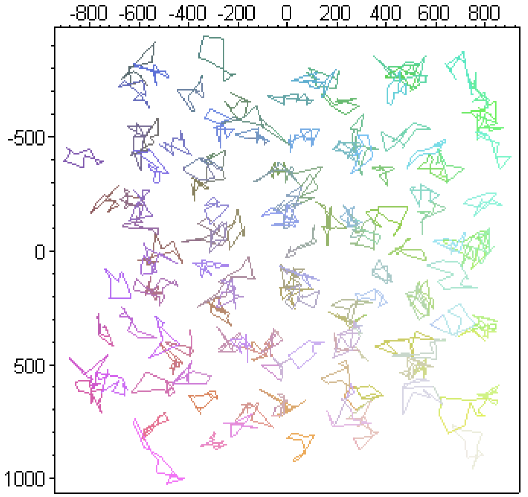
LPI for relativistic and non-relativistic MB Quantum systems

(Path integral Monte-Carlo method for relativistic matter)



Oleg V. Pavlovsky (MSU & ITEP, Moscow)

Alexander Ivanov (MSU, Moscow)

Alexander Novoselov (MSU & ITEP, Moscow)

Motivation

Lattice QFT and Lattice QM

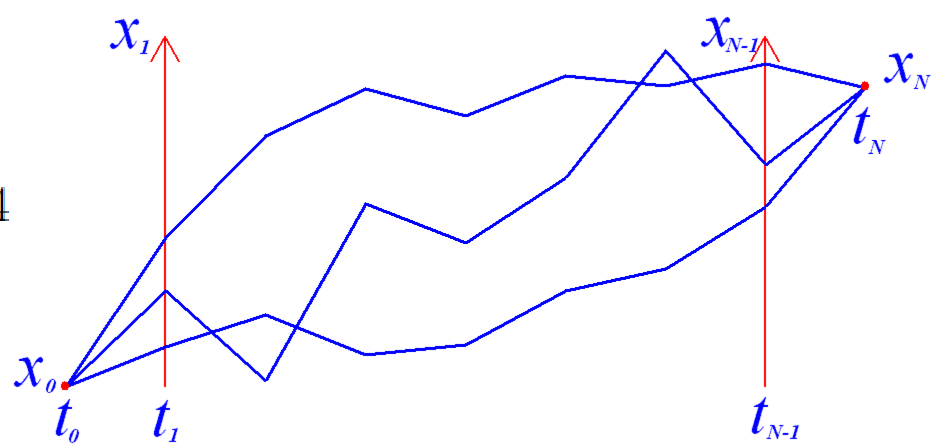
1. Euclidian QF – Boltzmann statistical system

$$\langle \mathbf{x}_0 | e^{-\beta H} | \mathbf{x}_{N_t} \rangle = \prod_{t=0}^{N_t-1} \langle \mathbf{x}_t | e^{-\tau H} | \mathbf{x}_{t+1} \rangle \equiv \prod_{t=0}^{N_t-1} e^{-S_t} \equiv e^{-S}$$

2. Path Integral approach

In numerical simulations

$$N_t \approx 10^3 - 10^4$$

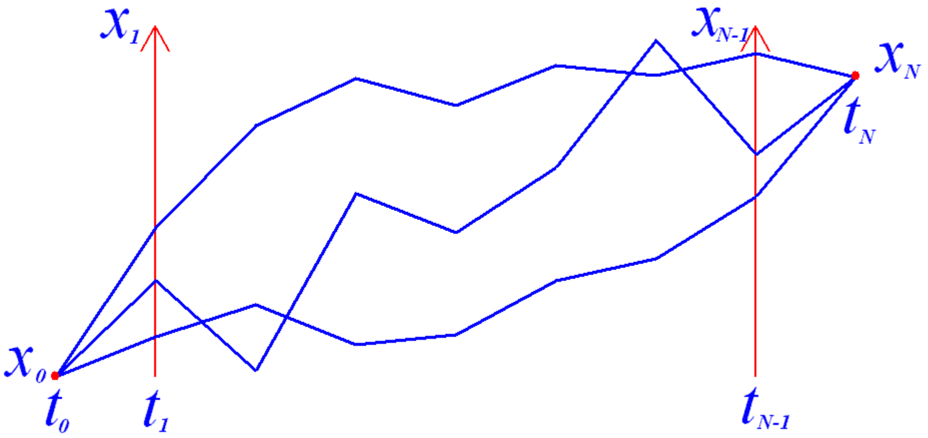


PIMC: non-relativistic case

$$Z = \int d\mathbf{x_0} \langle \mathbf{x}_0 | e^{-\beta H} | \mathbf{x}_0 \rangle = \int \mathcal{D}\mathbf{x} e^{-S}$$

$$\langle A \rangle = \frac{1}{Z} \int d\mathbf{x}_0 \langle \mathbf{x}_0 | A e^{-\beta H} | \mathbf{x}_0 \rangle = \frac{\int \mathcal{D}\mathbf{x} A e^{-S}}{\int \mathcal{D}\mathbf{x} e^{-S}}$$

Observable



Lattice QFT and Lattice QM

3. Monte – Carlo Method

$$Z = \int d\mathbf{x_0} \langle \mathbf{x}_0 | e^{-\beta H} | \mathbf{x}_0 \rangle = \int \mathcal{D}\mathbf{x} e^{-S}$$

$$\langle A \rangle = \frac{1}{Z} \int d\mathbf{x}_0 \langle \mathbf{x}_0 | A e^{-\beta H} | \mathbf{x}_0 \rangle = \frac{\int \mathcal{D}\mathbf{x} A e^{-S}}{\int \mathcal{D}\mathbf{x} e^{-S}}$$

$$\langle A \rangle = \int d\mu A(\mathbf{x})$$

$$d\mu = \frac{\mathcal{D}\mathbf{x} e^{-S}}{\int \mathcal{D}\mathbf{x} e^{-S}}$$

$$\langle A \rangle = \sum_{conf} P(\mathbf{x}) A(\mathbf{x}) \qquad P(\mathbf{x}) = \frac{e^{-S(\mathbf{x})}}{\sum_{conf} e^{-S(\mathbf{x})}}$$

$$\boxed{\langle A \rangle = \frac{1}{N_{conf}} \sum_{k=1}^{N_{conf}} A(\mathbf{x}_k)}$$

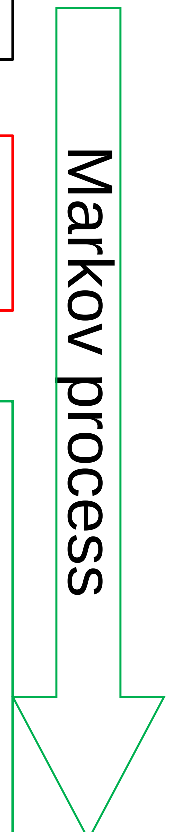
PIMC: generation of the equilibrium configurations

Initial configuration $\mathbf{x}_0$

«non-equilibrium» configuration

«equilibrium» configurations with

$$P(\mathbf{x}) = \frac{e^{-S(\mathbf{x})}}{\sum_{conf} e^{-S(\mathbf{x})}}$$



PIMC: non-relativistic and relativistic systems

For non-relativistic systems:

$$P(\mathrm{path}) \sim \exp\left(-S_{\mathrm{clas}}(\mathrm{path})\right)$$

Is it correct for relativistic systems?

Path Integrals: notation

Hamiltonian

$$H(p,q) = T(p) + V(q)$$

Evolution operator

$$U = \exp\left(-\beta\, H(p,q)\right)$$

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

$$e^{-(\beta_1+\beta_2)H} = e^{-\beta_1 H} e^{-\beta_2 H}$$

$$\rho(q_1,q_3;\beta_1+\beta_2) = \int dq_2 \rho(q_1,q_2;\beta_1)\rho(q_2,q_3;\beta_2)$$

$$e^{-\beta H} = (e^{-\tau H})^N$$

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

Path Integrals: notation

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

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

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

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

$$= \int \frac{dp}{2\pi} e^{-T(p)\tau - ip(q_0 - q_1)}$$

Path Integrals: notation

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

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

$$\underline{\langle q_0 | e^{-\tau T} | q_1 \rangle} = \int dp dp' \delta(p - p') \langle q_0 | p \rangle \langle p' | q_1 \rangle e^{-T(p)\tau}$$

$$\boxed{= \int \frac{dp}{2\pi} e^{-T(p)\tau - ip(q_0 - q_1)}}$$

Path Integrals: non-relativistic particle

$$T(p) = \frac{p^2}{2m}$$

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

$$= \frac{1}{\sqrt{2\pi\tau/m}} e^{-\frac{m(q_2-q_1)^2}{2\tau^2}\tau}$$

$$\rho(q_0, q_N; \beta) = \int dq_1 \ldots dq_{N-1} (2\pi\tau/m)^{-N/2} \exp\Big[-\sum_{i=1}^{N} \Big(\frac{m(q_i - q_{i-1})^2}{2\tau^2} + V(q_i)\Big)\tau\Big]$$

Path Integrals: non-relativistic particle

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$$\rho(q_0, q_N; \beta) = \int dq_1 \ldots dq_{N-1} (2\pi\tau/m)^{-N/2} \exp\Big[- \overbrace{\boxed{\sum_{i=1}^{N} \Big(\frac{m(q_i - q_{i-1})^2}{2\tau^2} + V(q_i) \Big) \tau}}^{S_{\text{clas}}(\text{path})} \Big]$$

Path Integrals: relativistic particle

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

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

Path Integrals: relativistic particle

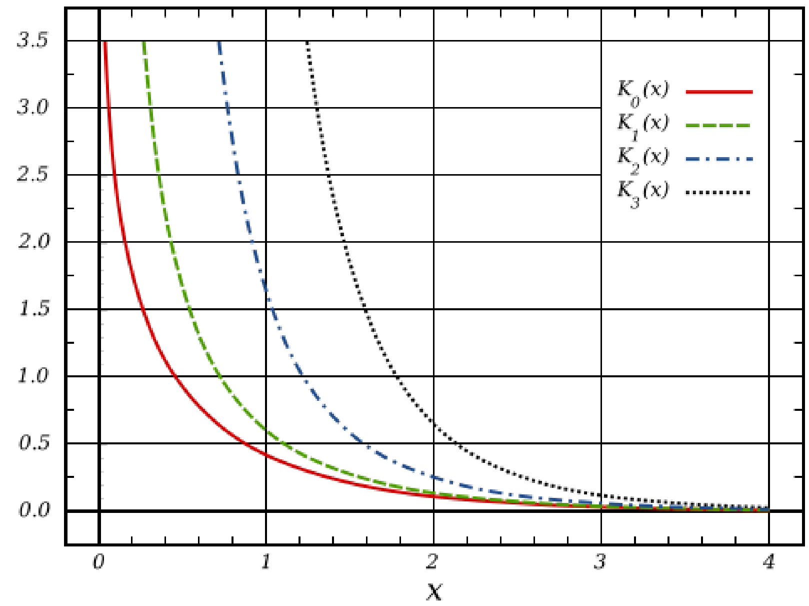
$$T(p) = \sqrt{p^2 + m^2}$$

$$\downarrow$$

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

$$= \frac{m\tau}{\pi\sqrt{\tau^2 + (q_1 - q_0)^2}} K_1(m\sqrt{\tau^2 + (q_1 - q_0)^2})$$

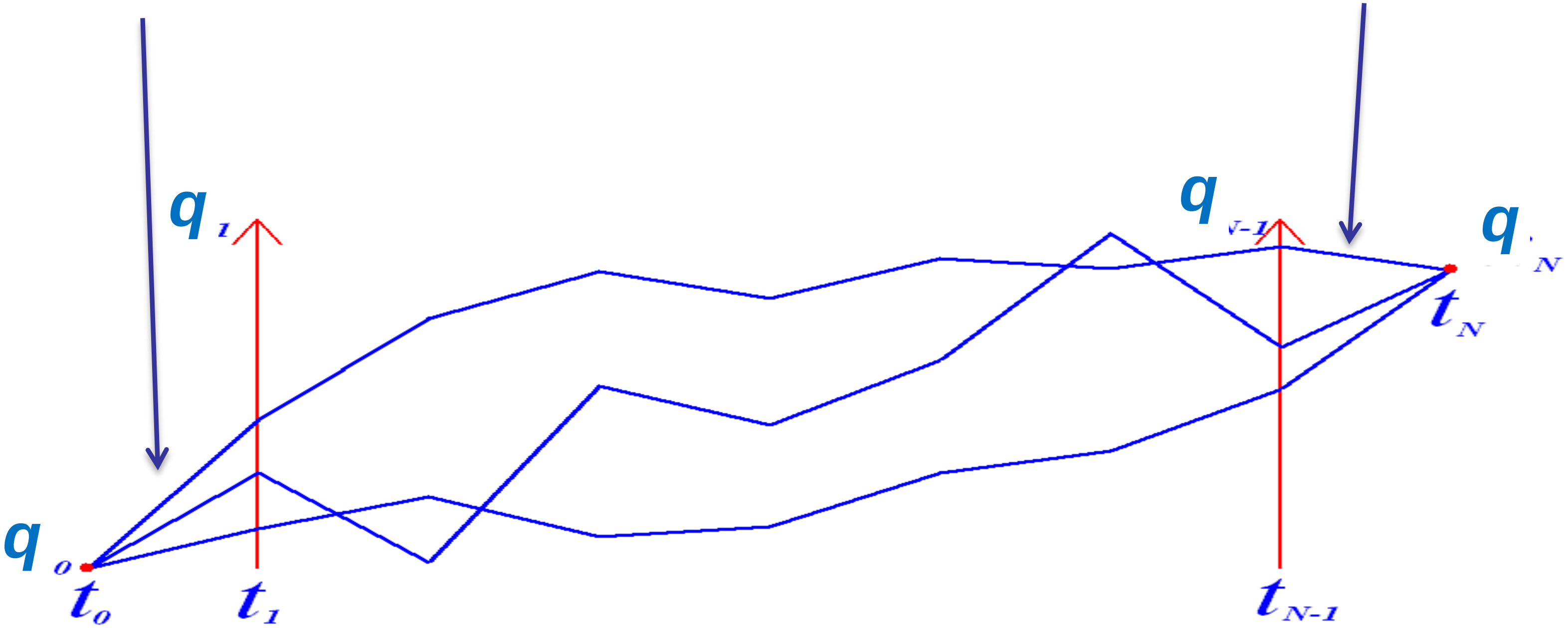
Modified Bessel function of 2nd kind (Macdonald)



Path Integrals: relativistic particle

$$\rho(q_0, q_N; \beta) =$$

$$= \int dq_1 \dots dq_{N-1} \frac{m\tau}{\pi\sqrt{\tau^2 + (q_1 - q_0)^2}} K_1(m\sqrt{\tau^2 + (q_1 - q_0)^2}) \dots \frac{m\tau}{\pi\sqrt{\tau^2 + (q_N - q_{N-1})^2}} K_1(m\sqrt{\tau^2 + (q_N - q_{N-1})^2})$$



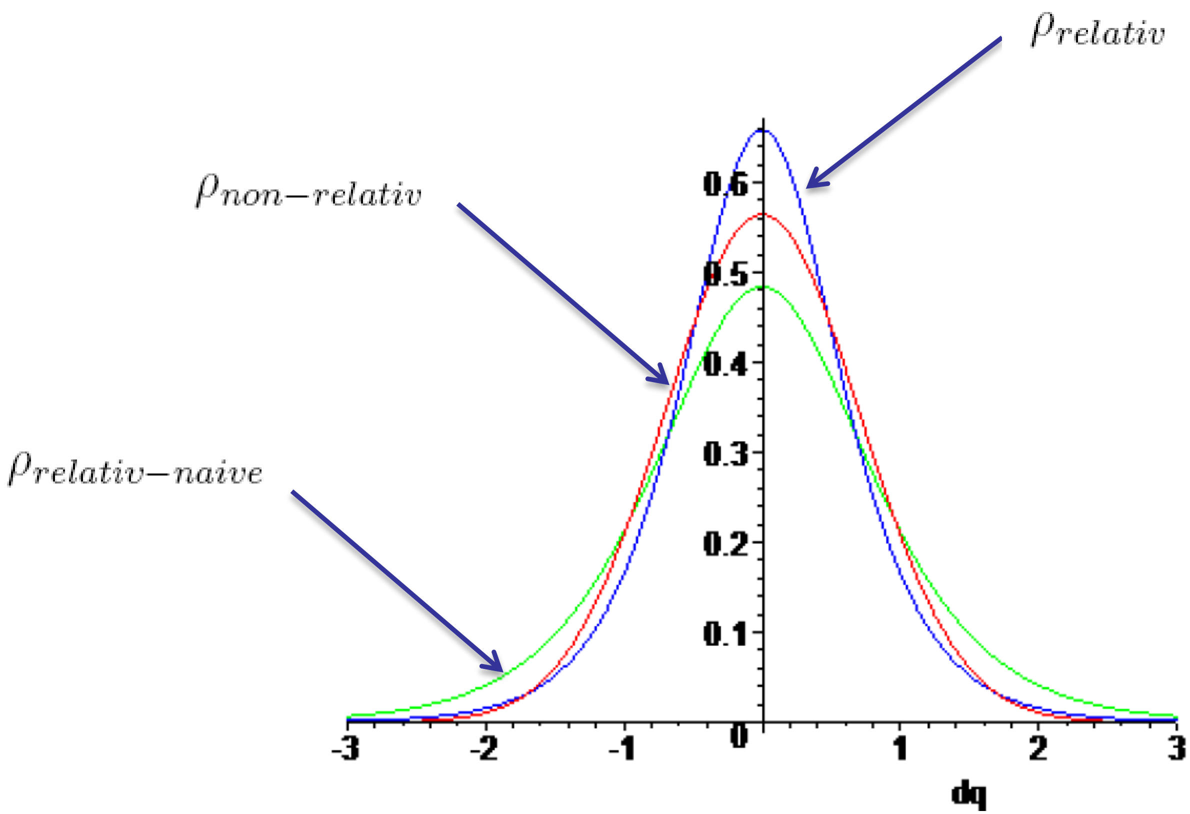
Path Integrals: relativistic particle

$$\cancel{\exp\left(-S_{\text{clas}}(\text{path})\right)}$$

$$\rho(q_0, q_N; \beta) = \int dq_1 \ldots dq_{N-1} \frac{m\tau}{\pi\sqrt{\tau^2 + (q_1 - q_0)^2}} K_1(m\sqrt{\tau^2 + (q_1 - q_0)^2}) \ldots$$

$$\ldots \frac{m\tau}{\pi\sqrt{\tau^2 + (q_N - q_{N-1})^2}} K_1(m\sqrt{\tau^2 + (q_N - q_{N-1})^2}) \exp\Big(-\sum_{i=1}^{N} V(q_i)\tau\Big).$$

Path Integrals: relativistic particle



Non-relativistic and ultra-relativistic limits

Non-Relativistic limit:

Class. Kin. Energy

Rest Mass

$$m\tau \gg 1, \ \frac{(q_1-q_0)^2}{\tau^2} \ll 1$$

$$\frac{m\tau}{\pi\sqrt{\tau^2+(q_1-q_0)^2}}K_1\left(m\sqrt{\tau^2+(q_1-q_0)^2}\right) \to \frac{1}{\sqrt{2\pi\tau/m}}e^{-\frac{m(q_2-q_1)^2}{2\tau^2}\tau - m\tau}.$$

Ultra-Relativistic limit:

$$\langle q_0|e^{-\tau T}|q_1\rangle = \int \frac{dp}{2\pi}e^{-|p|\tau - ip(q_0-q_1)} = \frac{1}{\pi}\frac{\tau}{\tau^2+(q_0-q_1)^2}$$

$$\langle q_1|H|q_0\rangle = -\frac{1}{\pi(q_0-q_1)^2}$$

Path Integrals: D+1 dim relativistic particle

$$T(p) = \sqrt{p_{q_1}^2 + \cdots + p_{q_d}^2 + m^2}$$

$$\downarrow$$

$$\langle q_0 | e^{-\tau T} | q_1 \rangle = \int \frac{dp_{q_1} \ldots dp_{q_d}}{(2\pi)^d} e^{-\sqrt{p_{q_1}^2 + \cdots + p_{q_d}^2 + m^2}\,\tau - i p_{q_1}(q_{10} - q_{11}) - \cdots - i p_{q_d}(q_{d0} - q_{d1})} =$$

$$= \left(\frac{m\tau}{\pi \sqrt{\tau^2 + (\mathbf{q_1} - \mathbf{q_0})^2}} \right)^{(d+1)/2} \frac{K_{(d+1)/2}(m\sqrt{\tau^2 + (\mathbf{q_1} - \mathbf{q_0})^2})}{(2\tau)^{(d-1)/2}}.$$

$$\rho(q_0, q_N; \beta) = \int dq_1 \ldots dq_{N-1} \left(\frac{m\tau}{\pi \sqrt{\tau^2 + (\mathbf{q_1} - \mathbf{q_0})^2}} \right)^{(d+1)/2} \frac{K_{(d+1)/2}(m\sqrt{\tau^2 + (\mathbf{q_1} - \mathbf{q_0})^2})}{(2\tau)^{(d-1)/2}} \cdots$$

$$\cdots \left(\frac{m\tau}{\pi \sqrt{\tau^2 + (\mathbf{q_N} - \mathbf{q_{N-1}})^2}} \right)^{(d+1)/2} \frac{K_{(d+1)/2}(m\sqrt{\tau^2 + (\mathbf{q_1} - \mathbf{q_0})^2})}{(2\tau)^{(d-1)/2}} \exp\left(-\sum_{i=1}^{N} V(q_i)\tau \right).$$

Path Integrals: 2+1 dim relativistic particles Model of Graphene

$$\langle q_0|e^{-\tau T}|q_1\rangle = \left(\frac{m\tau}{\pi\sqrt{\tau^2+(\mathbf{q_2}-\mathbf{q_1})^2}}\right)^{3/2}\frac{K_{3/2}(m\sqrt{\tau^2+(\mathbf{q_2}-\mathbf{q_1})^2})}{\sqrt{2\tau}}$$

$$K_{3/2}(x) = -\sqrt{\frac{\pi x}{2}}\frac{d}{dx}\left(\frac{e^{-x}}{x}\right)$$

$$\frac{\tau}{2\pi}\frac{1+m\sqrt{\tau^2+(\mathbf{q_2}-\mathbf{q_1})^2}}{(\tau^2+(\mathbf{q_2}-\mathbf{q_1})^2)^{3/2}} \quad \underline{e^{-m\sqrt{\tau^2+(\mathbf{q_2}-\mathbf{q_1})^2}}}$$

$$\rho(q_0,q_N;\beta) = \int D\,q(\tau)\;\; F[q(\tau)]\;\; e^{-S_{clas}[q(\tau)]}$$

Relativistic PIMC: one particle test

Relativistic harmonic oscillator

$$H = \sqrt{p^2 + m^2} + \frac{1}{2} m w^2 q^2$$

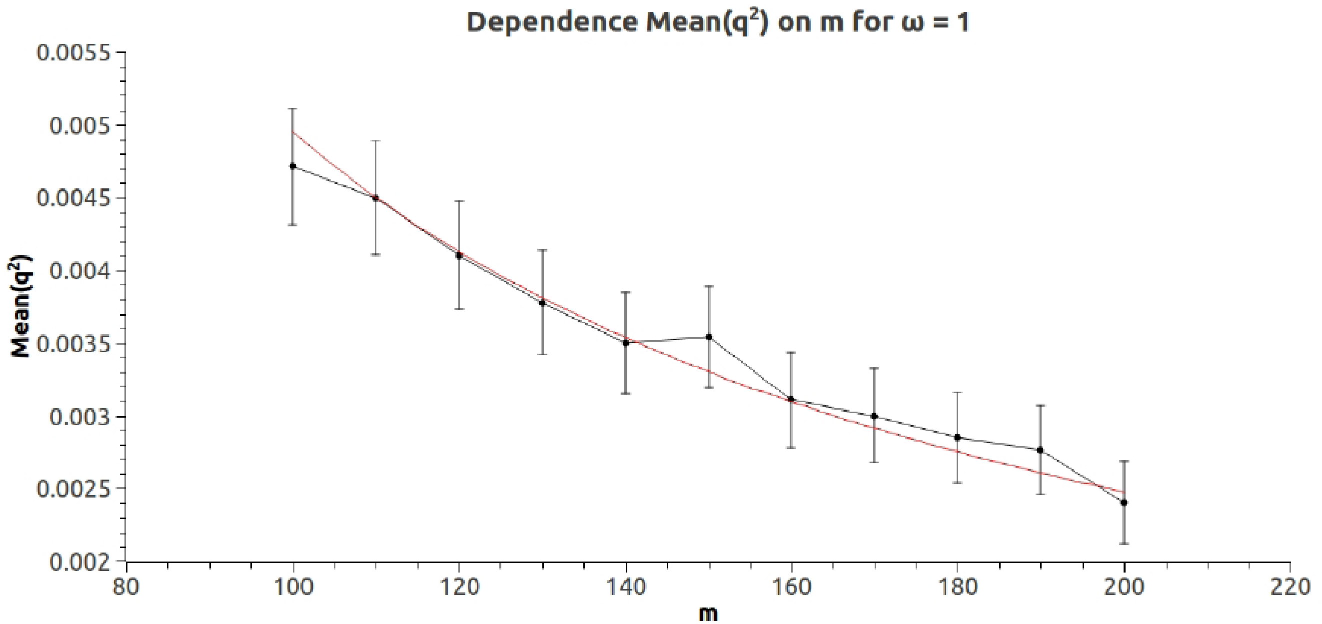
Metropolis Monte-Carlo algorithm

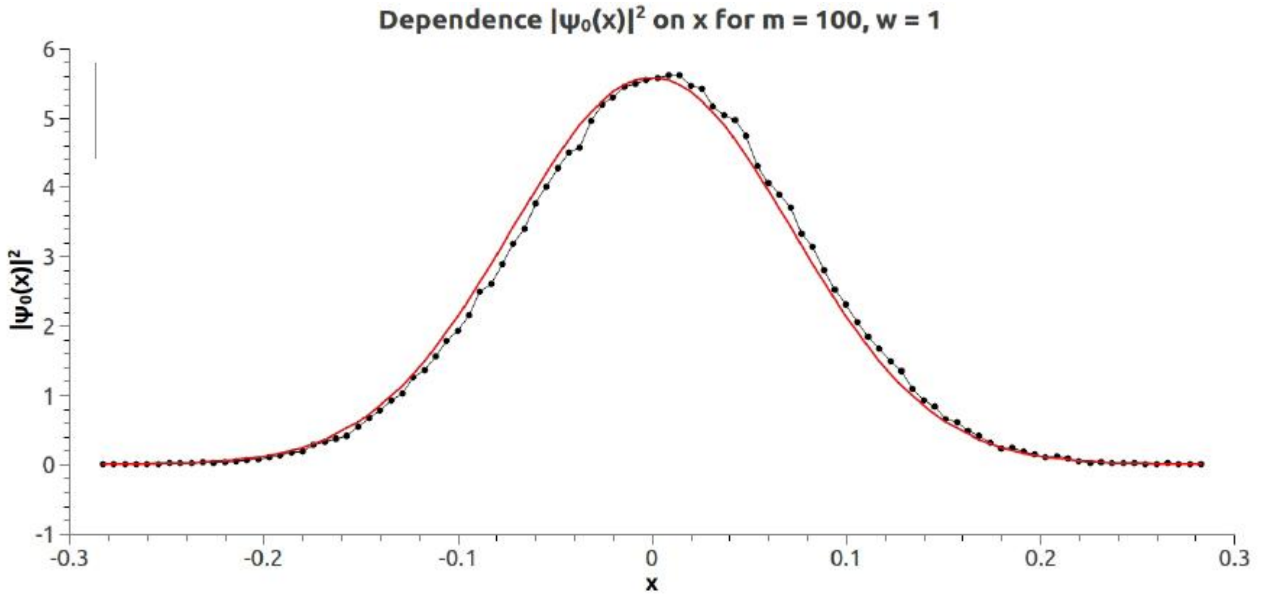
$$W(q_i, q_i') = T(q_i, q_i')A(q_i, q_i') - \delta(q_i - q_i')(1 - \int dq'' T(q_i, q_i'')A(q_i, q_i''))$$

$$A(q_i, q_i') = \min\left[1, \frac{P^{eq}(q_i')T(q_i', q_i)}{P^{eq}(q_i)T(q_i, q_i')}\right]$$

$$\left(\frac{m\tau}{\pi}\right)^2 \frac{K_1(m\sqrt{\tau^2 + (q_{i+1} - q_i)^2})K_1(m\sqrt{\tau^2 + (q_i - q_{i-1})^2})}{\sqrt{\tau^2 + (q_{i+1} - q_i)^2}\sqrt{\tau^2 + (q_i - q_{i-1})^2}}$$

Relativistic Harmonic oscillator





Problems for Solution:

1. Relativistic corrections in strong potentials
2. Thermodynamic properties of relativistic matters: Energy, Pressure, …
3. Equation of state of relativistic matters: $P(\rho)$
4. Transport coefficients: diffusion, viscosity, …

Energy: non-relativistic case

$$E = -\frac{1}{V}\frac{\partial}{\partial\beta}\Big(\mathrm{Ln}(Z)\Big)_V \qquad\qquad \beta = \tau N_t$$

$$Z \sim \int \frac{dp_n dq_n}{2\pi}\, e^{-\frac{p^2}{2m}\tau - ip_n(q_{n+1}-q_n)} = \int dq_n \sqrt{\frac{m}{2\pi\tau}}\, e^{-\frac{m(q_2-q_1)^2}{2\tau}}$$

$$\left\langle \frac{p^2}{2m} \right\rangle \sim \frac{\partial}{\partial\tau} \int dq_n \sqrt{\frac{m}{2\pi\tau}}\, e^{-\frac{m(q_2-q_1)^2}{2\tau}} \Rightarrow \frac{1}{2\tau} - \left\langle \frac{m(q_2-q_1)^2}{2\tau^2} \right\rangle$$

Energy: non-relativistic case

$$E = -\frac{1}{V}\frac{\partial}{\partial\beta}\Big(\mathrm{Ln}(Z)\Big)_V \qquad \beta = \tau N_t$$

$$E = \frac{1}{2\tau} - \left\langle \frac{m(q_2 - q_1)^2}{2\tau^2} - V(q_1) \right\rangle$$

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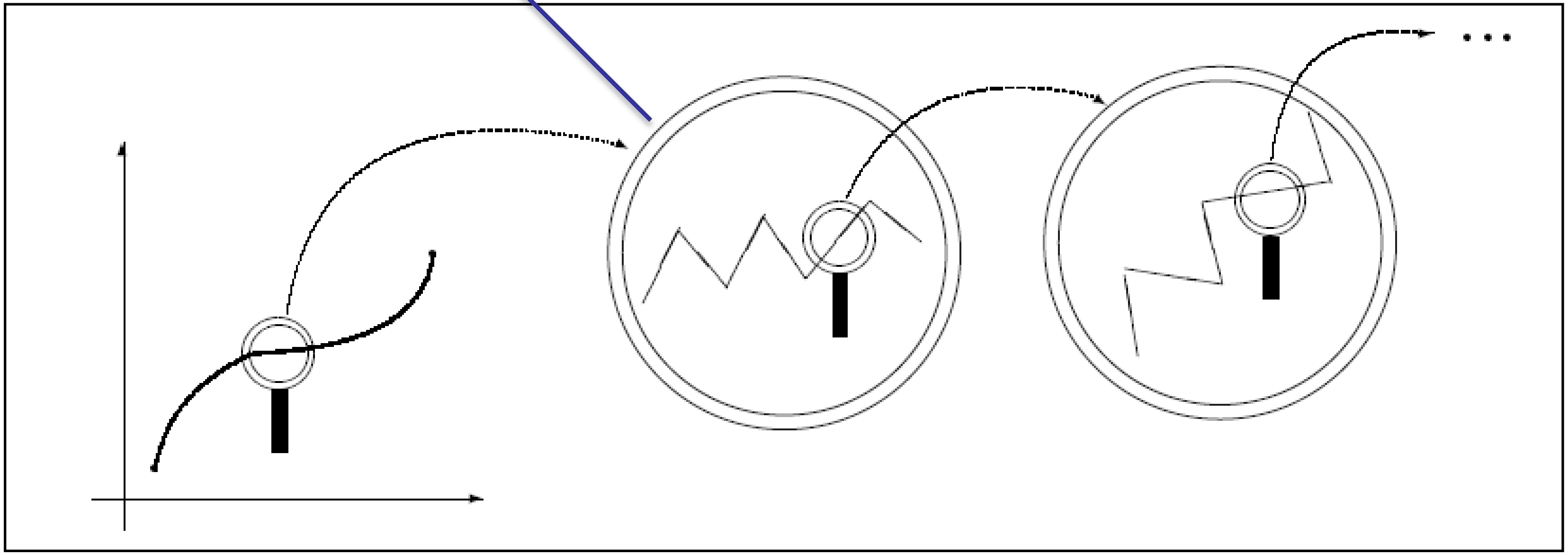

Energy: relativistic case

$$E = -\frac{1}{V}\frac{\partial}{\partial\beta}\Big(\mathrm{Ln}(Z)\Big)_V \qquad\qquad \beta = \tau N_t$$

$$Z \sim \int \frac{dp_n dq_n}{2\pi}\, e^{-\sqrt{p^2+m^2}\tau - ip_n(q_{n+1}-q_n)} = \int dq_n \frac{m\tau}{\pi\sqrt{\tau^2+(q_1-q_0)^2}} K_1(m\sqrt{\tau^2+(q_1-q_0)^2})$$

$$\langle\sqrt{p^2+m^2}\rangle \sim \frac{\partial}{\partial\tau}\int dq_n \frac{m\tau}{\pi\sqrt{\tau^2+(q_1-q_0)^2}} K_1(m\sqrt{\tau^2+(q_1-q_0)^2})$$

$$= \left\langle \frac{m\tau}{\sqrt{\tau^2+(q_1-q_0)^2}}\frac{K_0(m\sqrt{\tau^2+(q_1-q_0)^2})}{K_1(m\sqrt{\tau^2+(q_1-q_0)^2})} + \frac{\tau^2-(q_1-q_0)^2}{\tau(\tau^2+(q_1-q_0)^2)} \right\rangle$$

Pressure: non-relativistic case

$$P = \frac{1}{\beta}\frac{\partial}{\partial V}\Big(\mathrm{Ln}(Z)\Big)_{\beta}$$

$q \to a\, q$

$V \to a^3\, V$

$$P = \frac{1}{\beta}\frac{\partial}{\partial V}\Big(\mathrm{Ln}(Z)\Big)_{\beta} = \frac{1}{3\, N^3\, N_t \tau}\frac{\partial}{\partial a}\Big(\mathrm{Ln}(Z)\Big)_{\beta}\Big|_{a=1}$$

$$P = \frac{1}{3\, N^3\, N_t \tau}\frac{\partial}{\partial a}\int \frac{dp_n dq_n}{2\pi}\, e^{-\frac{p^2}{2m}\tau - i p_n (q_{n+1} - q_n)\, a - V(a\, q)\tau}$$

$$P = \frac{2}{3\, N^3}\left\langle \frac{m(q_2 - q_1)^2}{2\tau^2} - \frac{1}{2}\frac{\partial V(q)}{\partial q}\, q \right\rangle$$

Pressure: relativistic case

$$P = \frac{1}{\beta}\frac{\partial}{\partial V}\Big(\mathrm{Ln}(Z)\Big)_{\beta}$$

$$P = \frac{1}{3\,N^3\,N_t\tau}\frac{\partial}{\partial a}\int \frac{dp_n dq_n}{2\pi}\, e^{-\sqrt{p^2+m^2}\tau - ip_n(q_{n+1}-q_n)\,a - V(a\,q)\tau}$$

$$P = \left\langle \frac{(q_1-q_0)^2}{\tau^2+(q_1-q_0)^2}\left[2+m\sqrt{\tau^2+(q_1-q_0)^2}\,\frac{K_0(m\sqrt{\tau^2+(q_1-q_0)^2})}{K_1(m\sqrt{\tau^2+(q_1-q_0)^2})}\right] - \frac{1}{2}\frac{\partial V(q)}{\partial q}\,q\right\rangle$$

Conclusion:

1. PIMC method for Relativistic Systems have been formulated.

2. Expressions for the Energy and Pressure for Relativistic Systems have been found.

3. Some problems have been studied numerically for a test of the approach.

4. Transport coefficients: diffusion, viscosity, … in progress

5. Generalization of this approach on the another theories will be studied (Born-Infeld theory, bosonic string theory…)