Monte-Carlo calculations for Relativistic Oscillator

Generalization of Path Integral Metropolis Algorithm

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Abstract

Simple Path Integral Metropolis Algorithm has been generalized for relativistic kinetic energy. In this work average of x^2, kinetic T and potential V energy, correlation function $x(t)x(t+\tau)$, probability density $\rho(x)$ are calculated. Each observable value has been checked for nonrelativistic limit(big mass).

Introduction

The model of the Harmonic Oscillator is one of the most popular in physics. The Path Integral Monte-Carlo methods are well developed for this model. A lot of work are made in this field. We considered the model of oscillator, which has a relativistic kinetic energy instead of usual classical. Kinetic energy T, potential energy V, average of x square $\langle x^2\rangle$, density of probability $\rho(x)$, correlation function $\langle x(t)x(t+\tau)\rangle$ are calculated for the case of relativistic harmonic oacillator.

Designations

$x(t)$ - the path to be integrated, $t \in [0,T]$ and we took periodic bound conditions : $x(0) = x(T)$. m is the mass of particle and ω is frequency. p is the momentum. Hamiltonian function is

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

$\beta = 1/\theta$ - inverse temperature for this system. We considered limit of large β ($\beta \geq 10$). N_p - count of paths, N_s - count of sweeps, N_t - count of time slices, N - count of attemptions to change value in one time scile, $\tau = a$ - time step.

Mathematical Section

$\rho(x, x'; \beta)$ is position-space density matrix:

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

Discretization $\tau = T/N_t = \beta/N_t$ Matrix element of kinetic energy $T = \sqrt{p^2+m^2}$ was calculated

$$\langle x_{i-1}|e^{-\tau T}|q\rangle = \frac{m\tau}{\pi\sqrt{\tau^2+(q-x_{i-1})^2}}K_1(m\sqrt{\tau^2+(q-x_{i-1})^2}).$$

Finally,

$$\rho(x_{i-1}, x_i; \tau) = \frac{m\tau}{\pi\sqrt{\tau^2+(x_i-x_{i-1})^2}}K_1(m\sqrt{\tau^2+(x_i-x_{i-1})^2})e^{-V(x_i)\tau},$$

$$\rho(x_0, x_{N_t}; \beta) = \int\dots\int dx_1\dots dx_{N_t}\rho(x_0, x_1; \tau)\dots\rho(x_{N_t-1}, x_{N_t}; \tau).$$

Observable values

Densities of probability were calculated by formula

$$\rho(x) = |\psi(x)|^2 = \frac{1}{\Delta x N_t N_p}\sum_i^{\text{all paths}}\theta(\Delta x - |x_i - x|).$$

Kinetic energy of relativistic oscillator

$$\langle\sqrt{p^2+m^2} - m\rangle = \langle\frac{m\tau}{\sqrt{\tau^2+(x_{n+1}-x_n)^2}}\frac{K_0(m\sqrt{\tau^2+(x_{n+1}-x_n)^2})}{K_1(m\sqrt{\tau^2+(x_{n+1}-x_n)^2})} + \frac{\tau^2-(x_{n+1}-x_n)^2}{\tau(\tau^2+(x_{n+1}-x_n)^2)} - m\rangle$$

Results

Paths for different masses at fixed $\omega = 1$ were calculated.

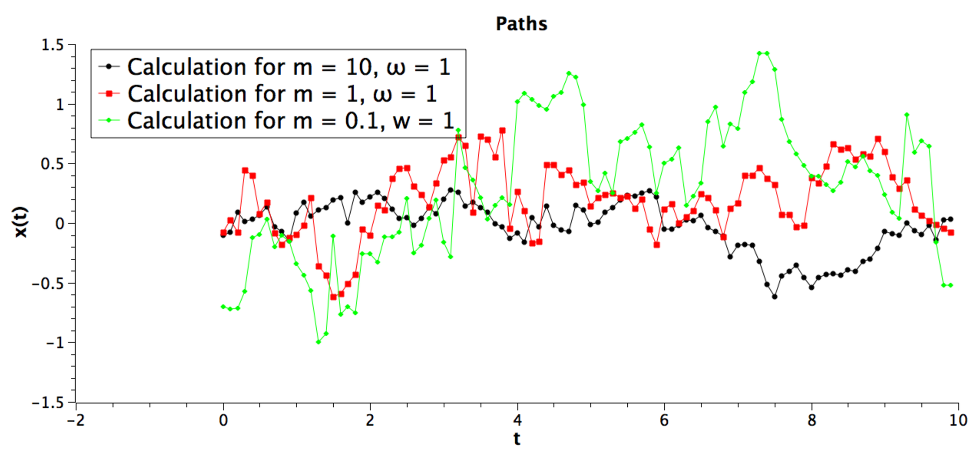

Figure 1: Dependence of some x(t) on t.

We calculated dependence $\langle x^2\rangle$ on m and ω over paths were generated with relativistic density matrix.

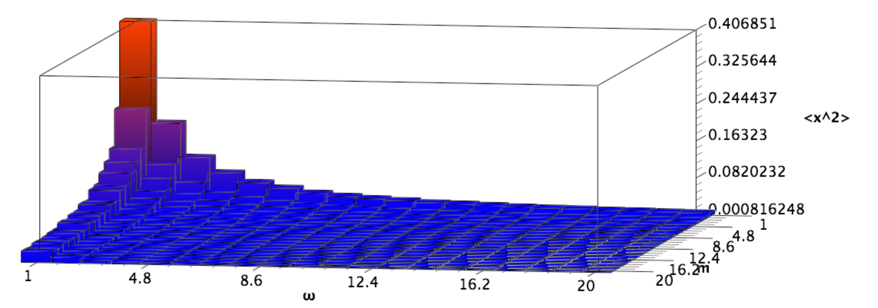

Figure 2: Dependence $\langle x^2\rangle$ on m and ω for $N_p = 100$, $N_s = 1000$, $N_t = 100$, $\tau = 0.1$, $N = 10$.

The next figure is more informative

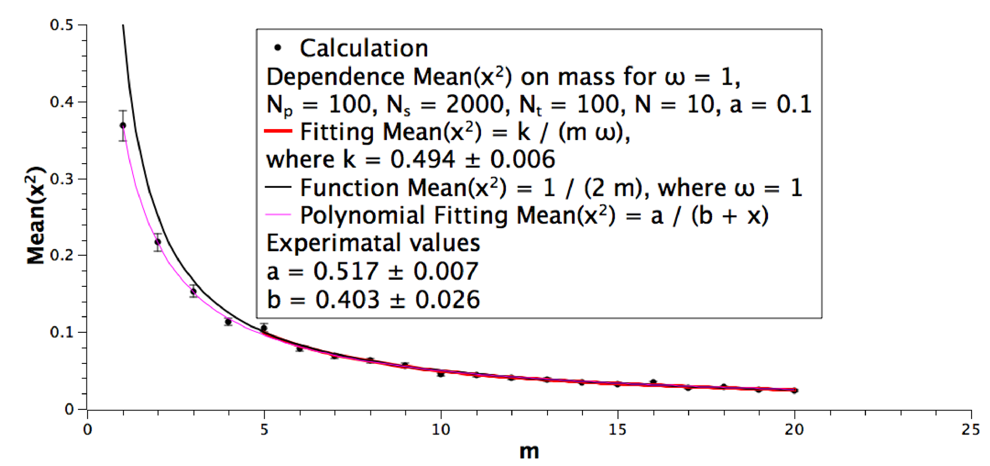

Figure 3: Dependence $\langle x^2\rangle$ on m for $\omega = 1$, $N_p = 100$, $N_s = 2000$, $N_t = 100$, $\tau = 0.1$, $N = 10$.

We see good agreement with nonrelativistic limit at mass more, than 5 for $\omega = 1$. At lower masses, there is a relativistic effect - average of x^2 is lower, than in nonrelativistic limit, which has a good agreement with polynomial fitting.

Typical figures for correlation functions

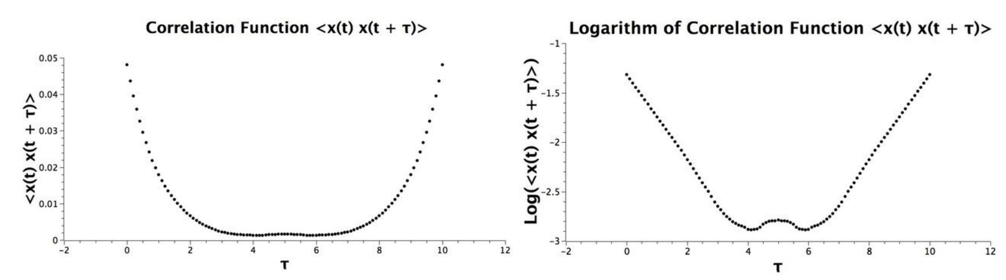

Figure 4: Correlation Function and Logarithm of Correlation Function for $N_p = 1000$, $N_s = 2000$, $N_t = 100$, $\tau = 0.1$, $N = 10$, $m = 10$, $\omega = 1$.

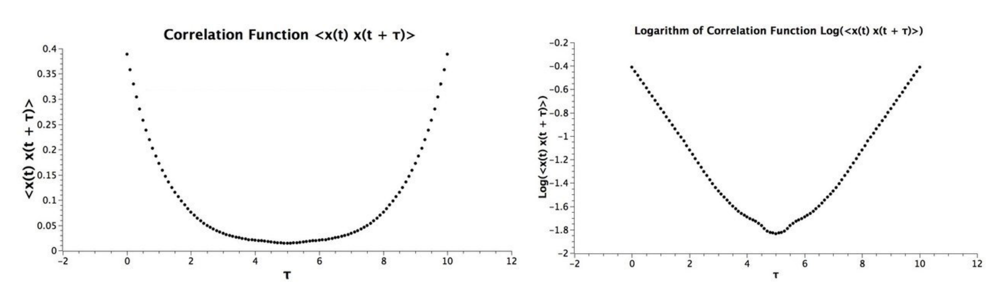

Figure 5: Correlation Function and Logarithm of Correlation Function for $N_p = 1000$, $N_s = 2000$, $N_t = 100$, $\tau = 0.1$, $N = 10$, $m = 1$, $\omega = 1$.

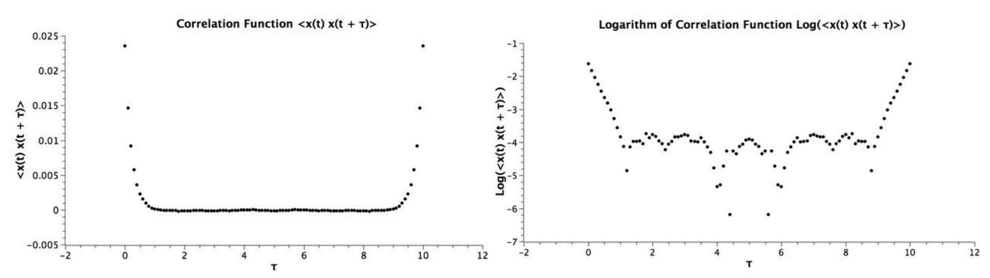

Figure 6: Correlation Function and Logarithm of Correlation Function for $N_p = 1000$, $N_s = 2000$, $N_t = 100$, $\tau = 0.1$, $N = 10$, $m = 1$, $\omega = 10$.

Inspite of changes in hamiltonian function, probability densities were fitted gaussian excellentlly. Although, at ultrarelativistic limit probability density describes by Airy function.

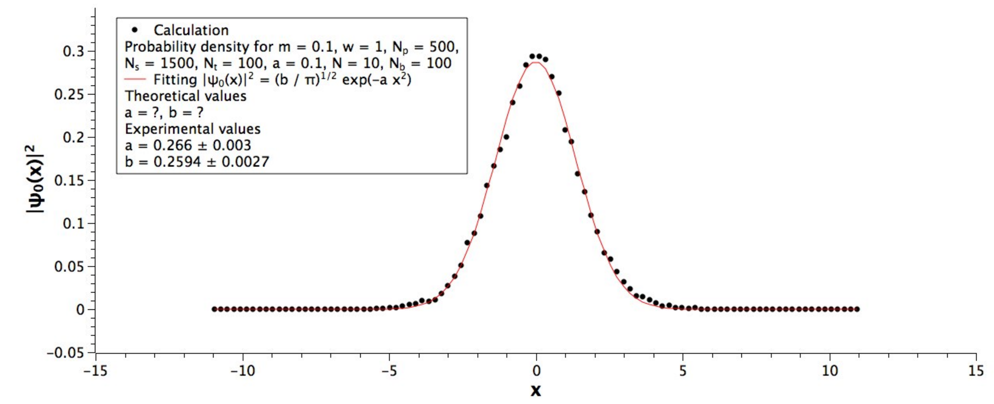

Figure 7: Probability density for $m = 0.1$, $\omega = 1$, $N_p = 500$, $N_s = 1500$, $N_t = 100$, $\tau = 0.1$, $N = 10$, $N_b = 100$.

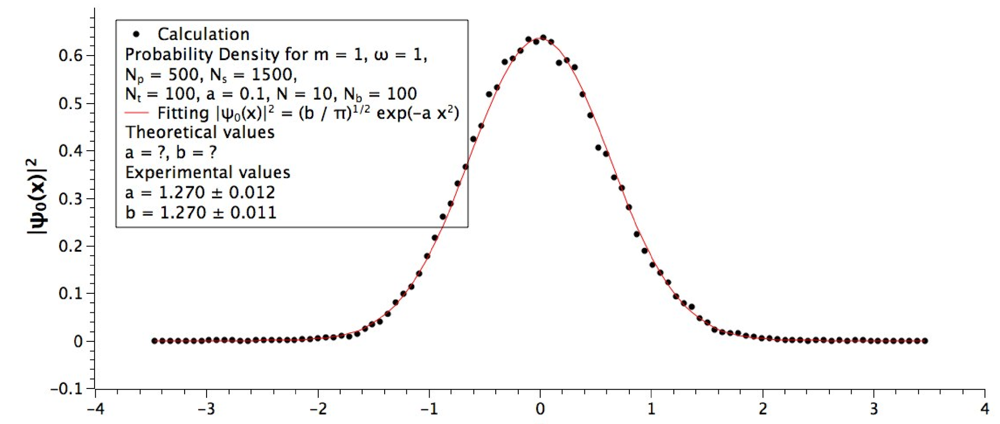

Figure 8: Probability density for $m = 1$, $\omega = 1$, $N_p = 500$, $N_s = 1500$, $N_t = 100$, $\tau = 0.1$, $N = 10$, $N_b = 100$.

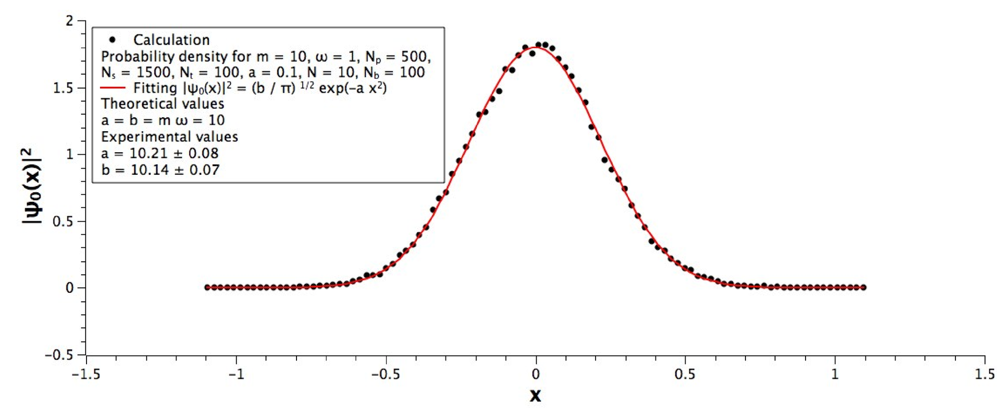

Figure 9: Probability density for $m = 10$, $\omega = 1$, $N_p = 500$, $N_s = 1500$, $N_t = 100$, $\tau = 0.1$, $N = 10$, $N_b = 100$.

At the limit $m \gg \omega$, nonrelativistic limit has been achieved. We obtained good fitting with probability density of main state of usual harmonic oscillator. Results for energy

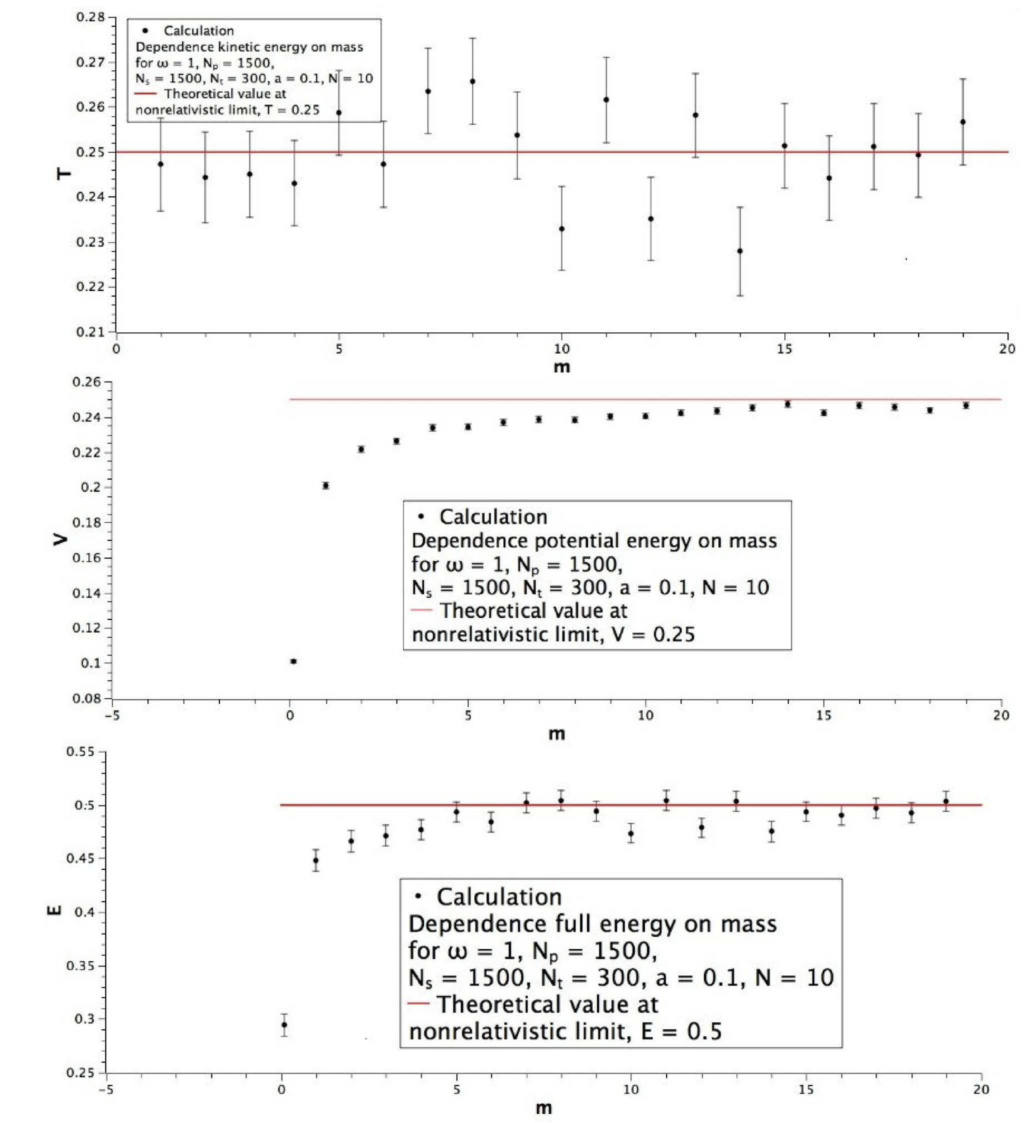

Figure 10: Dependence energy for $\omega = 1$, $N_p = 1500$, $N_s = 1500$, $N_t = 300$, $\tau = 0.1$, $N = 10$.

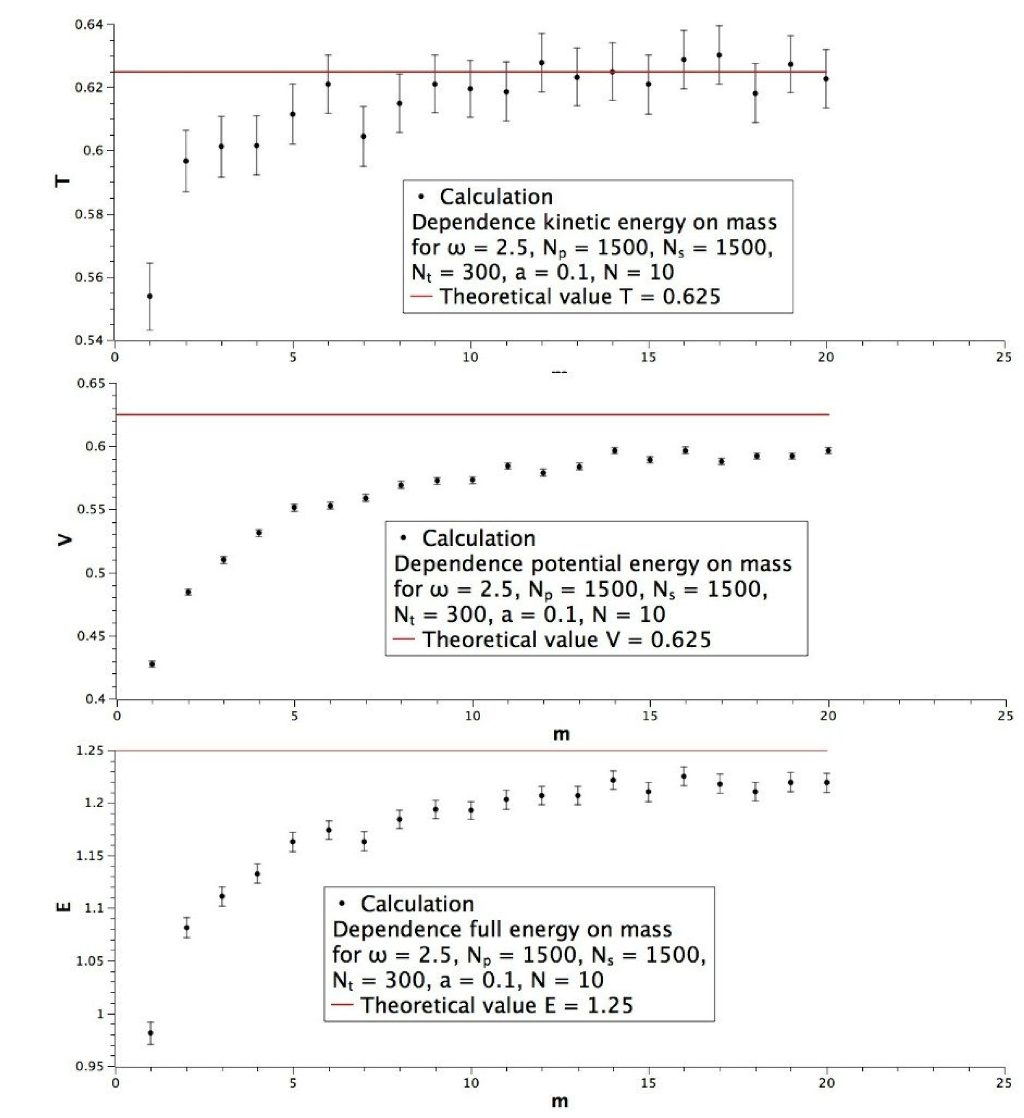

Figure 11: Probability density for $\omega = 2.5$, $N_p = 1500$, $N_s = 1500$, $N_t = 300$, $\tau = 0.1$, $N = 10$.

Conclusions

The Path Integral Metropolis Algorithm has been generalized for relativistic kinetic energy. The expression of kinetic energy observable was found. We calculated observable values for this model and checked them for nonrelativistic limit.