

Physics 205 links

- [cytoplasmic streaming movie](#)
- [cytoplasmic streaming/kinesin model](#)

Polymers in a Vacuum???

You wouldn't expect to find them in a vacuum. . .

But you do!

"One day in February of 1985, instead of using Cobalt Ultra Fine Metal Powder (UFMP) as a matrix, I mistakenly used a glycerin-UFMP mixed matrix. I noticed this mistake immediately, but I thought, "Mottai-nai!" at the idea of throwing the mixture away. If I allowed the glycerin to evaporate, I thought that I could still make use of the UFMP, so I placed the mixture in the vacuum chamber to dry it out. Thinking that I could even speed up the drying process by irradiating the mixture with the laser, I switched on the laser beam. On top of that, anxious to confirm the elimination of the glycerin as soon as possible, I kept the spectrometer running and monitored the results. And then, I noticed a signal peak I had never before seen mixed in with the noise peaks. I think because up to that point I had always felt annoyance at the sight of that noise wave data in the experiments, I noticed a slight difference. The signal peak that I had never seen before now appeared at the same position no matter how many times I ran the experiment."

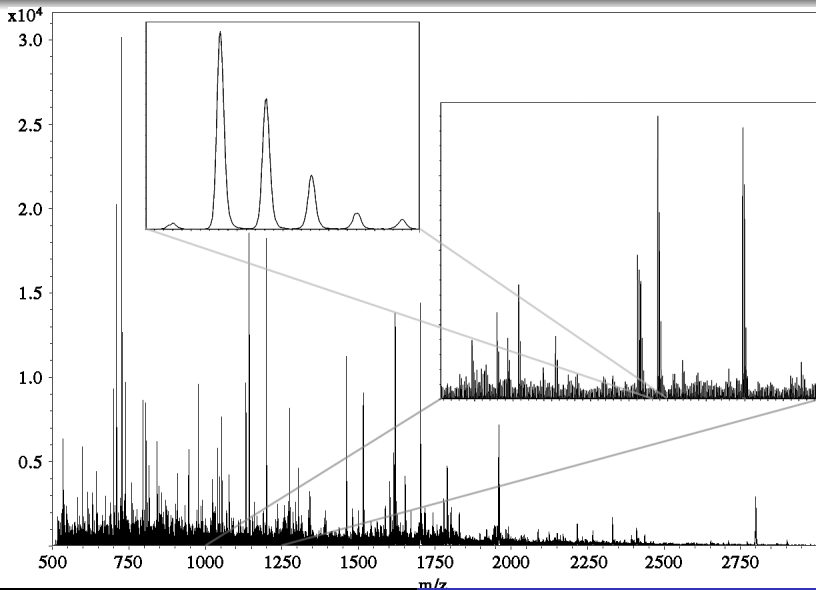


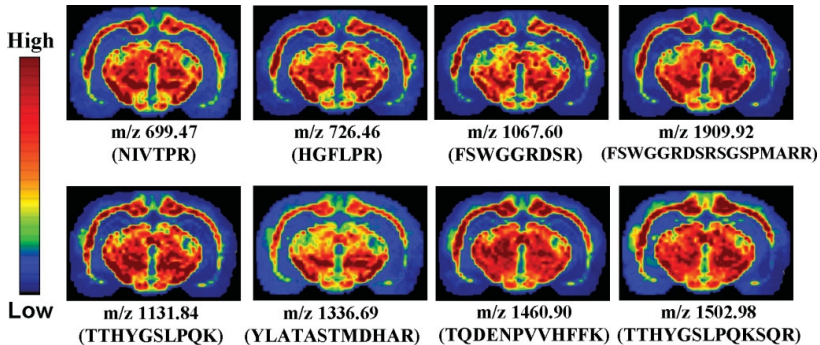
Koichi Tanaka, 2002 Nobel Prize in Chemistry

This led to a huge advance in biology and medicine. For example “Matrix-assisted Laser Desorption/Ionization” (MALDI) “Imaging Mass Spectrometry” (IMS).

The mass of molecules of order 10^5 Daltons can be measured to an accuracy of 1 part in 10^6 .

An example of a use of this is in understanding cancer and its diagnosis.





Drawback

You get the mass accurately but not the chemical sequence.

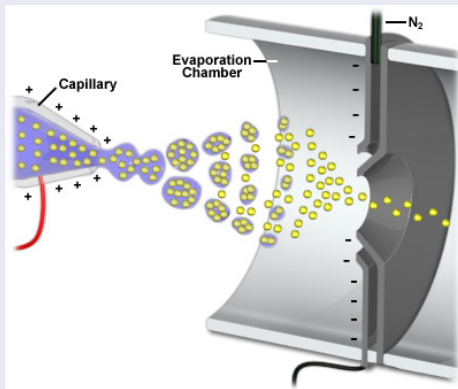
Additional probes of internal dynamics should provide more information about the chemical species

Drawback

You get the mass accurately but not the chemical sequence.

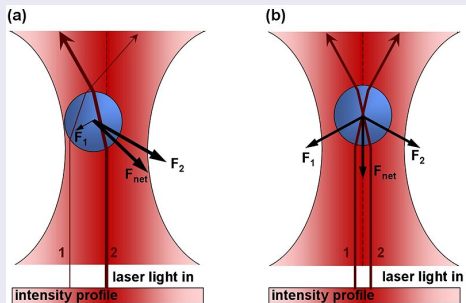
Additional probes of internal dynamics should provide more information about the chemical species

Alternate method: Electro spray Ionization



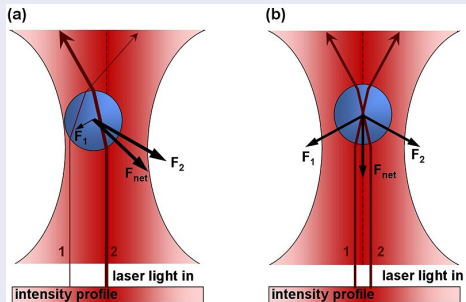
Developed by John Bennett Fenn, (2002 Nobel Prize in Chemistry).

Optical trap



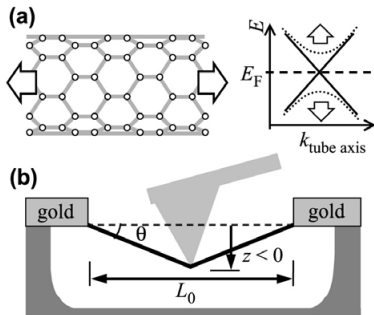
Put DNA in evacuated optical trap

Optical trap



Put DNA in evacuated optical trap

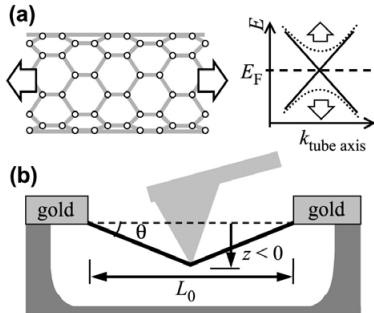
Suspend a molecule over a trench



Minot et al, PRL (2003)

May be possible to extend to DNA

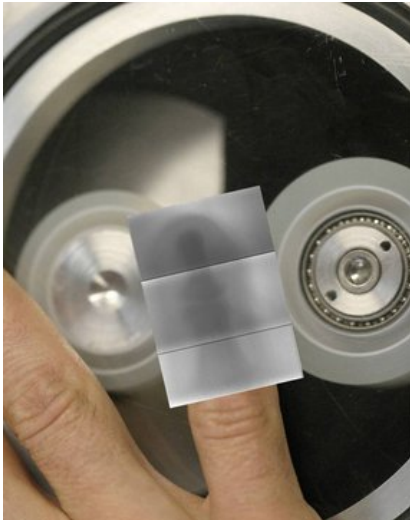
Suspend a molecule over a trench



Minot et al, PRL (2003)

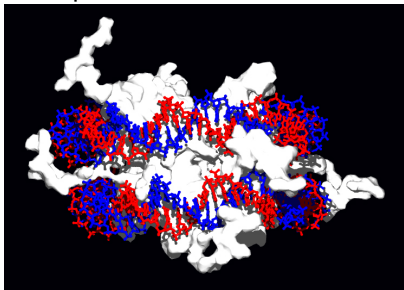
May be possible to extend to DNA

X-Ray's from Scotch Tape



Camara, Escobar, Hird, and
Putterman, Nature (2008)

Studying polymers in a vacuum gives you information about the mass distribution of a polymer.
Take proteins that bind to DNA



- In solution the mass is essentially irrelevant.
- In a vacuum the dynamics are very sensitive to the mass.
- This would then help to determine the presence of proteins on DNA.

- In solution the mass is essentially irrelevant.
- In a vacuum the dynamics are very sensitive to the mass.
- This would then help to determine the presence of proteins on DNA.

Polymers in Interstellar Media

Many different kinds of polymers have also been detected in interstellar media. (Thaddeus et al (1998)).



Conservation Laws

Because a single polymer in a vacuum is isolated you have three conservation laws:

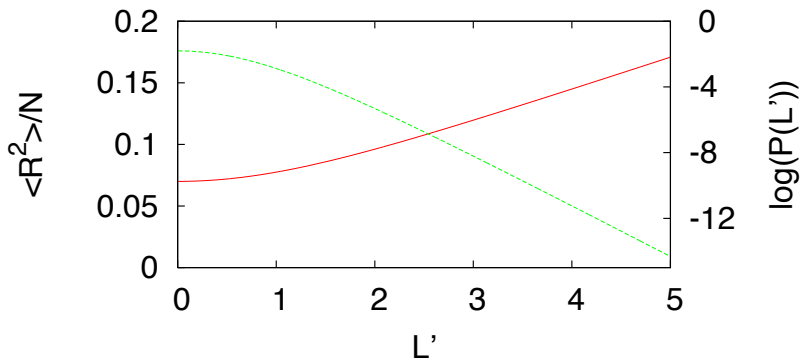
Conservation of Energy
Conservation of Momentum
Conservation of Angular Momentum

$$\zeta(\beta, k) = \int e^{-\frac{mk^2}{2\beta} \sum_i (x_i^2 + y_i^2) - \beta\Phi} \delta^{(3)}(\mathbf{r}_{cm}) \prod_{i=1}^N d^3r_i$$

$$\beta\Phi = \frac{3}{2l^2} \left(\sum_{i=1}^{N-1} |\mathbf{r}_{i+1} - \mathbf{r}_i|^2 + |\mathbf{r}_N - \mathbf{r}_1|^2 \right)$$

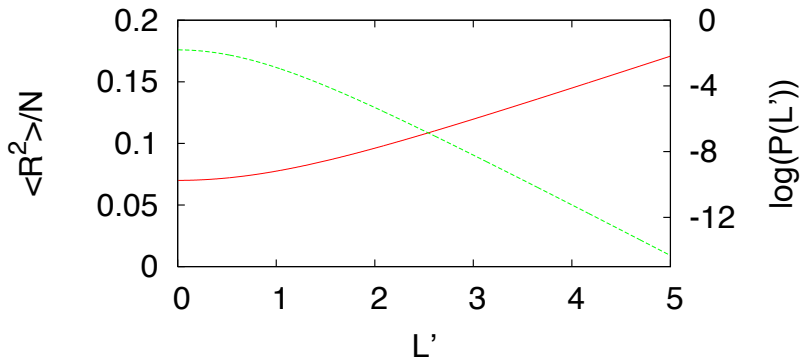
Performing the functional integration, $\frac{R_g^2}{Nl^2}$ is

$$\frac{(2L' (3 + \pi^2) + L' (-6 + \pi^2) \cosh[L'\pi] + 3 (-1 + L'^2) \pi \sinh[L'\pi])}{36\pi(2L'\pi + L'\pi \cosh[L'\pi] - 3\sinh[L'\pi])}$$



For $L=0$, $R_g^2/(Nl^2) = (1 + 15/\pi^2)/36 \approx 0.07$.

Without L-conservation $R_g^2/(Nl^2) = (1/12) \approx 0.083$

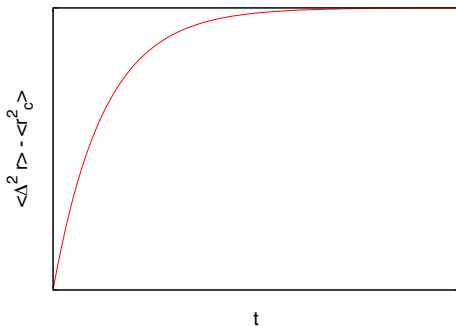


For $L=0$, $R_g^2/(Nl^2) = (1 + 15/\pi^2)/36 \approx 0.07$.

Without L-conservation $R_g^2/(Nl^2) = (1/12) \approx 0.083$

Dynamics

In a liquid, motion is highly damped.
Consider the average square displacement vs time



What does this look like for a polymer in a vacuum?

Internal Damping

Polymer solutions have hydrodynamic drag.

But also “Cerf friction”, or internal damping of chains.

$$f(s) \propto \frac{\partial \mathbf{r}}{\partial t} ???$$

In a vacuum, take $r(s) \rightarrow r(s) + vt$.

But f can't change!

Internal Damping

Polymer solutions have hydrodynamic drag.

But also “Cerf friction”, or internal damping of chains.

$$f(s) \propto \frac{\partial \mathbf{r}}{\partial t} ???$$

In a vacuum, take $r(s) \rightarrow r(s) + vt$.

But f can't change!

In a vacuum

$$f(s) \propto \frac{\partial^3 \mathbf{r}}{\partial t \partial^2 s}$$

Model needs to be sufficiently nonlinear

In a vacuum

$$f(s) \propto \frac{\partial^3 \mathbf{r}}{\partial t \partial^2 s}$$

Model needs to be sufficiently nonlinear

Vacuum Langevin Eqn

$$\frac{\partial^2 \mathbf{r}}{\partial t^2} = \left(1 + C \frac{\partial}{\partial t}\right) \frac{\partial^2 \mathbf{r}}{\partial s^2} + \xi(\mathbf{s}, \mathbf{t})$$

Eigenmodes: $\Omega_k \equiv \omega_k + i\lambda_k$.

Damping $\lambda_k \propto k^2$ for small k and $\omega_k \propto k$.

$$g(t) = \left\langle \frac{1}{N} \sum_{i=1}^N |\mathbf{r}_i(t) - \mathbf{r}_i(0)|^2 \right\rangle$$
$$\propto \text{Re} \sum_k \frac{\Omega_k (1 - \exp(i\Omega_k t))}{\omega_k k^2}$$

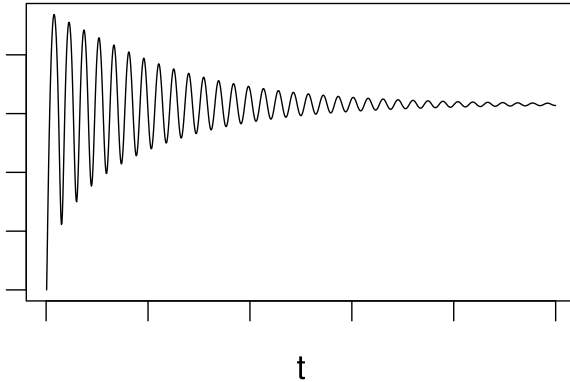
Vacuum Langevin Eqn

$$\frac{\partial^2 \mathbf{r}}{\partial t^2} = \left(1 + C \frac{\partial}{\partial t}\right) \frac{\partial^2 \mathbf{r}}{\partial s^2} + \xi(\mathbf{s}, \mathbf{t})$$

Eigenmodes: $\Omega_k \equiv \omega_k + i\lambda_k$.

Damping $\lambda_k \propto k^2$ for small k and $\omega_k \propto k$.

$$g(t) = \left\langle \frac{1}{N} \sum_{i=1}^N |\mathbf{r}_i(t) - \mathbf{r}_i(0)|^2 \right\rangle$$
$$\propto \text{Re} \sum_k \frac{\Omega_k (1 - \exp(i\Omega_k t))}{\omega_k k^2}$$



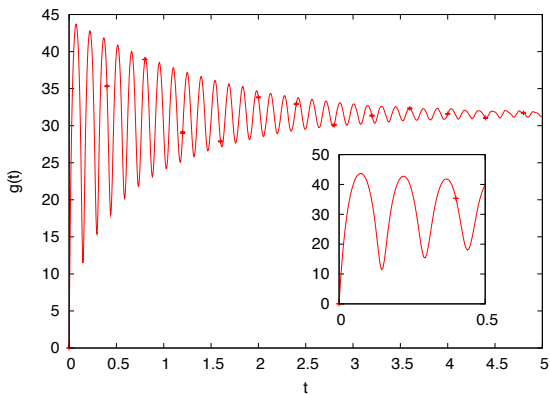
$$\text{Period} \propto N, T_{rel} \propto N^2$$

Simulation

- Rigid links
- Freely rotating
- Solves Newton's Laws
- Algorithm obeys conservation laws + keeps links fixed length.
- Efficient method, $\mathcal{O}(N)$ to move N link chain one time step

Ideal Chain

No interactions i.e. an “ideal chain”.



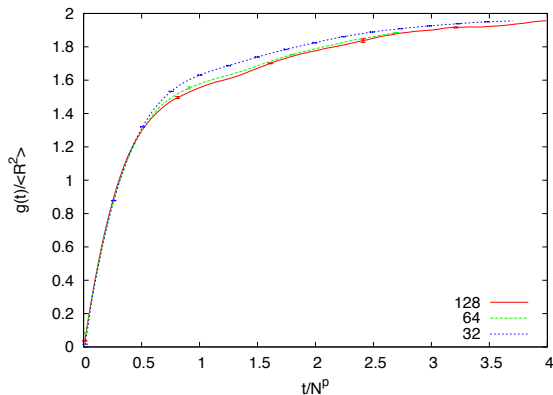
$$T_{rel} \propto N^{(1.85 \pm .15)}$$

Repulsive Interaction

$$\beta V(r) = 2(1 - (r/l)^2)^5.$$

$$\langle R^2 \rangle \propto N^\nu, \nu = .596 \pm .01 \text{ in 3d.}$$

Numerical Scaling



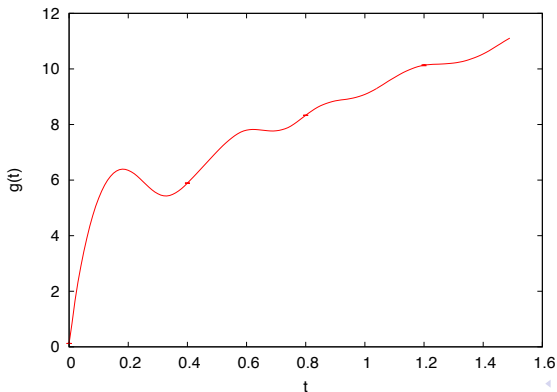
$$T_{rel} \propto N^p, \text{ with } p = 1.15 \pm .05.$$

Charged

Now lets also put charges on the two ends.

$$N = 32$$

$$\langle \text{end to end distance} \rangle = 10.0 \quad (l = 1)$$



Microcanonical averages

$$\overline{\langle \hat{O} \rangle} = \text{Tr}(\rho_{micro, \langle E \rangle} \hat{O})$$

(bar means time average).

$$\rho_{micro, E_0} \equiv \frac{1}{\mathcal{N}_{states}} \sum_{E_0 < E < E_0 + \Delta E} |E\rangle \langle E|$$

and:

$$S_{thermo} = -\text{Tr}(\rho_{micro} \ln \rho_{micro})$$

The Eigenstate Thermalization Hypothesis

ETH

$$\text{Tr}(\rho_E \hat{O}) = \text{Tr}(\rho_{\text{micro}, E} \hat{O})$$

$$\rho_E = |E\rangle\langle E|$$

The expectation value of \hat{O} will vary very little between neighboring energy levels for large N , implying that the expectation value of \hat{O} in any energy eigenstate is the microcanonical average (at that energy).

The Eigenstate Thermalization Hypothesis

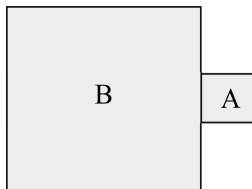
ETH

$$\text{Tr}(\rho_E \hat{O}) = \text{Tr}(\rho_{\text{micro}, E} \hat{O})$$

$$\rho_E = |E\rangle\langle E|$$

The expectation value of \hat{O} will vary very little between neighboring energy levels for large N , implying that the expectation value of \hat{O} in any energy eigenstate is the microcanonical average (at that energy).

Two Systems in Contact



Reduced density matrix

$$\rho_A \equiv \text{Tr}_B \rho$$

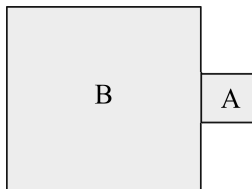
becomes mixed because it is entangled with B .

Now we define

entanglement entropy of A with B

$$S_{Ent}(A, B) \equiv -\text{Tr}(\rho_A \ln \rho_A).$$

Two Systems in Contact



Reduced density matrix

$$\rho_A \equiv \text{Tr}_B \rho$$

becomes mixed because it is entangled with B .

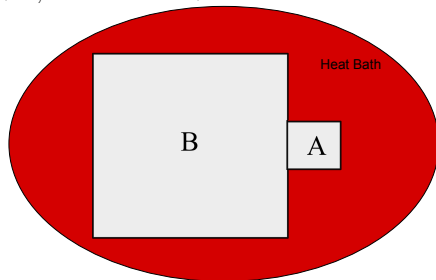
Now we define

entanglement entropy of A with B

$$S_{Ent}(A, B) \equiv -\text{Tr}(\rho_A \ln \rho_A).$$

Now consider

$$\rho_{A,micro} \equiv \text{Tr}_B \rho_{micro}$$



$$S_{Ent,micro}(A, B) \equiv -\text{Tr}(\rho_{A,micro} \ln \rho_{A,micro})$$

$$S_{thermo}(A) = S_{Ent,micro}(A, B) = -\text{Tr}(\rho_{A,micro} \ln \rho_{A,micro})$$

Calabrese and Cardy (2009), Korepin (2004)

Self-Entanglement Hypothesis

Is

$$S_{thermo}(A) = -\text{Tr}(\rho_A \ln \rho_A)?$$

or equivalently

$$-\text{Tr}(\rho_A \ln \rho_A) = -\text{Tr}(\rho_{A,micro} \ln \rho_{A,micro})?$$

compare with ETH:

$$\text{Tr}(\rho_E \hat{O}) = \text{Tr}(\rho_{micro,E} \hat{O})$$

Self-Entanglement Hypothesis

Is

$$S_{thermo}(A) = -\text{Tr}(\rho_A \ln \rho_A)?$$

or equivalently

$$-\text{Tr}(\rho_A \ln \rho_A) = -\text{Tr}(\rho_{A,micro} \ln \rho_{A,micro})?$$

compare with ETH:

$$\text{Tr}(\rho_E \hat{O}) = \text{Tr}(\rho_{micro,E} \hat{O})$$

Self-Entanglement Hypothesis

Is

$$S_{thermo}(A) = -\text{Tr}(\rho_A \ln \rho_A)?$$

or equivalently

$$-\text{Tr}(\rho_A \ln \rho_A) = -\text{Tr}(\rho_{A,micro} \ln \rho_{A,micro})?$$

compare with ETH:

$$\text{Tr}(\rho_E \hat{O}) = \text{Tr}(\rho_{micro,E} \hat{O})$$

Outline

- 1 Introduction
- 2 Thermodynamic Entropy and the Wave Function
- 3 Numerical Tests**
 - 1d Models
 - Entanglement Entropy
 - 2d Model
- 4 Conclusions

1d Hard Core Bosons and Spinless Fermions

$$H_B = \sum_{i=1}^L \left[-t \left(b_i^\dagger b_{i+1} + h.c. \right) + V n_i^b n_{i+1}^b - t' \left(b_i^\dagger b_{i+2} + h.c. \right) + V' n_i^b n_{i+2}^b \right],$$

and

$$H_F = \sum_{i=1}^L \left[-t \left(f_i^\dagger f_{i+1} + h.c. \right) + V n_i^f n_{i+1}^f - t' \left(f_i^\dagger f_{i+2} + h.c. \right) + V' n_i^f n_{i+2}^f \right].$$

1d Hard Core Bosons and Spinless Fermions

$$H_B = \sum_{i=1}^L \left[-t \left(b_i^\dagger b_{i+1} + h.c. \right) + V n_i^b n_{i+1}^b - t' \left(b_i^\dagger b_{i+2} + h.c. \right) + V' n_i^b n_{i+2}^b \right],$$

and

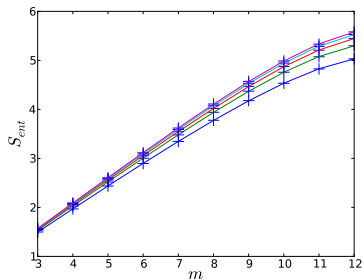
$$H_F = \sum_{i=1}^L \left[-t \left(f_i^\dagger f_{i+1} + h.c. \right) + V n_i^f n_{i+1}^f - t' \left(f_i^\dagger f_{i+2} + h.c. \right) + V' n_i^f n_{i+2}^f \right].$$

- We consider periodic BC's ($k=1$ sector) with $N = 27$ lattice sites
- 6 particles.
- We look at $V = t = 1$, and
- $V' = t' = 0.0$ (integrable) or $V' = t' = 0.96$ (non-integrable)
- We change the number of sites in A , denoted m , and see how $S_{ent}(m)$ varies.

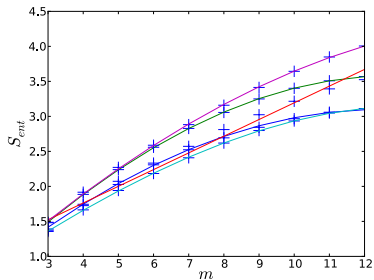
1d Hard Core Bosons

10966 states total in the $k = 1$ sector.

Non-integrable



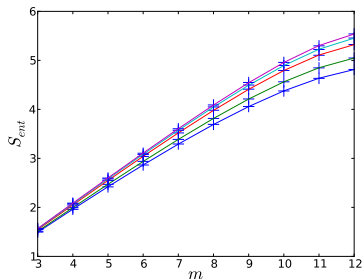
Integrable:



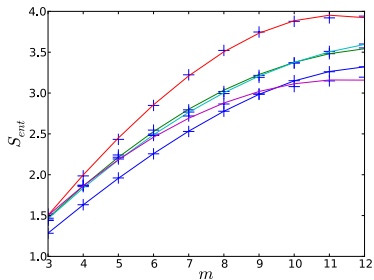
1d Spinless Fermions

10966 states total in the $k = 1$ sector.

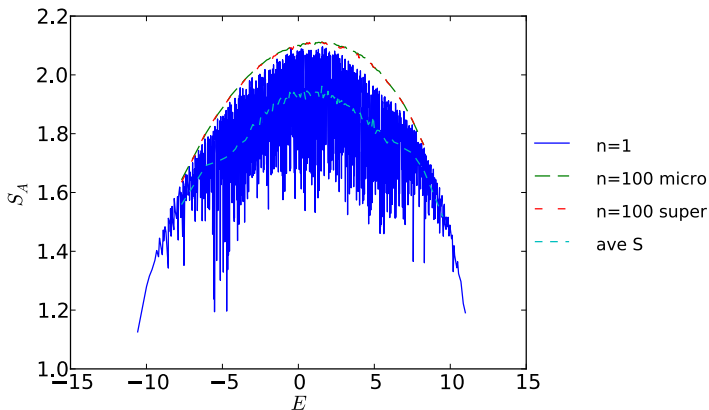
Non-integrable



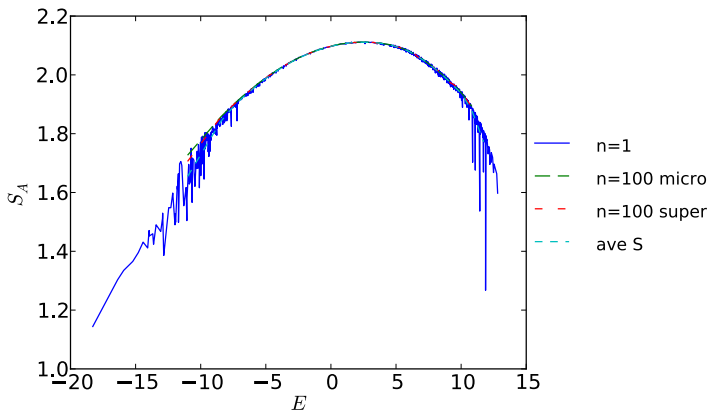
Integrable:



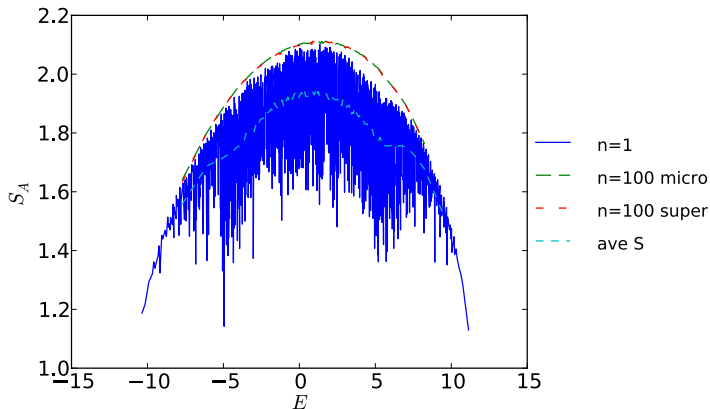
1d Hard Core Bosons, Integrable, $m=4$



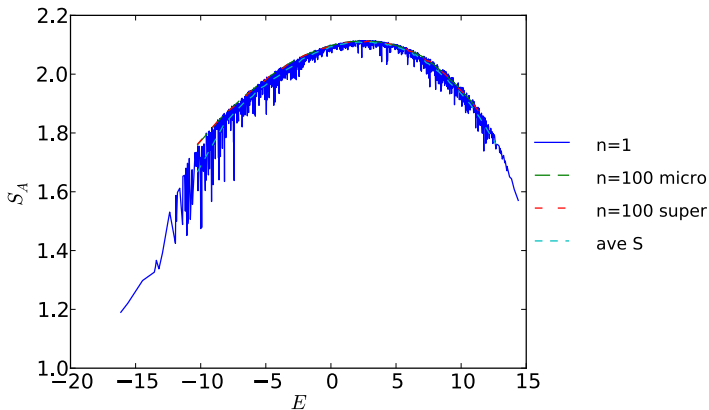
1d Hard Core Bosons, Generic, $m=4$



1d Spinless Fermions, Integrable, $m=4$



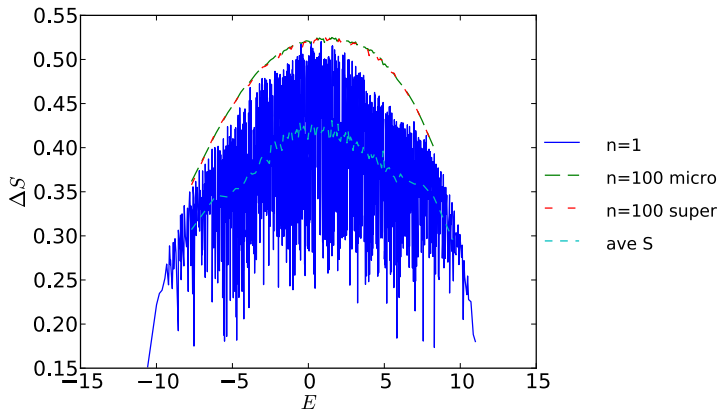
1d Spinless Fermions, Generic, $m=4$



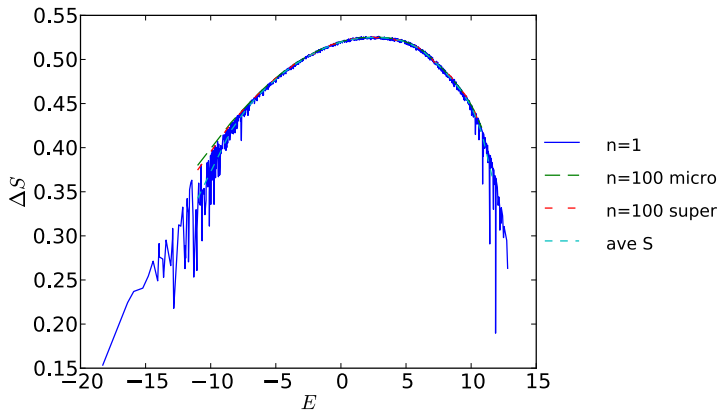
Entanglement Entropy Difference

We can consider the difference in entanglement entropy $\Delta S \equiv S_{ent}(4) - S_{ent}(3)$, which should be a measure of the entropy per site.

ΔS for Hard Core Bosons, Integrable



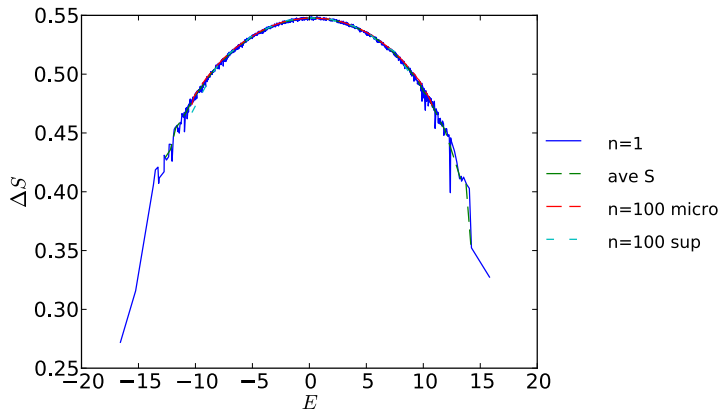
ΔS for Hard Core Bosons, Generic



2d Hard Core Bosons

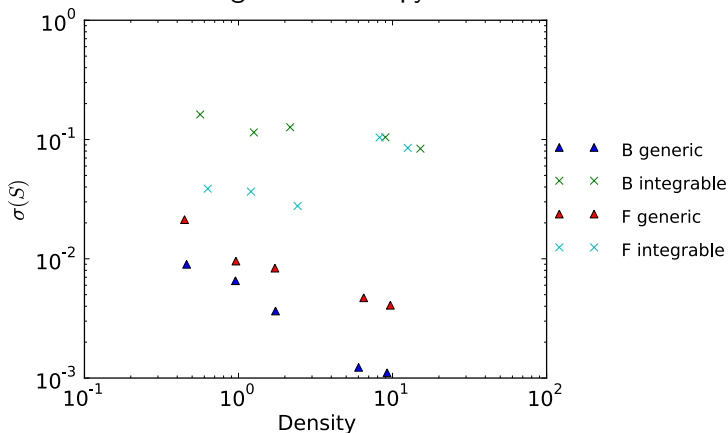
- 5×5 square lattice
- 6 particles
- Nearest neighbor repulsive potential = 0.1
- periodic boundary conditions.

2d Hard Core Bosons Entropy



Comparison of Generic and Integrable fluctuations

The standard deviation of the entanglement entropy $S_{ent}(A, B)$ is plotted against the density of states. This is done around the point of maximum entanglement entropy.



Evolution from more general initial conditions

Over long times, the energy eigenvector components of non-integrable wave functions will have random phases. So we consider wave functions that are the superposition of 100 contiguous eigenvectors with Gaussian random complex phases. These are the red dashed lines above.

Outline

- 1 Introduction
- 2 Thermodynamic Entropy and the Wave Function
- 3 Numerical Tests
- 4 Conclusions

Conclusions

- Knowledge of neighboring levels is not necessary to determine the entropy
- A complete knowledge of the system's quantum state, does not affect its behavior with respect to macroscopic measurements of the entropy.
- For long times, a system in a pure state and one in an statistical ensemble have identical thermodynamic entropies in the limit of large systems.
- This is because the entropy in such experiments measures the system's self-entanglement, not the lack of knowledge of it.

Conclusions

- Knowledge of neighboring levels is not necessary to determine the entropy
- A complete knowledge of the system's quantum state, does not affect its behavior with respect to macroscopic measurements of the entropy.
- For long times, a system in a pure state and one in an statistical ensemble have identical thermodynamic entropies in the limit of large systems.
- This is because the entropy in such experiments measures the system's self-entanglement, not the lack of knowledge of it.

Conclusions

- Knowledge of neighboring levels is not necessary to determine the entropy
- A complete knowledge of the system's quantum state, does not affect its behavior with respect to macroscopic measurements of the entropy.
- For long times, a system in a pure state and one in an statistical ensemble have identical thermodynamic entropies in the limit of large systems.
- This is because the entropy in such experiments measures the system's self-entanglement, not the lack of knowledge of it.

Conclusions

- Knowledge of neighboring levels is not necessary to determine the entropy
- A complete knowledge of the system's quantum state, does not affect its behavior with respect to macroscopic measurements of the entropy.
- For long times, a system in a pure state and one in an statistical ensemble have identical thermodynamic entropies in the limit of large systems.
- This is because the entropy in such experiments measures the system's self-entanglement, not the lack of knowledge of it.