First-principles simulations of Bose gasses using stochastic gauges

P. Deuar, P. D. Drummond and K. V. Kheruntsyan

Department of Physics, University of Queensland

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Two basic types of simulations:

Dynamics:

$$\dot{\hat{\boldsymbol{\rho}}} = -\frac{\boldsymbol{i}}{\boldsymbol{\hbar}}\left[\hat{\boldsymbol{H}} \;\;,\;\; \hat{\boldsymbol{\rho}}\right]$$

Thermal equilibrium:

$$\dot{\hat{\boldsymbol{\rho}}}_{\boldsymbol{u}} = -\frac{\mathbf{1}}{\mathbf{2}}\left[\hat{\boldsymbol{H}} - \boldsymbol{\hbar\mu}\hat{\boldsymbol{N}} \;\;,\;\; \hat{\boldsymbol{\rho}}_{\boldsymbol{u}}\right]_{+}$$

with $t = 1/(\hbar k_B T)$

Suppose we have up to

N particles/energy levels
in M orbitals/modes.

Direct approach intractable for any substantial number of particles/modes: Have to solve

$$\propto N^M \quad \text{or} \quad \propto M^N$$

equations.

Gauge P representation

Expand state in coherent state basis

$$\hat{\rho}_u = \int P(\overrightarrow{\alpha}, \overrightarrow{\beta}, \theta) \frac{|\overrightarrow{\boldsymbol{\alpha}} >< \overrightarrow{\boldsymbol{\beta}}^*|}{< \overrightarrow{\boldsymbol{\beta}}^* | \overrightarrow{\boldsymbol{\alpha}} >} \boldsymbol{e}^{\boldsymbol{\theta}} d^{2M}\overrightarrow{\alpha}\ d^{2M}\overrightarrow{\beta}\ d^2\theta$$

- Occupation of each mode is distributed like in a coherent state.
- Each mode has two coherent state amplitudes α and β.
- Also an overall phase and weight θ
- Density matrix with N^M complex elements maps to a distribution over just $\boldsymbol{2}M + 1$ complex variables $\theta, \overrightarrow{\alpha}, \overrightarrow{\beta}$.
- In principle, state is described to desired accuracy by generating a sufficient number of samples (each only of size $2M + 1$) from this distribution. (PRIMARY MOTIVATION!)

All observables can be calculated

$$< \hat{A} >= \quad \mathrm{Tr}\left[\hat{\rho}_u \hat{A}\right] \quad / \ \mathrm{Tr}\left[\hat{\rho}_u\right]$$

$$= \int P e^{\theta} \frac{< \overrightarrow{\beta}^* | \hat{A} | \overrightarrow{\alpha} >}{< \overrightarrow{\beta}^* | \overrightarrow{\alpha} >} \Big/ \int P e^{\theta}$$

$$= \sum_i e^{\theta} \ F_A(\overrightarrow{\alpha}_i, \overrightarrow{\beta}_i) \Big/ \sum_i e^{\theta}$$

- Each observable has corresponding function F_A of the coherent amplitudes.
- Expectation values are weighted (e^{θ}) averages of F_A over trajectories.
- One simulation gives information about all observables

How to sample the variables

- Start with easy-to-sample state.
  e.g. in thermodynamics, state at $T \to \infty$ (i.e. $t = 1/(k_B \hbar T) \to 0$) is simple.

$$\hat{\rho}_u = \exp\left\{-\hat{N} \lim_{T\to\infty} [\mu(T)/k_B T]\right\}$$

- convert master equation for $\hat{\rho}$ (involving $\hat{a}, \hat{a}^\dagger$), to Fokker-Planck equation for distribution P (involving variables $\overrightarrow{\alpha}$, $\overrightarrow{\beta}$, θ and their derivatives.) Use

$$\begin{aligned} \hat{a}^\dagger|\alpha> &= \frac{\partial}{\partial\alpha}|\alpha> \\ \hat{a}|\alpha> &= \alpha|\alpha> \\ 0 &= \left[\frac{\partial}{\partial\theta} - 1\right] e^\theta \end{aligned}$$

- Then convert to stochastic equations for variables $\overrightarrow{\alpha}$, $\overrightarrow{\beta}$, θ.

- Randomly sample initial state

- evolve variables.

1D Interacting Bose gas

- Consider a thermal calculation — temperature drops as simulation "time" advances.

- Let the particle number be variable — needed for a continuously loaded system e.g. atom laser.

- Only a few exact results known, and only in the homogenous (un-trapped) case:
  Density, total and potential energy, pressure, $g_2(0)$.

- Would like to obtain others:
  Momentum distribution, second order correlation $g_2(x)$, and anything at all for trapped gas.

- Expand state on a lattice (size M) of free momentum modes k.

- Variables: coherent state amplitudes $\tilde{\alpha}(k)$
  and their inverse fourier transforms $\alpha(x)$.

- Variables: off-diagonal partners $\tilde{\beta}(k)$.
  Mean number of particles $\tilde{n}(k) = \tilde{\alpha}\tilde{\beta}^*$

- Variable: complex phase θ.

Kinetic Energy

$$\hat{H} += \frac{\hbar^2}{2m} \int dx \;\; \nabla^2 \hat{\Psi}^\dagger(x) \hat{\Psi}(x)$$

$\hat{\Psi}^\dagger(x)$ creates a boson at x.

$$\begin{aligned} \dot{\tilde{\alpha}}(k) &+= -k^2 \tilde{\alpha}(k)/2 \\ \dot{\tilde{\beta}}(k) &+= -k^2 \tilde{\beta}(k)/2 \\ \dot{\theta} &+= -k^2 \tilde{n}(k) \end{aligned}$$

Interactions

$$\hat{H} += \chi \int dx\ \hat{\Psi}^{\dagger 2}(x)\hat{\Psi}^{2}(x)$$

- Local interactions of strength χ.
- Correct as long as scattering length $a_o \ll \max[k]$.

$$\begin{aligned}
\dot{\alpha}(x) &+= -\alpha(x)\left[\chi n(x) - i\sqrt{\chi/}\ \xi_1(t)\right]/\Delta \\
\dot{\beta}(x) &+= -\beta(x)\left[\chi n(x)^* + i\sqrt{\chi/}\ \xi_2(t)\right]/\Delta \\
\dot{\theta} &+= -\chi n(x)^2/\Delta
\end{aligned}$$

- Gröss-Pitaevskii equations with added noise.
- Lattice spacing Δ in x.
- Gaussian noises $\xi_{1,2}(t)$ of variance $\sqrt{1/\delta t \Delta}$
- There is an instability when Re[n] < 0, which must be removed by using gauges

Stochastic Gauges

$$\hat{H} += 0 \times \int dx G_1(\alpha(x), \beta(x)) + G_2(\alpha(x), \beta(x))$$

- Due to $[\partial/\partial\theta - 1]e^{\theta}$, certain modifications of the equations do not change the physical system that is being simulated!

- Infinite family of ARBITRARY functions $G_{1,2}(\alpha, \beta)$ which can be inserted into equations in this way.

$$\begin{aligned} \dot{\alpha}(x) &+= -i\alpha(x)G_1 \\ \dot{\alpha}(x) &+= -i\beta(x)G_2 \\ \dot{\theta} &+= \sqrt{\chi/\Delta} \sum_{i=\{1,2\}} -G_i^2/2 + G_i\xi_i(t) \end{aligned}$$

- Appropriate choice of gauge functions G stabilizes the equations. e.g. $G_1 = G_2 = i\left[n(x) - \lfloor n(x) \rceil\right]\chi/\delta$

- The price you pay is additional variation in the weight e^{θ}.

Chemical Potential

$$-\hbar\mu(T)\hat{N} = \int dx\ \hat{\Psi}^\dagger(x)\hat{\Psi}(x)$$

$$\begin{aligned}
\dot{\alpha}(x) &+= \mu_e\alpha(x)/2 \\
\dot{\alpha}(x) &+= \mu_e\beta(x)/2 \\
\dot{\theta} &+= \mu_e n(x)
\end{aligned}$$

"Effective" chemical potential $\mu_e = \frac{\partial}{\partial t}(t\mu)$.

External Trap Potential

$$\hat{H} += \int dx\ V(x)\hat{\Psi}^\dagger(x)\hat{\Psi}(x)$$

Strength $V(x)$

$$\begin{aligned}
\dot{\alpha}(x) &+= -V(x)\alpha(x)/2 \\
\dot{\alpha}(x) &+= -V(x)\beta(x)/2 \\
\dot{\theta} &+= -V(x)n(x)
\end{aligned}$$

Parameters

An un-trapped interacting 1D bose gas has two important parameters.

Interaction strength

$$\gamma = \chi/\rho$$

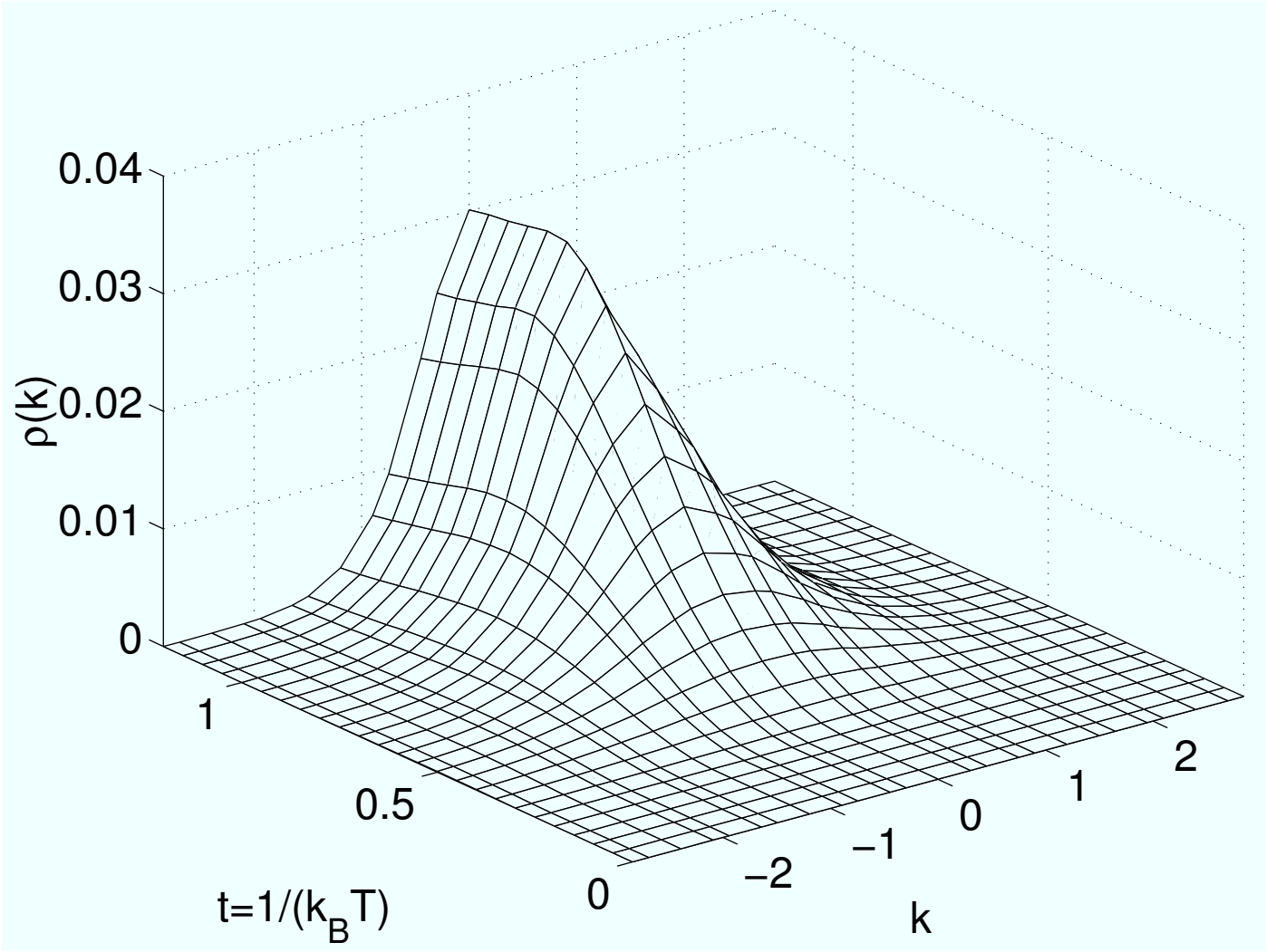
When $\gamma \to 0$ Non-interacting gas
When $\gamma \to \infty$ Tonks (hard sphere) gas

Relative temperature

$$\tau = \frac{T}{T_d} = \frac{T}{4\pi\rho^2}$$

T_d is the quantum degeneracy temperature.
When $\tau = 1$,
Interparticle separation $\approx$ de Broglie wavelength.
In 3D, critical temperature $T_c \approx T_d$.

momentum density



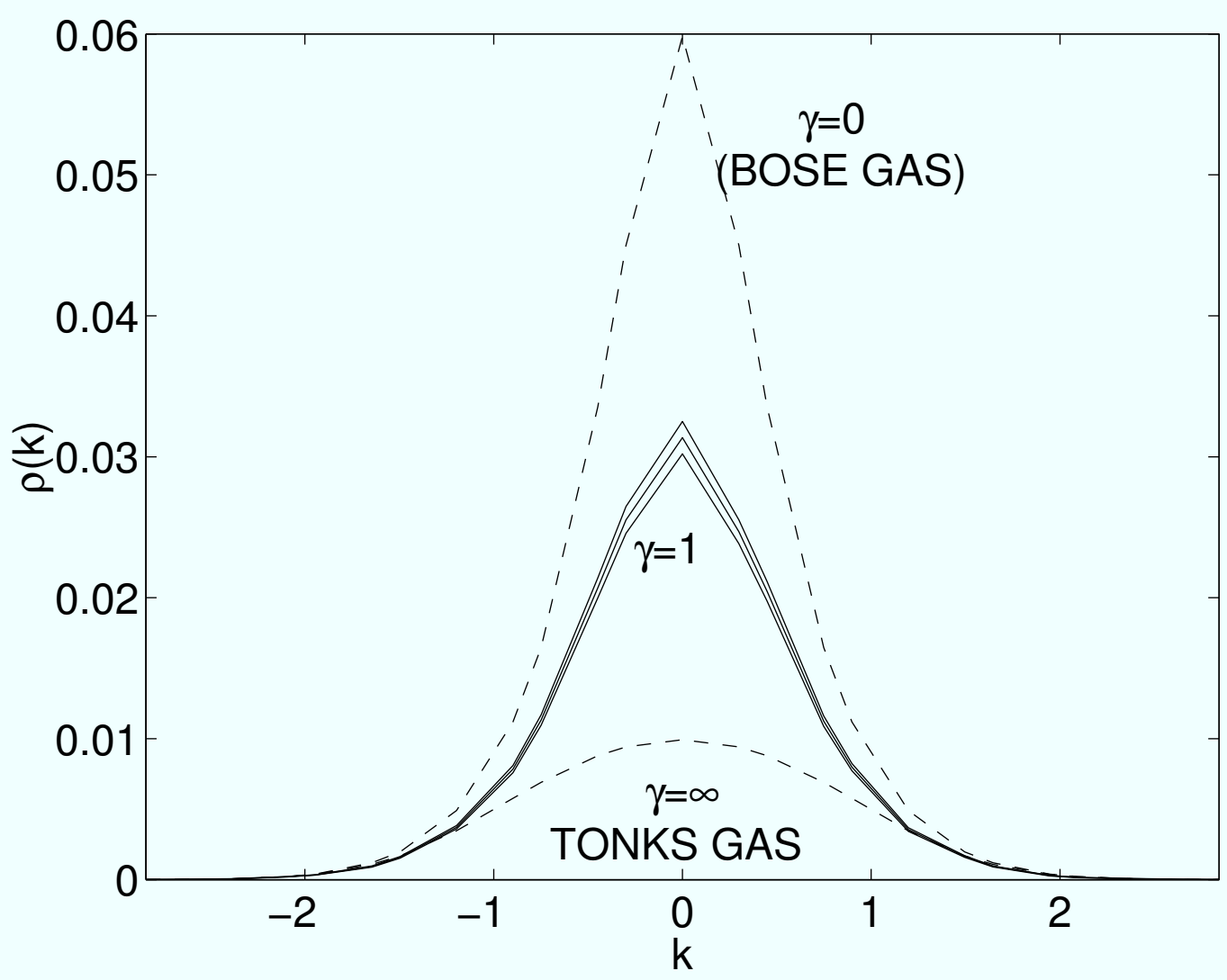
$\gamma = \tau = 1$ at $t = 1$

for $t < 0.25$, $\tau \approx 10^6$, γ rises from 0 to ≈ 600

for $0.25 < t < 1$, τ and γ decrease to 1

for $t > 1$, τ is $\approx$ constant, γ increases to ≈ 1.12

momentum density at $\gamma = \tau = 1$



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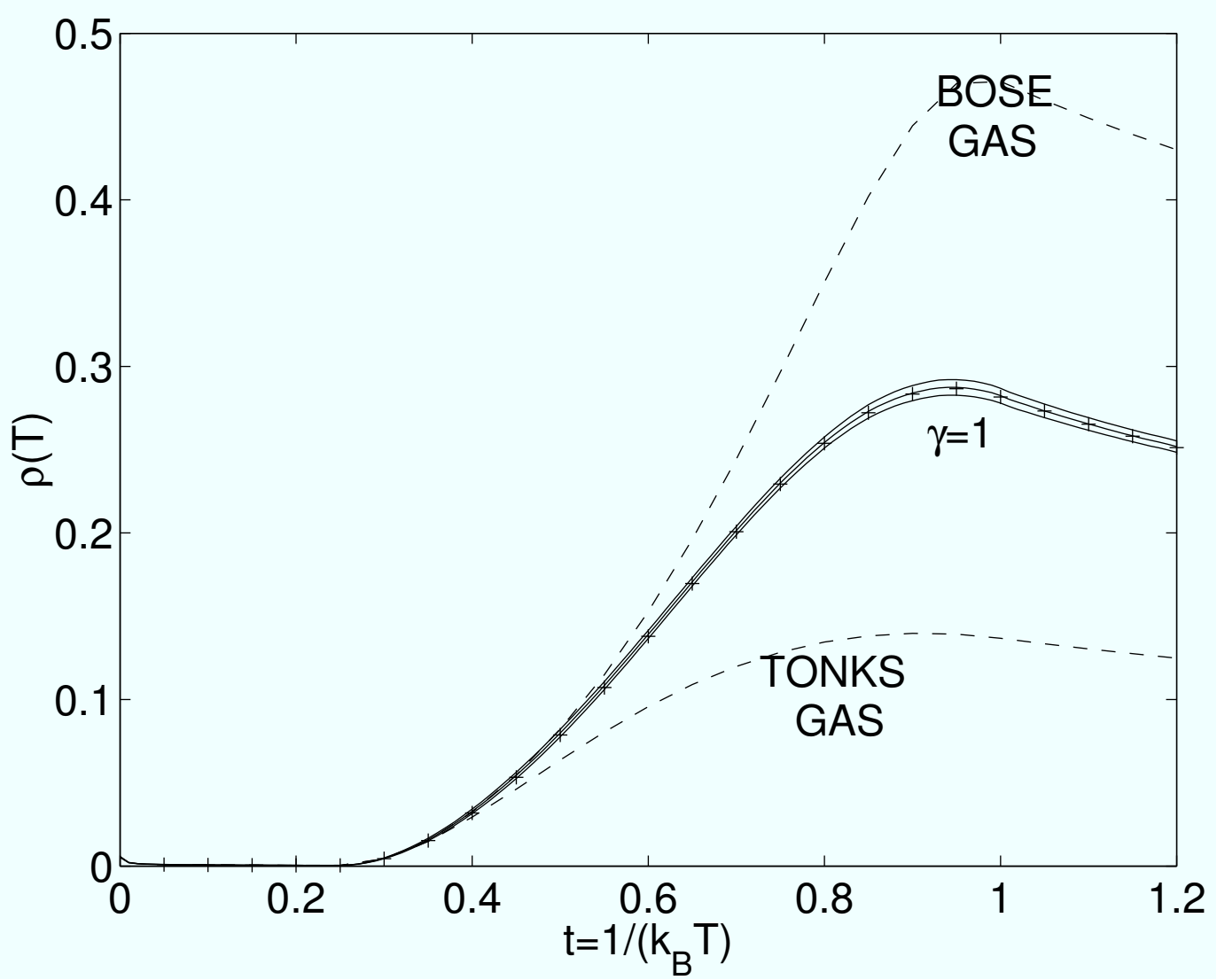
Comparison to exact results



Crosses indicate Yang&yang solution

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for $0.25 < t < 1$, τ and γ decrease to 1

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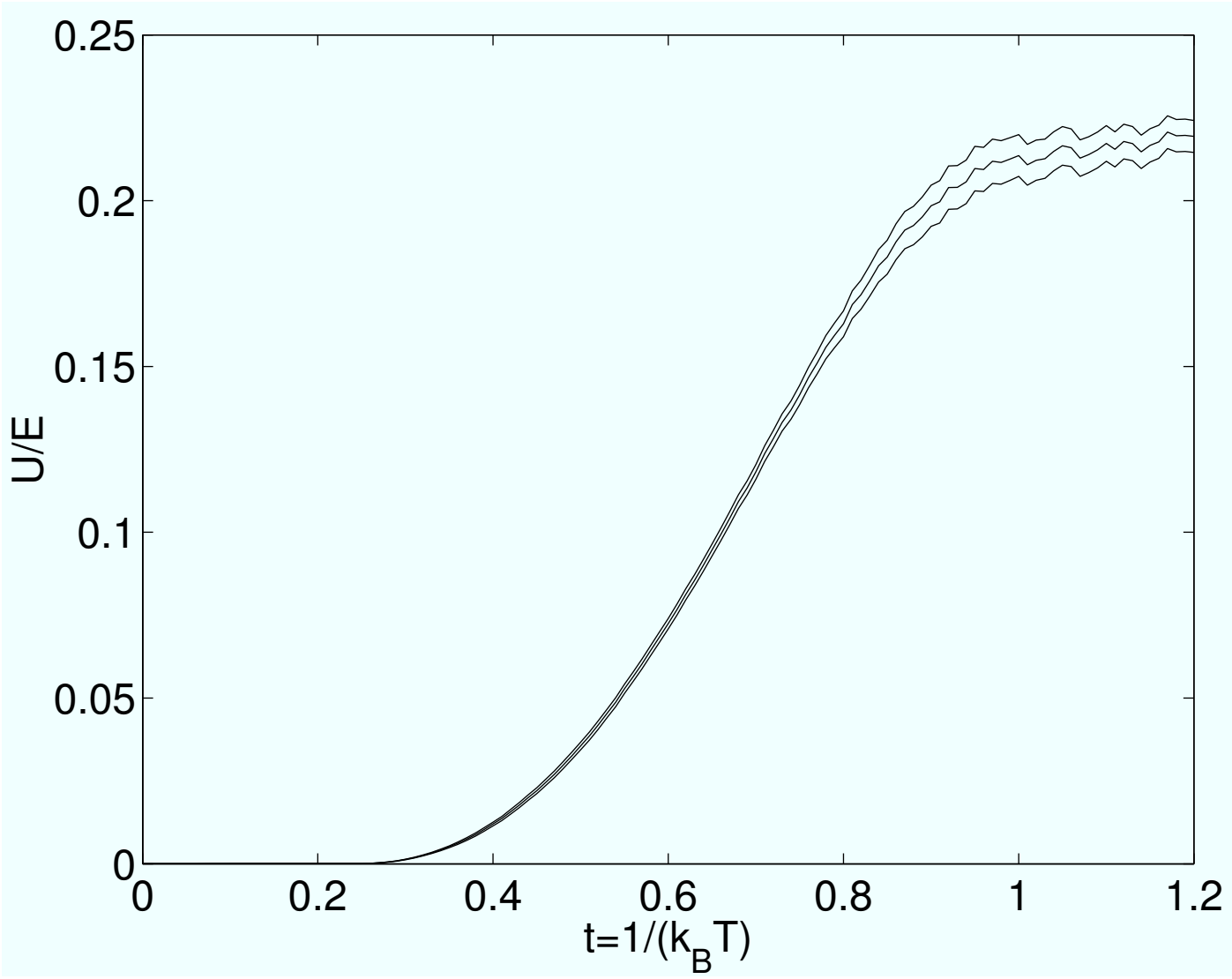
Potential energy fraction



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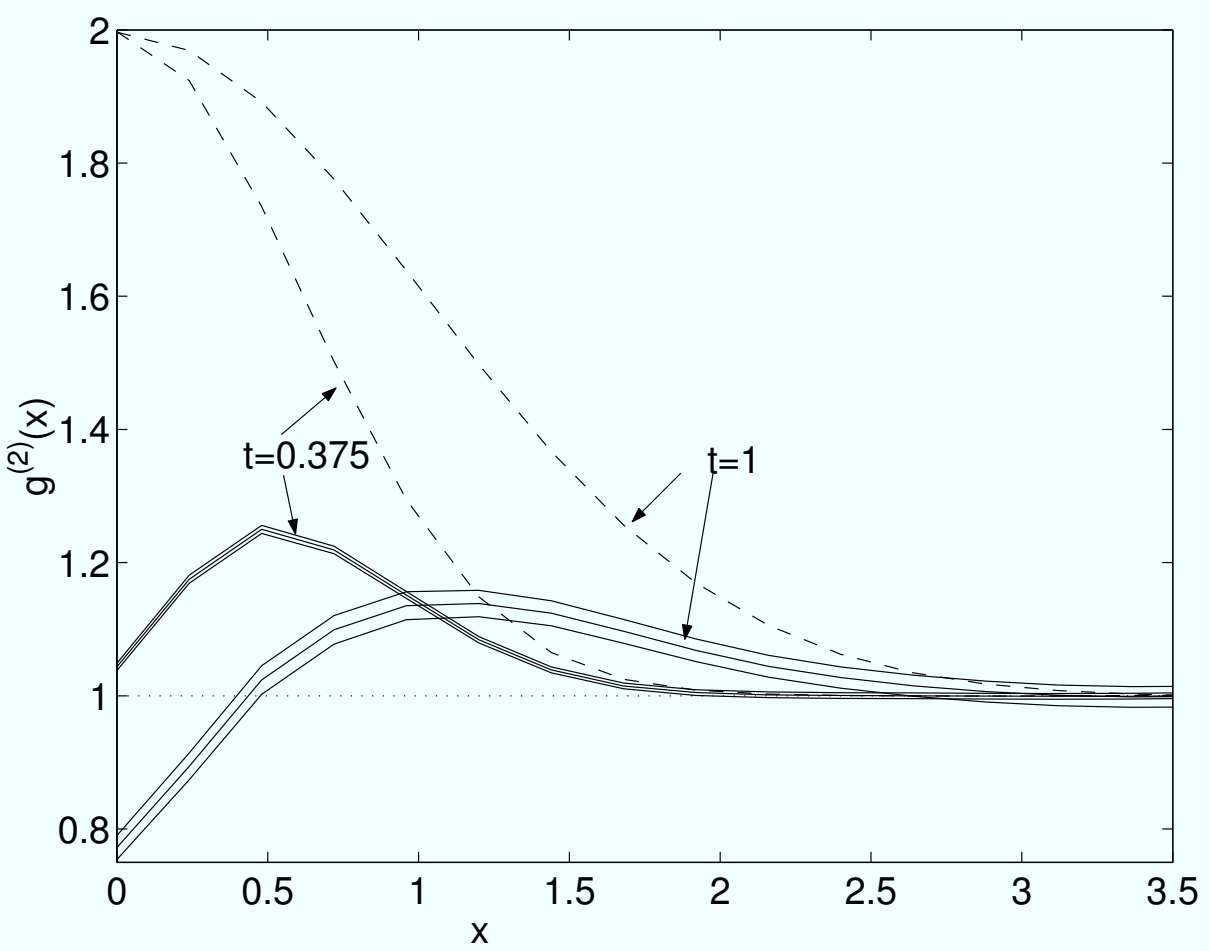
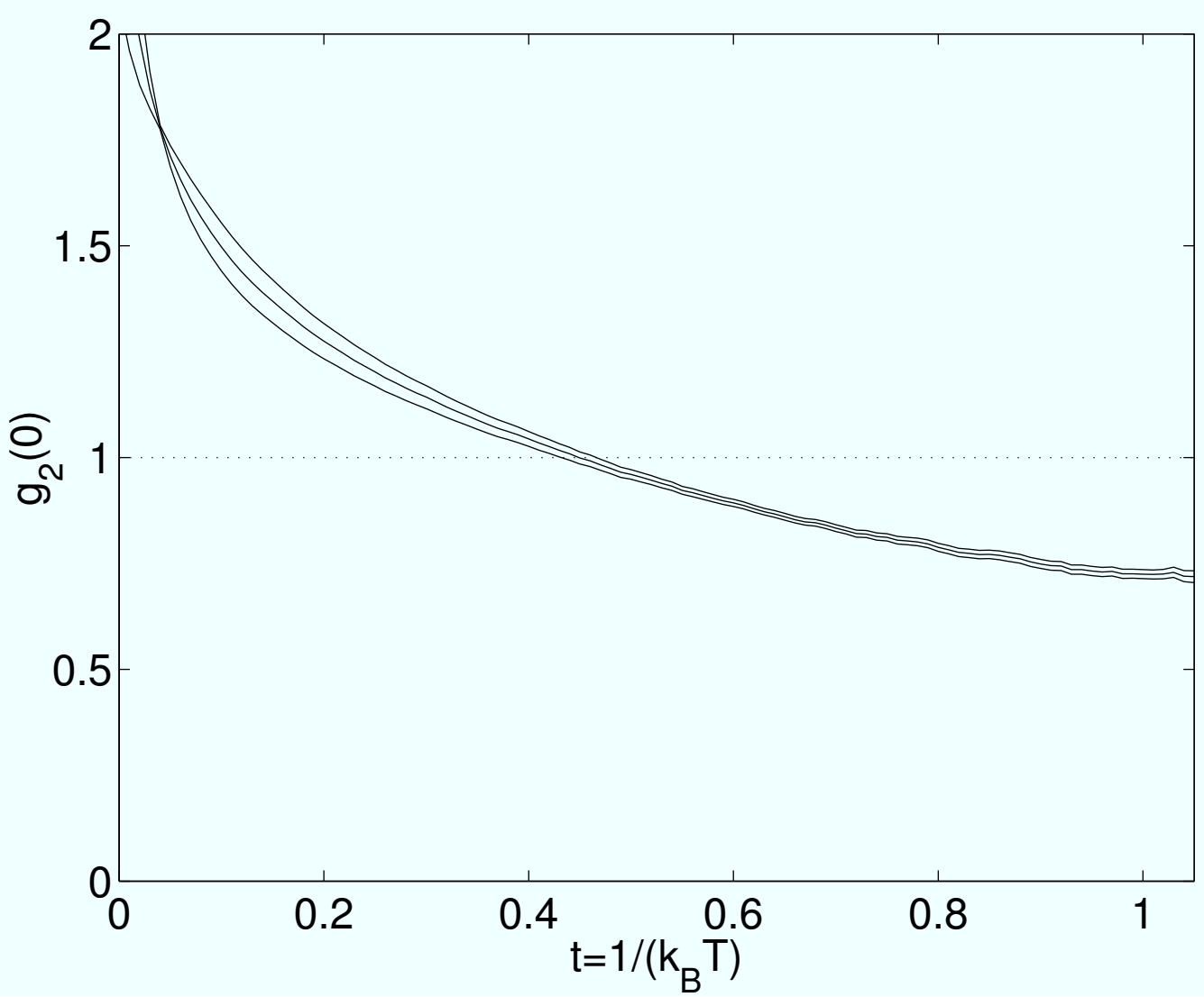
second order correlation function



$$g_2(x) = \frac{\int dy < \hat{N}(y)\hat{N}(y+x) >}{L\left[\int dx < \hat{N}(x) >\right]^2}$$

At $t = 0.375$, $\gamma \approx 165$, $\tau \approx 5800$.
At $t = 1$, $\gamma \approx 42$, $\tau \approx 139$.
Dashed lines indicate non-interacting gas.
$g_2(0) = 2$: Thermal state
$g_2(0) = 1$: Coherent state
$g_2(0) < 1$: Anti-bunching

second order correlation function



$\gamma = \tau = 10$ at $t = 1$

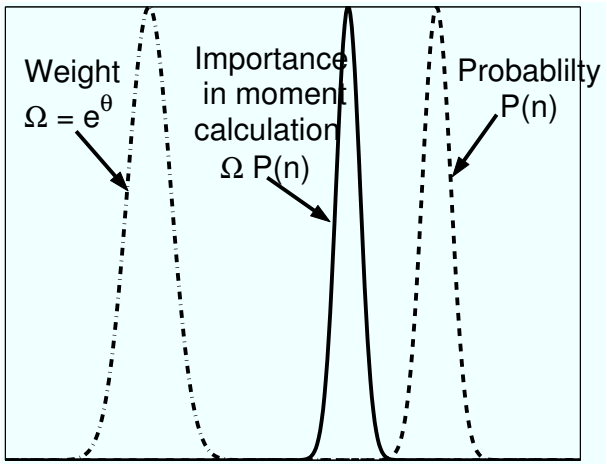
for $t < 0.25$, $\tau \approx 10^7$, γ rises from 0 to ≈ 5000

for $0.25 < t < 1$, τ and γ decrease to 10

for $t > 1$, τ is $\approx$ constant, γ increases to ≈ 11

Some difficulties

- Weights $e^{\mathrm{Re}[\theta]}$ evolve deterministically and exponentially, as a function of n.
  This can lead to the most significant trajectories not being sampled properly.

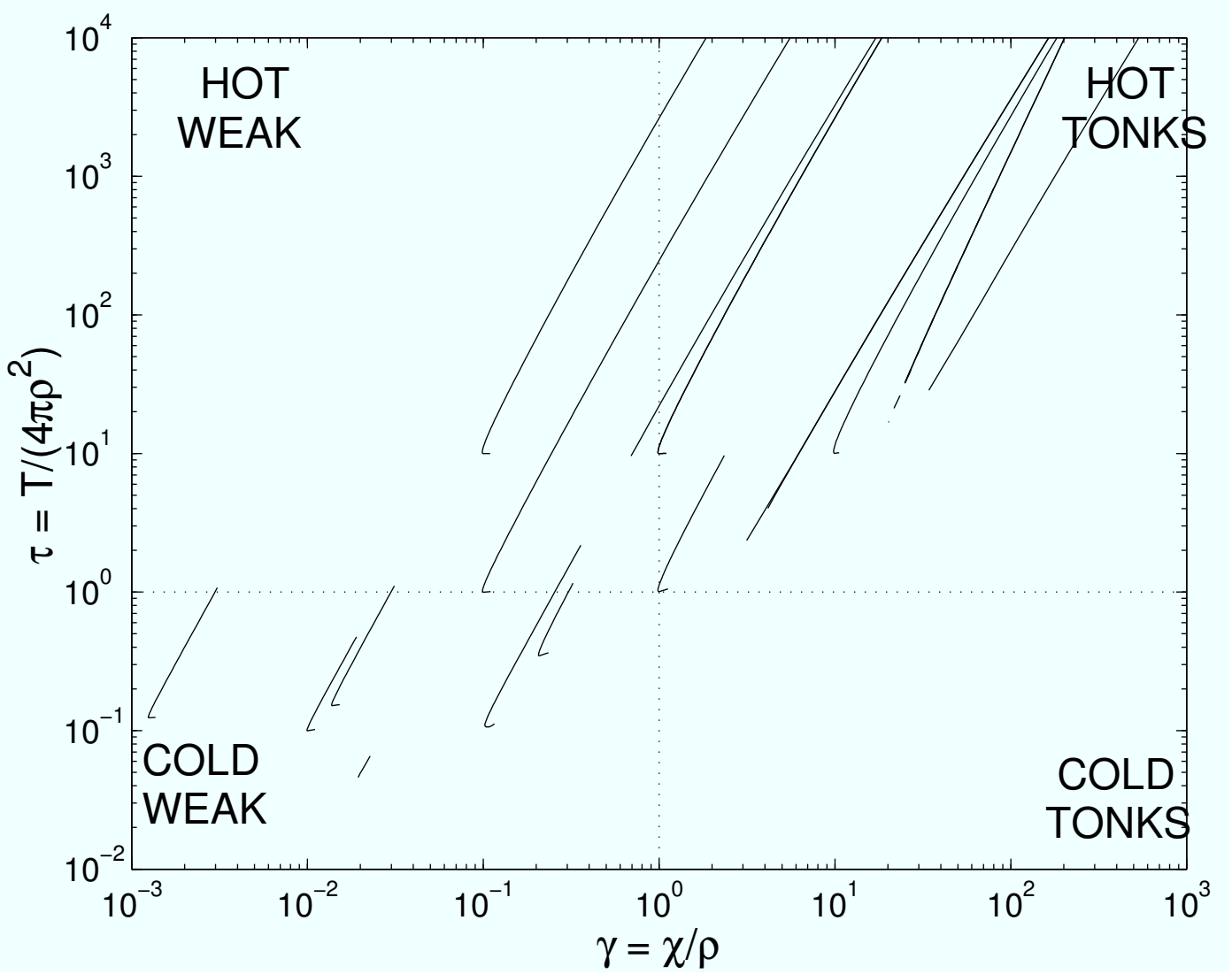


  This is particularly acute when System size (actual length) or interaction is big.

- Partial solution: Can try to $a\text{-}priori$ analytically predict the weight evolution
  — with varying success.

- One would like more of a "black box".

(Basic) Simulation Range



Metropolis Algorithm Sampling

- Previously sampled distribution $P(\overrightarrow{\alpha}, \overrightarrow{\beta}, \theta)$ using the the noises $\xi_i(x,t)$, random choice of initial state $\xi^0(x)$, and time evolution.

- Now try to sample the distribution

$$\Pi = e^{\mathsf{Re}[\theta]} P(\overrightarrow{\alpha}, \overrightarrow{\beta}, \theta)$$

  using the noises, time evolution and Metropolis rejection algorithm at a chosen temperature T.

- The value of Π can actually be worked out knowing only:

  1. the value of all the noises (hence their probability),
  2. and the value of the weight which is calculatedby using those noises to evolve the initial state and obtain θ.

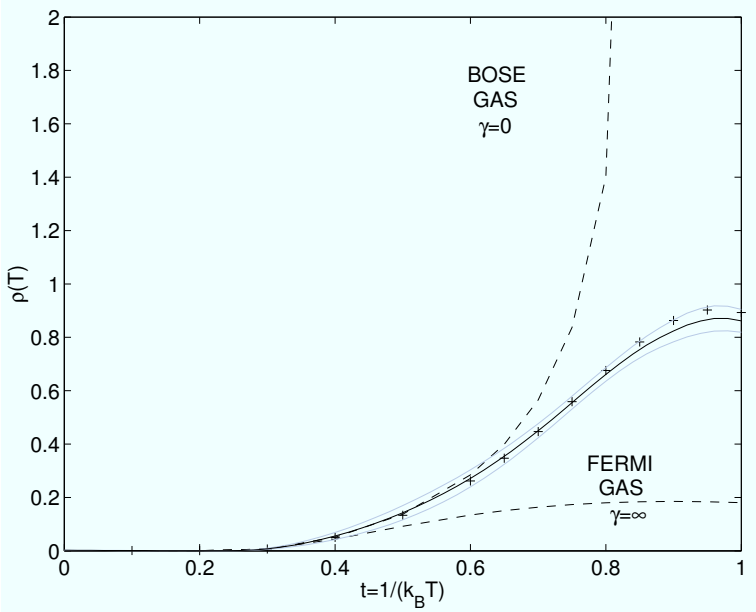
The algorithm

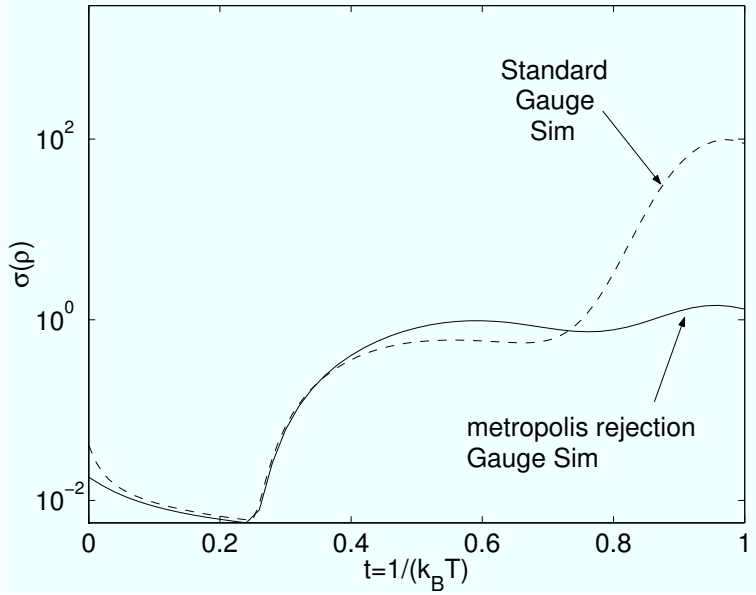
- initialize noises to some value $\xi_0(x,t)$
- choose a transition rule for the noises between iterations $T = \text{Prob}((\xi_n \to \xi')$.
- sample one new noise $\xi'(x,t)$ according to transition rule, leave rest as is $(\xi' = \xi_n)$.
- calculate ratio of probabilities

$$q = \frac{\Pi(\xi'))T(\xi' \to \xi_n(x,t))}{\Pi(\xi_n)T(\xi_n(x,t) \to \xi')}$$

- chance of accepting the new noise $(\xi_{n+1} = \xi')$ is $\min[1, q]$.
- iterate through all noises in simulation.
- after iterating through all noises, save current variables as a sample of the density matrix (at a range of temperatures). Repeat.
- calculate correlation time κ between samples.
- throw away first κ states, as being out of equilibrium.

Cold weakly-interacting gas



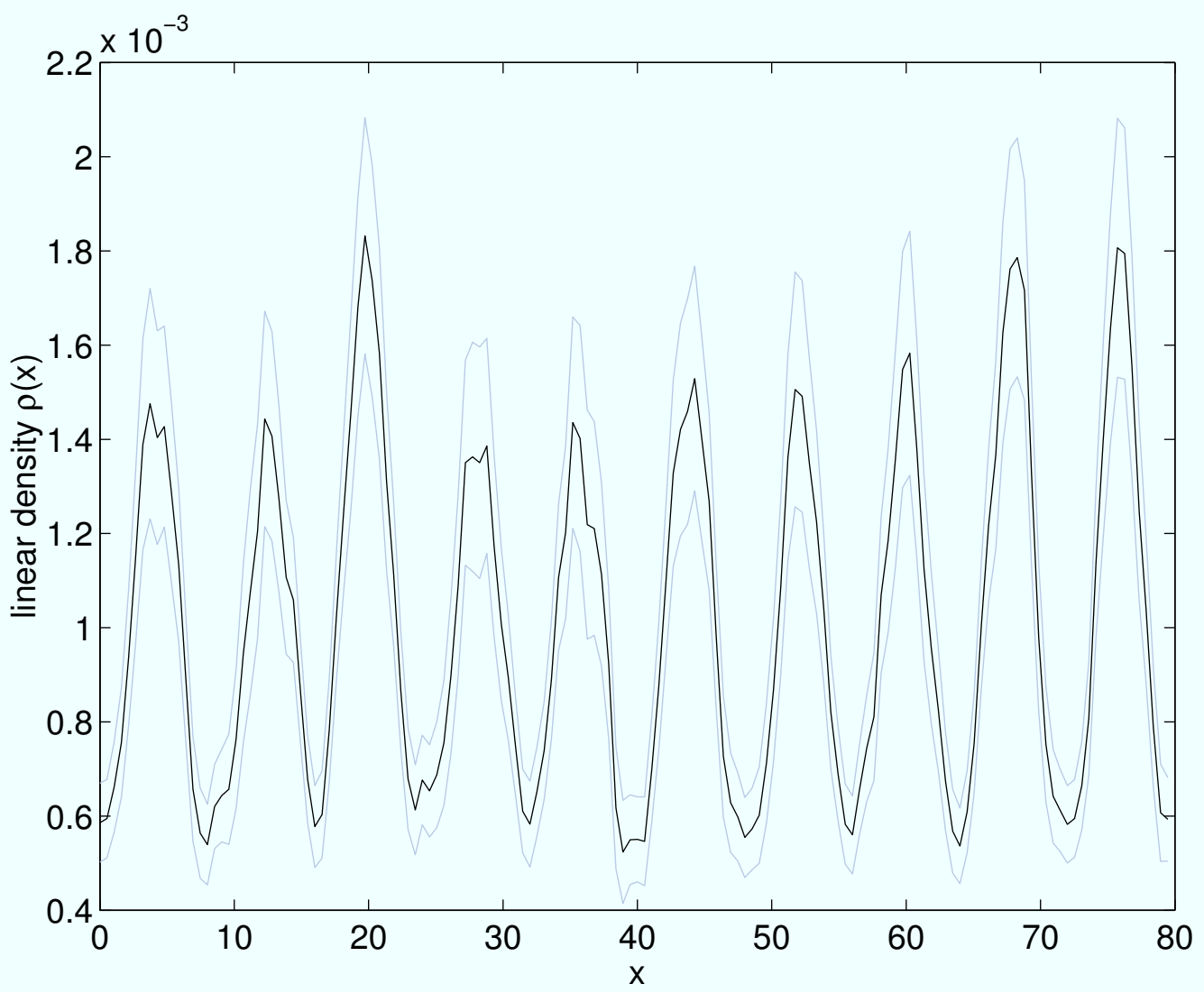


Number of samples required for a given accuracy

$$\propto \sigma^2$$

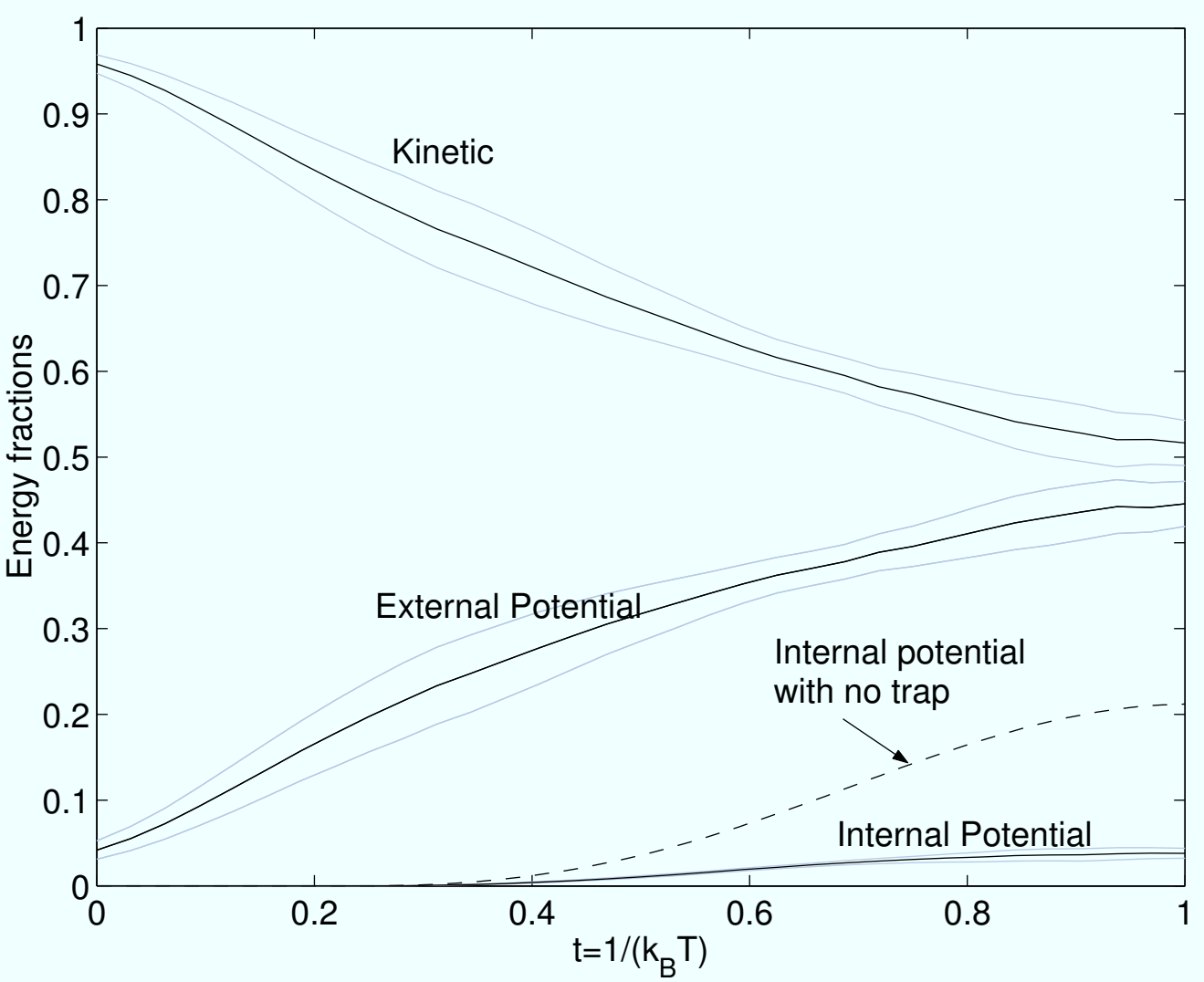
$$\gamma = \tau = 0.1 \text{ at } t = 0.1$$

Lattice of potential wells of middling strength



Same Temperature and chemical potential as for previous $\gamma = \tau = 1$ calculations.

Energy fractions



Same Temperature and chemical potential as for previous $\gamma = \tau = 1$ calculations. Same external potential lattice as on previous plot.

comparison to basic gauge calculation

- metropolis method takes $O(MS)$ longer to get a sample - have to perform evolution for each noise tried. [S is the number of time steps].

- However, Metropolis method is much more of a "black box".

- Excessive noise in Im$[\theta]$ can still be a problem, especially for a Tonks gas. May be solvable by judicious choice of gauge.

Possible advantages compared to a path-integral monte-carlo calculation

- Standard monte-carlo approach, varying particle positions, does not allow for varying particle number.

- A path Integral, varying coherent amplitudes would have calculation time for one sample $\propto (SM)M \log M$, but correlation time between samples τ often $O(S^2)$.

- Gauge calculation with Metropolis rejection: calculation time for one sample $\propto S(SM)M \log M$ but correlation time between samples τ appears to be typically $O(1)$.

- Gauge calculations give a sample of the actual density matrix — Allows subsequent dynamical evolution, and calculation of all desired moments.

- Gauge calculations give results for a range of temperatures (often the entire range from T upwards).

Some conclusions

- Can calculate a wide variety of properties of nonlinear Bose gases at thermal equilibrium, from first principles.

- Simulation scales polynomially with number of modes.

- For a wide variety of parameters, simulation does not require a lot of additional analytic work or optimisation.

- Method readily scalable to 2 or 3 dimensions.

- A Metropolis sampling procedure gives improved accuracy in some situations.

- Further improvement might be obtained by a more cunning choice of gauge, or sampling procedure.

Thankyou