral approach for quantum mechanical systems has a long history.[6,7] Today this approach is becoming more and more popular and find its application in high-energy physics.[3,4]

For the testing of the relativistic PIMC approach, we consider the relativistic oscillator problem in one space dimension. This problem can be studied by using of the standard Schrodinger equation approach in the momentum space and we will compare the results of this two approaches. Also, relativistic oscillator problem was studied analytically.[8,9]

In the next section, we briefly discuss the main statements of path integral formalism for relativistic quantum mechanical system.

2. Density Matrix for Monte Carlo Calculations

In this section, we consider the relativistic generalization of path integral formalism for quantum mechanics system at finite temperature. One can find the full consideration of this question in Ref. 1.

Average value of an operator A is

$$\langle A\rangle = \frac{\mathrm{tr}(Ae^{-\beta \mathrm{H}})}{\mathrm{tr}(e^{-\beta \mathrm{H}})}, \tag{1}$$

where operator $e^{-\beta \mathrm{H}}$ is density matrix and $\beta = 1/\theta$ is inverse temperature of the system to be considered. For PIMC method, we should consider zero temperature limit. Matrix element of density matrix in coordinate representation is

$$\rho(q, q'; \beta) = \langle q|e^{-\beta \mathrm{H}}|q'\rangle. \tag{2}$$

Then, we have for the average value of the operator A

$$\langle A\rangle = \frac{\int dqdq' \rho(q, q'; \beta)\langle q|A|q'\rangle}{\int dq\rho(q, q; \beta)}. \tag{3}$$

For the density matrix operator, we can write the expression

$$e^{-(\beta_1+\beta_2)\mathrm{H}} = e^{-\beta_1 H}e^{-\beta_2 \mathrm{H}}. \tag{4}$$

The same expression in coordinate representation is

$$\rho(q_1, q_3; \beta_1 + \beta_2) = \int dq_2 \rho(q_1, q_2; \beta_1)\rho(q_2, q_3; \beta_2). \tag{5}$$

Applied this property N_t times for the density matrix element, we have

$$e^{-\beta \mathrm{H}} = (e^{-\tau \mathrm{H}})^{N_t}, \tag{6}$$

where $\tau = \beta/N_t$. The same expression in coordinate representation is

$$\rho(q_0, q_N; \beta) = \int \ldots \int dq_1 dq_2 \ldots dq_{N-1}\rho(q_0, q_1; \tau)\rho(q_1, q_2; \tau) \ldots \rho(q_{N-1}, q_N; \tau). \tag{7}$$

Consider the Hamiltonian $\mathrm{H} = T(p) + V(q)$. Kinetic energy operator $T(p)$ is diagonal in momentum representation and potential energy operator $V(q)$ is diagonal in coordinate representation. We can separate kinetic and potential energy if τ is small, so

$$e^{-\tau(T+V)+\frac{\tau^2}{2}[T,V]} = e^{-\tau T}e^{-\tau V} \tag{8}$$

and if $\tau \to 0$

$$e^{-\tau(T+V)} \approx e^{-\tau T}e^{-\tau V}, \tag{9}$$

$$\rho(q_0, q_2; \tau) \approx \int dq_1 \langle q_0|e^{-\tau T}|q_1\rangle\langle q_1|e^{-\tau V}|q_2\rangle. \tag{10}$$

Potential energy is diagonal in coordinate representation, so

$$\langle q_1|e^{-\tau V}|q_2\rangle = e^{-\tau V(q_1)}\delta(q_2-q_1). \tag{11}$$

With the expression $\int |p\rangle \frac{dp}{2\pi}\langle p| = 1$, we obtain

$$\langle q_0|e^{-\tau T}|q_1\rangle = \int dpdp'\delta(p-p')\langle q_0|p\rangle\langle p'|q_1\rangle e^{-T(p)\tau}. \tag{12}$$

Taking into account $\langle q|p\rangle = e^{-iqp}$, we obtain

$$\langle q_0|e^{-\tau T}|q_1\rangle = \int \frac{dp}{2\pi} e^{-T(p)\tau - ip(q_0-q_1)}. \tag{13}$$

In relativistic case, the kinetic energy has the following form:

$$T(p) = \sqrt{p^2+m^2}. \tag{14}$$

So to calculate the matrix element, we must take the above integral over momentum with this form. Consider it in general case or, in other words, with general form of relativistic kinetic energy. We can calculate this integral over momentum with this $T(p)$

$$\begin{aligned}\langle q_0|e^{-\tau T}|q_1\rangle &= \frac{m\tau}{\pi\sqrt{\tau^2+(q_1-q_0)^2}}K_1(m\sqrt{\tau^2+(q_1-q_0)^2}\,)\\ &= \frac{m}{\pi\sqrt{1+(\frac{q_1-q_0}{\tau})^2}}K_1\left(m\tau\sqrt{1+\left(\frac{q_1-q_0}{\tau}\right)^2}\right),\end{aligned} \tag{15}$$

where $K_1(*)$ is modified Bessel function of the first-order. The general expression for matrix element is the following:

$$\begin{aligned}\rho(q'',q';\tau) &= \langle q''|e^{-\tau(T(p)+V(q))}|q'\rangle\\ &= \frac{m}{\pi\sqrt{1+(\frac{q''-q'}{\tau})^2}}K_1\left[m\tau\sqrt{1+\left(\frac{q''-q'}{\tau}\right)^2}\right]e^{-\tau V(q')}.\end{aligned} \tag{16}$$

One can find the multi-dimensional generalization of the expression (16)

$$\rho(\mathbf{q}'',\mathbf{q}';\tau) = \left(\frac{m\tau}{\pi\sqrt{\tau^2+(\mathbf{q}''-\mathbf{q}')^2}}\right)^{(d+1)/2}\frac{K_{(d+1)/2}(m\sqrt{\tau^2+(\mathbf{q}''-\mathbf{q}')^2})}{(2\tau)^{(d-1)/2}}\,e^{-\tau V(\mathbf{q}')}, \tag{17}$$

where $d = 1, 2, 3$ is the space dimensions.

3. PIMC Metropolis Algorithm

For PIMC Metropolis algorithm, we should know a part of the density matrix which corresponds to a fixed point q_i. One can find the discussion about this method and all

proofs in Ref. 10. Using (16), we can write

$$\pi(q_i) = \frac{m^2 K_1[m\tau\sqrt{1+(\frac{q_i-q_{i-1}}{\tau})^2}]K_1[m\tau\sqrt{1+(\frac{q_{i+1}-q_i}{\tau})^2}]}{\pi^2\sqrt{1+(\frac{q_i-q_{i-1}}{\tau})^2}\sqrt{1+(\frac{q_{i+1}-q_i}{\tau})^2}} e^{-\tau V(q_i)}. \tag{18}$$

To calculate path integral, we construct Markov chain which has the equilibrium state at fixed q_i proportional to $\pi(q_i)$. Transition probability for this Markov chain satisfies the equation

$$\int dq_i \pi(q_i) P(q_i \to q_i') = \pi(q_i'). \tag{19}$$

We want to obtain $\pi(q)$ as the limit of Markov chain, so we require the detailed balance condition

$$\pi(q_i)P(q_i \to q_i') = \pi(q_i')P(q_i' \to q_i). \tag{20}$$

In Metropolis algorithm, we can split transition probability

$$P(q_i \to q_i') = T(q_i \to q_i')A(q_i \to q_i'), \tag{21}$$

where $T(q_i \to q_i')$ is sampling distribution and $A(q_i \to q_i')$ is acceptance probability

$$A(q_i \to q_i') = \min\left[1, \frac{T(q_i' \to q_i)\pi(q_i')}{T(q_i \to q_i')\pi(q_i)}\right]. \tag{22}$$

If we know the density matrix in position representation, we can calculate expressions for average values of all observables. Using (16), we can obtain the average value of kinetic energy in general relativistic case (see Ref. 11),

$$\langle T(p)\rangle = \left\langle \frac{m\tau}{\sqrt{\tau^2+(\Delta q)^2}} \frac{K_0(m\sqrt{\tau^2+(\Delta q)^2})}{K_1(m\sqrt{\tau^2+(\Delta q)^2})} + \frac{\tau^2-(\Delta q)^2}{\tau(\tau^2+(\Delta q)^2)} \right\rangle. \tag{23}$$

We calculate the average values of the ground state full energy

$$\langle E(p,q)\rangle = \langle T(p) + V(q)\rangle \tag{24}$$

and correlation function

$$\langle q(t)q(t+n\tau)\rangle = \langle q_i q_{i+n}\rangle. \tag{25}$$

We have expressions for generating Markov chain and for calculating observables. Now, we can compare results obtained by Monte Carlo simulations and theoretical predictions.

4. Relativistic Oscillator Problem

Relativistic harmonic oscillator has the Hamiltonian

$$H = \sqrt{p^2+m^2} + \frac{1}{2}m\omega^2 q^2. \tag{26}$$

In order to test our approach and compare PIMC results with analytical expressions, let us consider the nonrelativistic ($m^2 \gg p^2$) and ultra-relativistic ($m^2 \ll p^2$) limits. In fact, there are only two-dimensional parameters m and ω, as we will see later, these conditions must be reformulated in terms of m and ω.

4.1. *Nonrelativistic limit*

In this section, the limit $m^2 \gg p^2$ is considered. We should understand it in terms of average values, it means that $m^2 \gg \langle p^2 \rangle$. Expanding the expression for kinetic energy $T(p) = \sqrt{p^2 + m^2}$, we obtain the following:

$$T(p) = \sqrt{p^2 + m^2} = m\left(1 + \frac{p^2}{2m^2} + O\left(\left(\frac{p}{m}\right)^4\right)\right) \approx m + \frac{p^2}{2m}. \tag{27}$$

Then, the nonrelativistic limit of the Hamiltonian (26) is the following:

$$\mathrm{H} = m + \frac{p^2}{2m} + \frac{1}{2} m\omega^2 q^2, \tag{28}$$

where m is the rest mass. So, we obtain simple harmonic oscillator. Energy and probability density of the ground state are well known for this Hamiltonian:

$$E_0 = m + \frac{\omega}{2}, \tag{29}$$

$$\rho(q) = |\psi(q)|^2 = \left(\frac{m\omega}{\pi}\right)^{\frac{1}{2}} \exp(-m\omega q^2), \tag{30}$$

where $\psi(q)$ is the wave function of this ground state. The virial theorem gives us the relation between kinetic and potential energy

$$\left\langle \frac{p^2}{2m} \right\rangle = \left\langle \frac{1}{2} m\omega^2 q^2 \right\rangle \quad \text{or} \quad \langle T(p) - m \rangle = \langle V(q) \rangle. \tag{31}$$

From this with (28), we obtain

$$\langle T(p) - m \rangle = \frac{1}{2}(E_0 - m) = \langle V(q) \rangle = \frac{\omega}{4}. \tag{32}$$

Correlation function $\langle q(t)q(t+s) \rangle$ for this system is the following:

$$\langle q(t)q(t+s) \rangle = \frac{1}{2m\omega} e^{-w|s|}. \tag{33}$$

We have a list of observables (29), (32), (33) to compare results with numerical calculations by PIMC.

We can formulate the nonrelativistic limit in terms of m and ω, that is necessary to distinguish different limits. Using (32), we can obtain $\langle p^2 \rangle \sim m\omega$ and $m \gg \omega$. It means that we consider heavy particles and soft potential in this case.

4.2. *Ultra-relativistic limit*

Our next step is the consideration of Hamiltonian (26) in the ultra-relativistic limit. Kinetic energy in this case has the following form:

$$T(p) = \sqrt{p^2 + m^2} = |p|\left(1 + \frac{m^2}{2p^2} + O\left(\left(\frac{m}{p}\right)^4\right)\right) \approx |p|. \tag{34}$$

It is enough to take only zero-order to describe the behavior of the system. We have

$$H = |p| + \frac{1}{2}m\omega^2 q^2. \tag{35}$$

We can solve the Schrodinger equation for this Hamiltonian in momentum representation and find the energy of ground state and corresponding probability density

$$E_0 = \lambda_0 (m\omega^2)^{1/3}, \tag{36}$$

where $\lambda_0 = 0.808617\ldots$,

$$\rho(q) = \frac{\int\int \frac{dpdk}{(2\pi)^2} \mathrm{Ai}((\frac{2}{m\omega^2})^{1/3}(|p| - \lambda_0))\mathrm{Ai}((\frac{2}{m\omega^2})^{1/3}(|k| - \lambda_0))e^{-i(p-k)q}}{\int \frac{dp}{2\pi}\mathrm{Ai}^2((\frac{2}{m\omega^2})^{1/3}(|p| - \lambda_0))}, \tag{37}$$

where $\mathrm{Ai}(x)$ is the Airy function of the first kind. The virial theorem for the Hamiltonian (35) gives us the relation between kinetic and potential energy

$$\langle T(p)\rangle = 2\left\langle V(q) = \frac{2\lambda_0}{3}(m\omega^2)^{1/3}\right\rangle. \tag{38}$$

From the virial theorem, we have $\langle |p|\rangle \sim (m\omega^2)^{1/3}$. In momentum representation, one can calculate that

$$\frac{\langle |p|\rangle^2}{\langle p^2\rangle} = \frac{20\alpha^3}{3(3 + 8\alpha^3)} = 0.615175\ldots, \tag{39}$$

where $\alpha = 2^{1/3}\lambda_0 = 1.018792\ldots$ is the first root of $\mathrm{Ai}'(-\alpha) = 0$. So $\langle |p|\rangle^2 \sim \langle p^2\rangle$, then we can obtain the ratio

$$\frac{m^2}{\langle p^2\rangle} \sim \left(\frac{m}{\omega}\right)^{4/3} \ll 1. \tag{40}$$

For ultra-relativistic case, we have the following expression for mass and "frequency", opposite to the nonrelativistic one: $\omega \gg m$. So, for the ultra-relativistic case, we have obtained one more list of observables for comparison with PIMC calculations.

5. Relativistic PIMC Results

5.1. *Nonrelativistic limit*

In this part, we compare the results obtained by PIMC program for $m \gg \omega$ case with theoretical predictions for harmonic oscillator. Taking into account features of PIMC

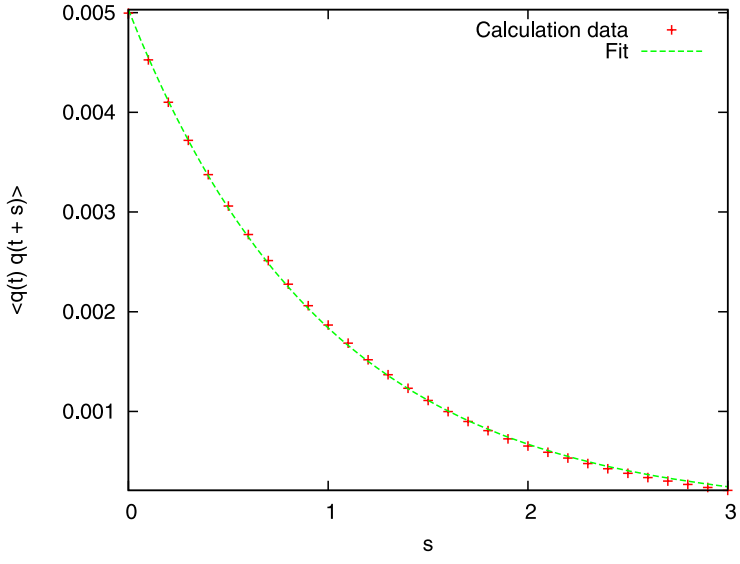

Fig. 1. (Color online) Correlation function for $m = 100$, $\omega = 1$.

metropolis algorithm is necessary to reach the limit of Markov chain and desired level of errors to compare results with analytical expressions.

For correlation function, we have a good agreement with the theoretical expression (33) (see Fig. 1). We fit it with the function

$$f\langle q(t)q(t+s)\rangle = a\ \exp(-b|s|), \tag{41}$$

where obtained values are $a = (503.0 \pm 1.4) \times 10^{-5}$ and $b = 1.006 \pm 0.004$. We know that these values for absolutely nonrelativistic harmonic oscillator are $a = 1/(2m\omega) = 500 \times 10^{-5}$ and $b = \omega = 1$.

Consider the results of PIMC program for energy. We have analytical expressions (32) (see Fig. 2).

The fit for the energy data is constant

$$\langle T(p)\rangle = a, \tag{42}$$

$$\langle V(q)\rangle = b. \tag{43}$$

It gives us $a = 0.251 \pm 0.003$, $b = 0.2476 \pm 0.0003$, while theoretical predictions are $a = b = \omega/4 = 0.25$.

As we can see, we have an agreement with the case of classical (absolutely nonrelativistic) harmonic oscillator in the limit of $m \gg \omega$ or nonrelativistic limit. Somewhere, we have an agreement with two or more standard deviations, it means that we should increase ratio of m and ω, but the computer time of calculations for this case is much longer.

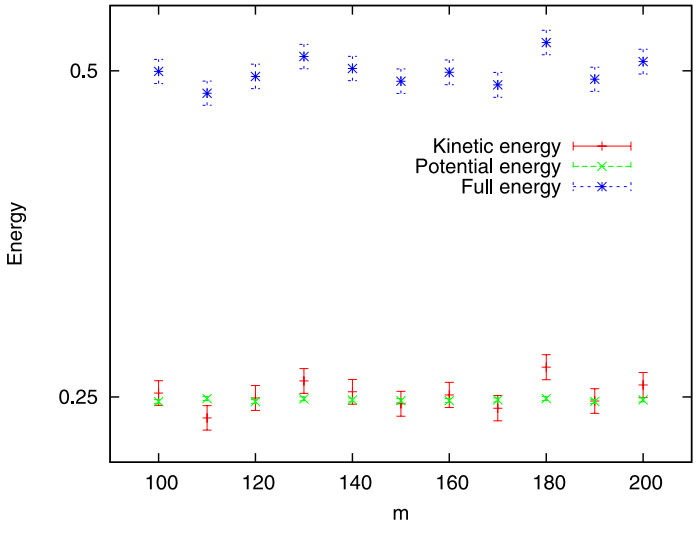

Fig. 2. (Color online) Dependence of energy on mass for $\omega = 1$.

5.2. *Ultra-relativistic limit*

In this section, we compare the results of PIMC metropolis with theoretical ones for $p^2 \gg m^2$ or $\omega \gg m$ limit.

For correlation function, see Fig. 3. We fit it with an exponential function

$$\langle q(t)q(t+s)\rangle = a\ \exp(-b|s|), \tag{44}$$

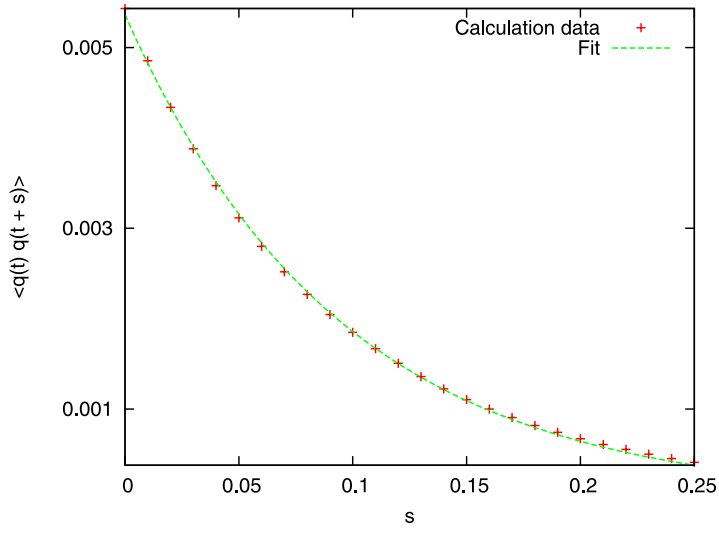

Fig. 3. (Color online) Dependence of correlation function $\langle q(t)q(t+s)\rangle$ on $|s|$ for $m = 0.1$, $\omega = 100$.

that gives us $a = (536.5 \pm 1.8) \times 10^{-5}$ and $b = 10.60 \pm 0.05$. We suppose the following expression for the correlation function:

$$\langle q(t)q(t+s)\rangle = q^2(0)e^{-(\lambda_1-\lambda_0)(m\omega^2)^{1/3}s}, \tag{45}$$

where $\lambda_1(m\omega^2)^{1/3}$ is the next energy level of the ultra-relativistic oscillator, and $\lambda_1 = 2.338\ldots$. Theoretical values are $a = 0.539$ and energy gap $b = 10.47$. We have an agreement with theoretical expression for correlation function, so we can continue the comparison of results.

Let us consider the calculations of energy for ultra-relativistic oscillator and compare them with analytical expressions (38) (see Fig. 4). The fitting of PIMC results with functions

$$\langle T(p)\rangle = \frac{2}{3}a(m\omega^2)^{1/3}, \tag{46}$$

$$\langle V(q)\rangle = \frac{1}{3}b(m\omega^2)^{1/3}, \tag{47}$$

$$\langle E(p,q)\rangle = c(m\omega^2)^{1/3} \tag{48}$$

gives the following values: $a = 0.801 \pm 0.004$, $b = 0.812 \pm 0.004$ and $c = 0.804 \pm 0.003$. Theoretical values are $a = b = c = \lambda_0 = 0.8086\ldots$.

As a result, the PIMC calculations for relativistic oscillator have a perfect agreement in ultra-relativistic limit with the theoretical results obtained from the Hamiltonian (35).

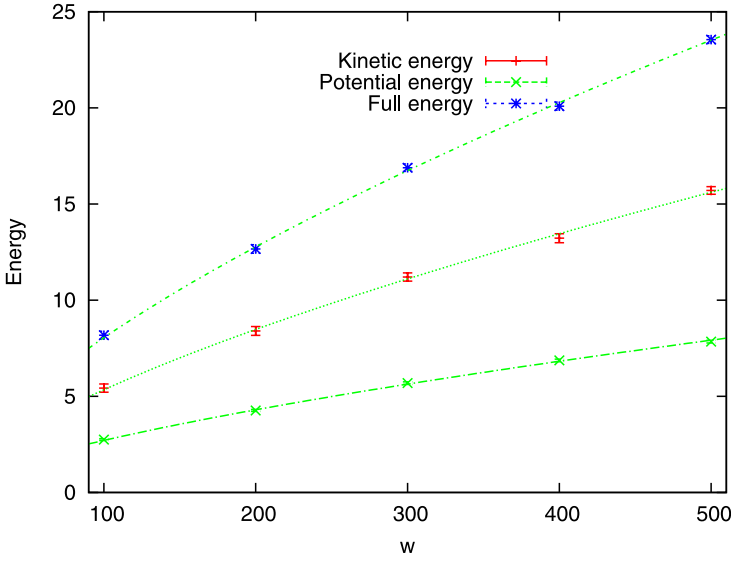

Fig. 4. (Color online) Dependence of energy on ω for $m = 0.1$.

6. Comparison with the Schrodinger Equation Approach

The Hamiltonian of the relativistic oscillator is

$$\hat{\mathrm{H}} = \sqrt{\hat{p}^2 + m^2} + \frac{1}{2} m\omega^2 \hat{q}^2. \tag{49}$$

It is a quadratic form of coordinate and a more complicated function of momentum, in contrast with most nonrelativistic Hamiltonians. It is convenient to use momentum representation $\hat{p} = p$, $\hat{q} = i\frac{\partial}{\partial p}$. Then, the Schrodinger equation will have the form

$$\frac{m\omega^2}{2} \frac{\partial^2 \Psi_p}{\partial p^2} + (\sqrt{p^2 + m^2} + E)\Psi_p = 0. \tag{50}$$

It is equivalent to the Schrodinger equation for potential $V = \sqrt{q^2 + a^2}$ in coordinate space and can be solved by similar methods. The resulting function $\Psi_p(p)$ can be later transformed into $\Psi_q(q)$ by Fourier transform, the energy levels E_i do not depend on representation.

Equation (50) can be transformed to dimensionless variables $\tilde{p} = p/m = p/mc$, $\tilde{E} = E/m = E/mc^2$, $\tilde{\omega} = \omega/m = \omega\hbar/mc^2$

$$\frac{\tilde{\omega}^2}{2} \Psi_p'' + (\tilde{E} - \sqrt{\tilde{p}^2 + 1})\Psi_p = 0, \tag{51}$$

where $'$ denotes a derivative by momentum p. This equation contains only one parameter $\tilde{\omega}$, which controls the derivative. If $\tilde{\omega} \ll 1$, the wave function is well localized near the minimum of the "potential" (in momentum representation) i.e. this situation corresponds the non relativistic case $\tilde{p} \to 0$. Respectively, if $\tilde{\omega} \gg 1$, the wave function is not much localized, that corresponds the ultra-relativistic case $\tilde{p} \to \infty$. In both cases, we should understand the momentum as its average absolute value.

For $\tilde{\omega} \ll 1$, $\tilde{p} \to 0$, the asymptotic form of the equation is

$$\frac{\tilde{\omega}^2}{2} \Psi_p'' + \left(\tilde{E} - 1 - \frac{\tilde{p}^2}{2}\right)\Psi_p = 0. \tag{52}$$

It is similar to Schrodinger equation for classical oscillator. Corresponding wave functions and energy levels are

$$\Psi_{pn} = \frac{\sqrt[4]{\tilde{\omega}/\pi}}{\sqrt{2^n n!}} \exp(-\tilde{\omega}\tilde{p}^2/2) H_n(\sqrt{\tilde{\omega}}\tilde{p}), \tag{53}$$

$$\tilde{E}_n = 1 + \tilde{\omega}(n + 1/2). \tag{54}$$

The asymptotic form of Eq. (51) for $\tilde{\omega} \gg 1$, $\tilde{p} \to \infty$ is

$$\frac{\tilde{\omega}^2}{2} \Psi_p'' + (\tilde{E} - \tilde{p})\Psi_p = 0. \tag{55}$$

Its solution, regular at infinity, is the Airy function of the first kind

$$\Psi_p = A * \mathrm{Ai}\left(\left(\frac{\sqrt{2}}{\omega}\right)^{2/3}(\tilde{p}-\tilde{E})\right) \sim e^{-\frac{2\sqrt{2}}{3\omega}(\tilde{p}-\tilde{E})^{3/2}}. \tag{56}$$

Corresponding energy levels are

$$\tilde{E}_n = (3\pi\tilde{\omega}n)^{2/3}/2. \tag{57}$$

Equation (51) was numerically solved by shooting method for $10^{-5} \leq \tilde{\omega} \leq 10^5$. As the asymptotic behavior at infinity is an exponential decay, shooting was performed from $\pm\infty$ with arbitrary small constant as the boundary condition. The stitch was made in zero. The parameter of shooting is the energy E. We required relative accuracy 10^{-6} in energy levels. Eigenfunctions $\Psi_{pm}(p)$ and eigenvalues E_n (for 10 lowest levels) were obtained. Eigenfunctions in coordinate representation $\Psi_n(x)$ were calculated by Fourier transform. This numerical solution of Schrodinger equation can be used to verify the PIMC results.

In Figs. 5 and 6, one can find the results of PIMC simulations of the total energy of the ground state at $\omega = 1$. In nonrelativistic limit, the energy of the ground state equals to $\omega/2 = 0.5$. The green line is the result of Schrodinger equation approach. One can see that PIMC results are in good agreement with the results of the Schrodinger equation approach. After analyzing, we have found out that PIMC method can be applied for very strong potentials.

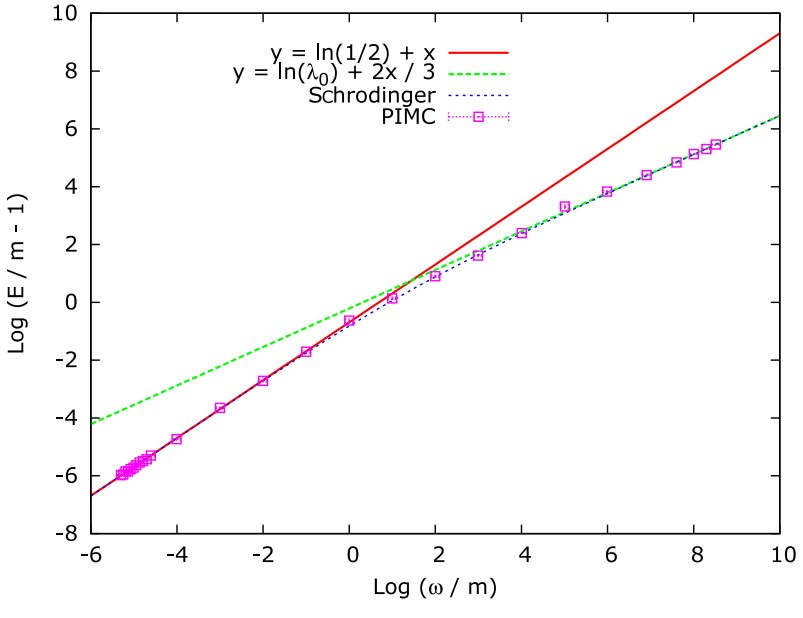

Fig. 5. (Color online) PIMC simulations for total energy of the relativistic oscillator ground state, $\omega = 1$. The green line is the results of Schrodinger equation approach.

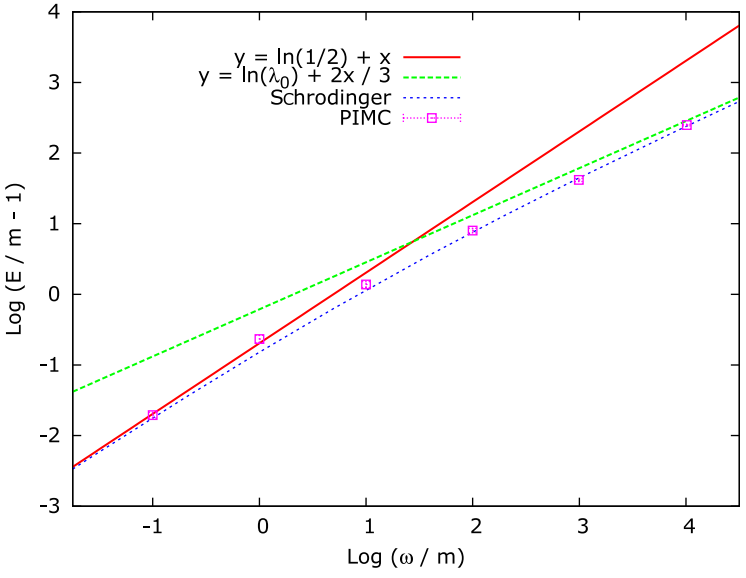

Fig. 6. (Color online) PIMC simulations for total energy of the relativistic oscillator ground state, $\omega = 1$. The green line is the results of Schrodinger equation approach. High resolution plot for intermediate area.

7. Conclusion

The main goal of our work is to construct relativistic generalization of the PIMC method. We plan to use this method to investigate the properties of the relativistic quantum media with instantaneous interactions between the particles. The last condition gives us a possibility to avoid the problem with correctness of the many-body quantum–mechanical interaction. Of course, there are many interesting applications that one can find in relativistic quantum chemistry and condensed matter physics.

To test our approach, we study a simple one-dimensional system with quadratic external potential — relativistic harmonic oscillator. This system gives us the possibility to test our approach because relativistic harmonic oscillator can be studied by solving Schrodinger equation in momentum space. The comparison of the results of these two approaches has shown that our relativistic generalization of PIMC method can be used for the investigation of quantum systems which contain relativistic particles. It is very essential to emphasize that in ultra-relativistic, some special considerations are needed to solve the problem of thermalization configuration.

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