PROBLEM SET 2

Physics 219A, Spring 2014

Due Wednesday, April 16

[1.] In class we computed the density of states $N(E)$ for N free particles,

$$H = \sum_{l=1}^{N} \frac{p_l^2}{2m}, \tag{1}$$

directly from the definition. Do the calculation by a second method:
a. First, show

$$Z(\beta) = \int d\Gamma e^{-\beta H} \tag{2}$$

is the Laplace transform of $N(E)$.
b. Compute $Z(\beta)$ by combining Eqns. 1 and 2 and doing the resulting (trivial) Gaussian integrals.
c. Compute $N(E)$ using your expression for $Z(\beta)$ from part (b) and the usual techniques for computing an inverse Laplace transform. You should get the same result we got in class.

[2.] The ideal relativistic gas. This problem can be done by following the computation done in class for the non-relativistic case where the energy-momentum dispersion relation is quadratic. In fact, the algebra is slightly simpler. You might want to get $N(E)$ using the approach of problem (1).
a. Calculate $N(E) = \int d\Gamma \delta(E - H)$ for N free classical particles in the extreme relativistic limit,

$$H = \sum_l c p_l. \tag{3}$$

b. Find the equation of state and the specific heat.
c. Find the single particle momentum distribution function.

[3.] Consider a single simple harmonic oscillator,

$$H = \frac{1}{2} m\omega^2 x^2 + \frac{1}{2m} p^2 \tag{4}$$

in the microcanonical ensemble.
a. Draw a "phase space" picture of the trajectory of the particle assuming it has energy E. Can you predict what the probability distributions $P(x)$ and $P(p)$ of position and momentum might look like from this picture?
b. Compute the density of states $N(E)$.
c. Compute $P(x)$ and $P(p)$. Does your answer agree with your prediction from (a)?

d. In the canonical ensemble, as we have discussed in class, we imagine the oscillator in contact with a heat bath at temperature T rather than having some fixed energy E. What are $P(p)$ and $P(x)$ in that case? Where are they peaked? How do they compare with the microcanonical result of (c)?
e. Should we fret about the difference? After all, the different ensembles are supposed to be equivalent!

[4.] Consider N independent particles each of which can assume two energy levels 0 and ϵ. Denote by n_0 the number of particles in the energy level 0 and by n_1 the number in level ϵ.
a. What is the relation between the energy E and n_1?
b. What is the relation between the entropy S and n_1?
c. Using $1/T = dS/dE$, compute $E(T)$. Make a plot of the result for $N = 128$ particles. For the plot, choose $k_B = \epsilon = 1$.
d. On the same plot, show the canonical result

$$\langle E \rangle (T) = \frac{N}{e^{1/T} + 1}. \tag{5}$$

What do you conclude?
e. Comment on what happens to the temperature for energies $E > N\epsilon/2$. Do you know a physical system which has this sort of behavior?

(a) $N(E) = \int d\Gamma\, \delta(E-H)$ so the Laplace transform of $N(E)$ is $\int d\beta\, e^{-\beta E} N(E) = \int d\beta\, e^{-\beta E} \int d\Gamma\, \delta(E-H)$

$$= \int d\Gamma\, e^{-\beta H} = Z(\beta)$$

(b) $$Z(\beta) = \int d^{3N}x\, d^{3N}p\; e^{-1/2m \sum p_\ell^2\, \beta}$$

$$= V^N \left[\int dp\; e^{-\beta\, 1/2m\, p^2}\right]^{3N}$$

$$= V^N \left[2\pi m/\beta\right]^{3N/2}$$

(c) $$N(E) = 1/2\pi i \int_{c-i\infty}^{c+i\infty} d\beta\, Z(\beta)\, e^{+\beta E}$$

$$= \frac{1}{2\pi i} V^N (2\pi m)^{3N/2} \int_{c-i\infty}^{c+i\infty} d\beta\, \beta^{-3N/2} e^{+\beta E}$$

pole of order $3N/2$

$$= \frac{1}{2\pi i} V^N (2\pi m)^{3N/2}\, 2\pi i\, \frac{1}{(\frac{3N}{2}-1)!} \left(\frac{d}{d\beta}\right)^{\frac{3N}{2}-1} e^{\beta E}\Big|_{\beta}$$

$$= V^N (2\pi m)^{3N/2}\, E^{3N/2-1}\, \Gamma\left(\tfrac{3N}{2}\right)$$

where I used $\Gamma(n) = (n-1)!$

This result agrees with the one derived in class.

1. The Relativistic Gas of free particles

a) $$Z(\beta) = \int d\Gamma\, e^{-\beta H} = V^N \int d^3p_1 \dots \int d^3p_N\, e^{-\beta(cp_1 + \dots cp_N)}$$

$$= V^N h^{-3N} \left[\int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta\, d\theta \int_0^{\infty} p^2 e^{-\beta c p}\, dp \right]^N$$

$$= (4\pi V/h^3)^N \left[\int_0^{\infty} p^2 e^{-\beta c p}\, dp \right]^N$$

$$\boxed{Z(\beta) = \left(\frac{8\pi V}{h^3 c^3 \beta^3} \right)^N}$$

Recall that

$$Z(\beta) = \int d\Gamma\, e^{-\beta H} = \int dE \int d\Gamma\, e^{-\beta E}\, \delta(E - H)$$

$$Z(\beta) = \int dE\, e^{-\beta E} N(E)$$

so Z is the Laplace transform of N. Do inverse Laplace transform to get N from Z

$$N(E) = \frac{1}{2\pi i} \int_{0^+ - i\infty}^{0^+ + i\infty} \left(\frac{8\pi V}{\beta^3 h^3 c^3} \right)^N e^{+\beta E}\, d\beta$$

$$= \frac{1}{2\pi i} (2\pi i) \left(\frac{8\pi V}{h^3 c^3} \right)^N \frac{1}{(3N-1)!} \frac{d^{3N-1}}{d\beta^{3N-1}} e^{+\beta E}$$

So $$\boxed{N(E) = \left(\frac{8\pi V}{h^3c^3}\right)^N E^{3N-1} / (3N-1)!}$$

As for $E = p^2/2m$ dispersion, key feature is rapid growth of $N(E)$ with E.

b) $$P = 1/\beta \,\partial/\partial V\,(\ln Z) = kT \frac{1}{Z}\frac{\partial Z}{\partial V}$$

$$= \left(\frac{h^3c^3\beta^3}{8\pi V}\right)^N \left(\frac{8\pi}{h^3c^3\beta^3}\right)^N N V^{N-1} = \frac{N}{V} k_B T$$

so $$\boxed{PV = Nk_BT}$$

c) $$n(p) = \sum_i \langle \delta(|\vec{p}_i| - p)\rangle$$

$$= N \langle \delta(|\vec{p}_1| - p)\rangle$$

$$= N \frac{1}{N(E)} \int d^3p_1 \ldots d^3p_N \; \delta(|\vec{p}_1| - p)\,\delta(E - H)$$

$$= N \, 1/N(E)\, V\frac{4\pi p^2}{h^3} \underbrace{\int d^3p_2 \ldots d^3p_N \, \delta[E - cp - (cp_1 + cp_2 \cdots}_{N(E-cp) \text{ for } N-1 \text{ particles}}$$

$$= \frac{NV}{h^3} \frac{(3N-1)!}{E^{3N-1}} \left(\frac{h^3c^3}{8\pi V}\right)^N 4\pi p^2 \left(\frac{8\pi V}{h^3c^3}\right)^{N-1} (E-cp)^{3N-4} \frac{1}{(3N-}$$

$$n(p) = N \, \overbrace{(3N-1)(3N-2)(3N-3)}^{\approx (3N)^3} \, \frac{1}{E^3} \, 4\pi p^2 \, \frac{c^3}{8\pi} \left(1 - \frac{cp}{E}\right)^3$$

It is an easy exercise to show that $\langle E \rangle = 3N k_B T$. (Eg compute $\langle E \rangle = -\partial/\partial\beta \ln Z$!) Then, also writing $3N-4 \approx 3N$

$$\boxed{n(p) = N \frac{c^3}{2} p^2 \frac{1}{(k_B T)^3} e^{-cp/k_B T}}$$

where I used $(1 - x/N)^N \Rightarrow e^{-x}$ for N large.

We can check normalization

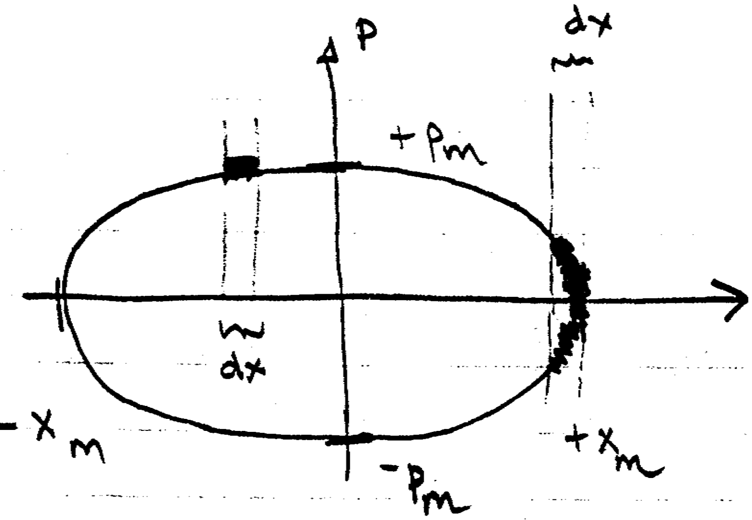
$$\int_0^\infty n(p)\,dp = N \, c^3/2 \, (k_B T)^3 \int_0^\infty p^2 e^{-cp/k_B T} dp$$

$$= N \, c^3/2 \, (k_B T)^{-3} \left(\frac{k_B T}{c}\right)^3 \underbrace{\int_0^\infty u^2 e^{-u} du}_{2}$$

$$= N \quad \checkmark\checkmark$$

3-1

(a)



$$x_m = \left[2E/m\omega^2\right]^{1/2}$$

$$p_m = \left[2mE\right]^{1/2}$$

I expect $P(x)$ to be peaked near $x = \pm x_m$ and likewise $P(p)$ peaked near $p = \pm p_m$. To see this consider slices of fixed dx and note that a lot more of the ellipse is contained in the slice for x near $\pm x_m$ than x away from $\pm x_m$

(b) $$N(E) = \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dp \; \delta\left(E - p^2/2m - \tfrac{1}{2} m\omega^2 x^2\right)$$

Use $\delta\left[f(p)\right] = 1/\left|f'(p_0)\right| \; \delta(p - p_0)$ where $f(p_0) =$

Here $f(p) = E - p^2/2m - \tfrac{1}{2} m\omega^2 x^2$

$$p_0 = \left[2m\left(E - \tfrac{1}{2} m\omega^2 x^2\right)\right]^{1/2}$$

Note, p_0 exists iff $E > \tfrac{1}{2} m\omega^2 x^2$ so the limits $\pm\infty$ on our x integral get shrunk down

(4b cont'd)

$$N(E) = \int_{-\infty}^{\infty} dx \; \frac{m}{p_0} \underbrace{\int_{-\infty}^{\infty} \delta(p - p_0)\, dp}_{\substack{=1 \text{ if a } p_0 \text{ exists, which} \\ \text{happens iff } |x| < x_m}}$$

$$= \int_{-x_m}^{x_m} \left[m / 2(E - \tfrac{1}{2} m\omega^2 x^2) \right]^{1/2} dx$$

Let $x = \sqrt{2E/m\omega^2}\, \sin\theta = x_m \sin\theta$

$$dx = x_m \cos\theta \, d\theta$$

$$N(E) = \int_{-\pi/2}^{\pi/2} x_m \cos\theta \, d\theta \left(m/2E \right)^{1/2} 1/\cos\theta$$

$$= x_m (m/2E)^{1/2} \pi = \left(2E/m\omega^2 \; m/2E \right)^{1/2} \pi$$

$N(E) = \pi/\omega$ ← Interesting that it is E independent!

Interpretation: One energy level per ω tro

$\boxed{E_n = (n+1/2)\hbar\omega \text{ suggests } N(E) = 1/\omega}$

Check dimensions: What are units of $N(E)$

$N(E) = \int dx\, dp\, \delta(E - H)$ ← NB δ function has units $1/E$

$[N(E)] = L \; ML/T \; 1/ML \ldots = T$

Indeed $1/\omega$ has units of T.

(c) $$P(x) = N(E)^{-1} \int dp\, \delta(E - \tfrac{1}{2}m\omega^2 x^2 - p^2/2m)$$

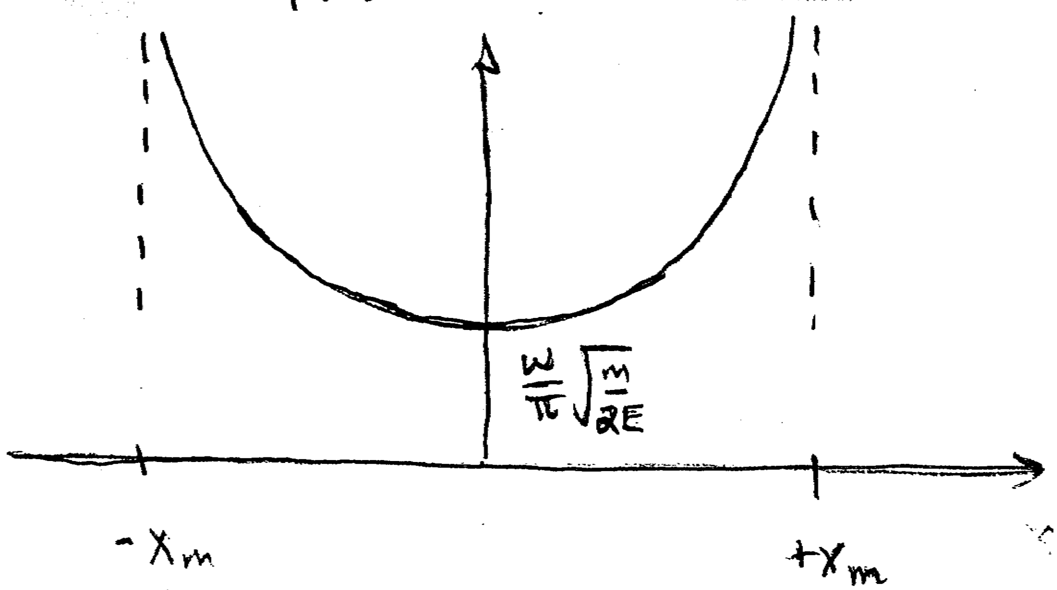
Clearly, $\int dx\, p(x) = 1$ as desired. In words, this formula for $p(x)$ says integrate over all possible p values consistent with the desired x and the known E. The $N(E)$ out front ensures normalization.

Using algebra from (4b):

$$P(x) = \frac{\omega}{\pi}\left[m/2(E - \tfrac{1}{2}m\omega^2 x^2)\right]^{1/2}$$

(Check $p(x)$ has dimensions $1/L$!)

Sketch $p(x)$



This has expected peaks (in fact, singularities) at $X = \pm X_m$ as predicted from picture in (a). Similar result for $P(p)$....

3-4

(d) $$\rho(x) = \left[\frac{2\pi k_B T}{m\omega^2}\right]^{-1/2} e^{-\frac{1}{2} m\omega^2 x^2 / k_B T}$$

$$\rho(p) = \left[2\pi m k_B T\right]^{-1/2} e^{-\frac{1}{2} p^2 / m k_B T}$$

These are peaked at $x=0$ and $p=0$.

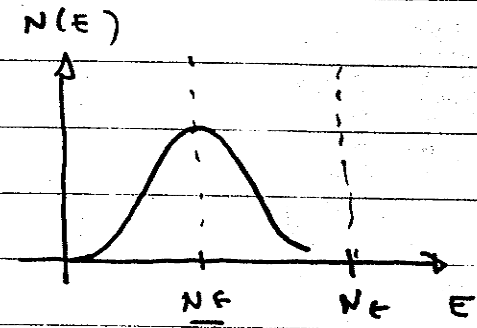
Very different from 4c!

(e) Microcanonical $\leftrightarrow$ Canonical Equivalence is guaranteed <u>only</u> in thermodynamic limit. So there is no contradiction here

(Huang 7-3)

N free particles energy levels 0, ϵ

compute S, T etc

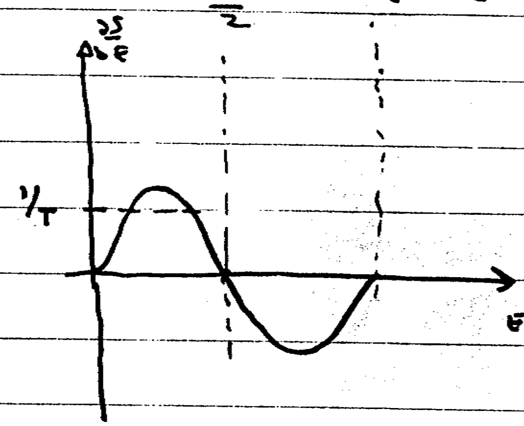


$$N(E) = \binom{N}{n_0} \quad \text{where} \quad E = n_0 \epsilon$$

$$S = + k_B \ln N(E)$$

Note peculiar thing: N(E) is <u>not</u> an increasing function of E → This leads to negative temperatures

$$1/k_BT = \partial S/\partial E$$



$$\frac{\Delta S}{\Delta E} = \left[\binom{N}{n_0+1} - \binom{N}{n_0}\right]\frac{1}{\epsilon}$$

$$= \frac{N!}{(n_0+1)!(N-n_0-1)!} - \binom{N}{n_0} = \binom{N}{n_0}\left[\frac{N-n_0}{n_0+1} - 1\right]$$

when $N_0 < N/2$ $\quad \frac{\Delta S}{\Delta E} > 0$, as clear from the picture

Write a little program with table of

	$n_0 (= E/\epsilon)$	N(E)	$S = (k_B)\ln N(E)$	$1/T$	T
set $\epsilon = 1$	0				
$k_B = 1$	1				
	2				

Then plot E(T).

4-2

Canonical Result

$$\langle E \rangle = \frac{N \epsilon e^{-\beta\epsilon}}{1 + e^{-\beta\epsilon}} = \frac{N \epsilon}{e^{\beta\epsilon} + 1}$$

We set $\epsilon = 1 = k_B$

$$\langle E \rangle = N / e^{1/T} + 1$$

4-3

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c       CODE TO ANALYZE HUANG'S TWO STATE PROBLEM

        implicit none
        integer n0,n1,N
        real*8 s,s0,ds

        write (6,*) 'enter N'
        read  (5,*) N

        s0=0.d0
        write (38,*) '   n0     n1            S
     1         1/T=dS         T'
        do 100 n1=1,N
             n0=N-n1
             s=s0+dlog(dfloat(n0+1)/dfloat(n1))
             ds=s-s0
             write (38,990) n0,n1,s,ds,1.d0/ds
             s0=s
100     continue
990     format(2i6,3f14.4)

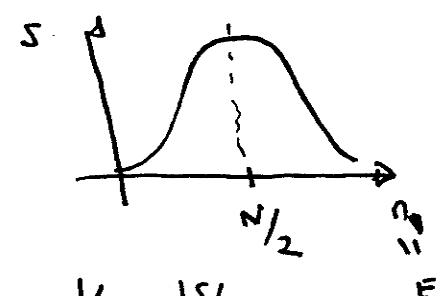
        end
```

$$\left.\begin{matrix} n_1 & \text{---}\ \epsilon \\ n_0 & \text{---}\ 0 \end{matrix}\right\} N$$

$n_0 + n_1 = N$

$E = n_1 \epsilon$

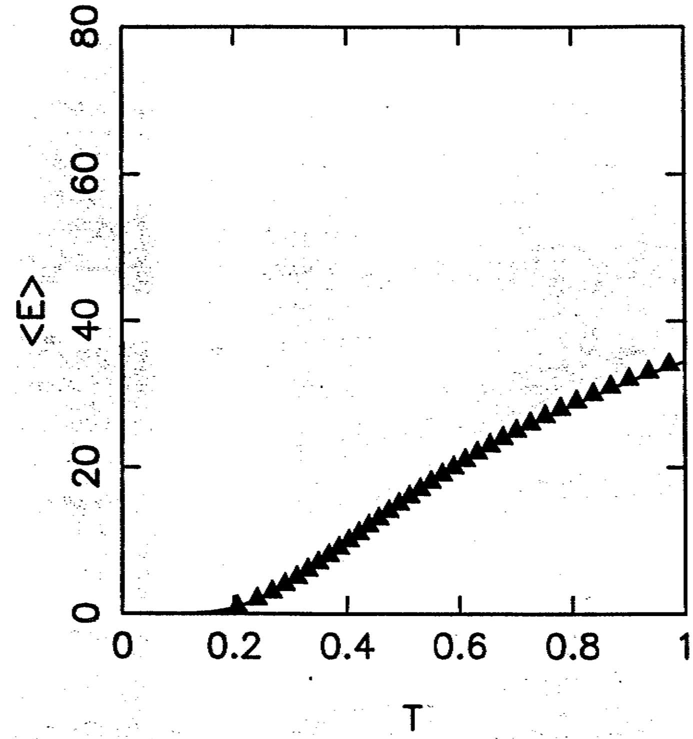
$S = \ln \binom{N}{n_0}$



$1/T = dS/dE$

4-4

N=128 two-state systems



$\boxed{\epsilon = k_B = 1}$

▲ microcanonical

$1/T = \frac{dS}{dE}$

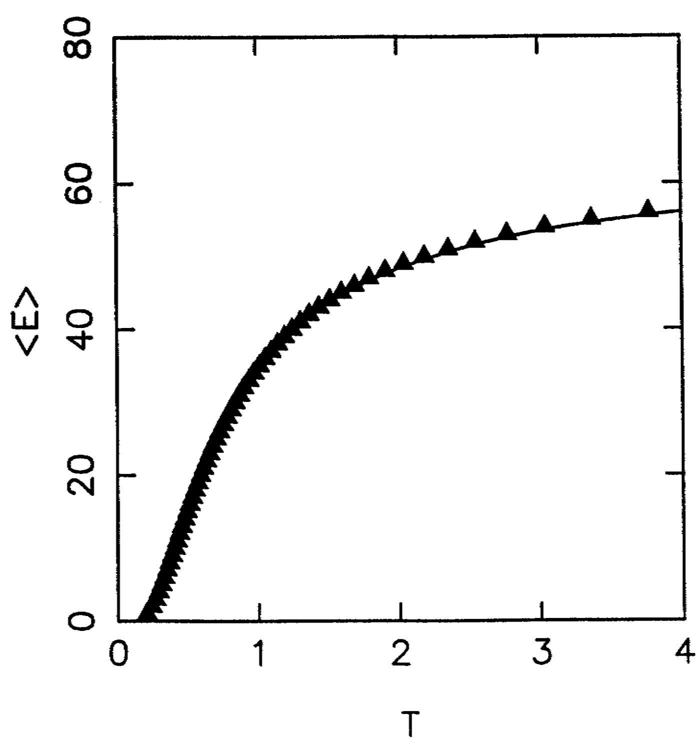
$E = n_1 \epsilon$

$S = \ln\binom{N}{n_0}$

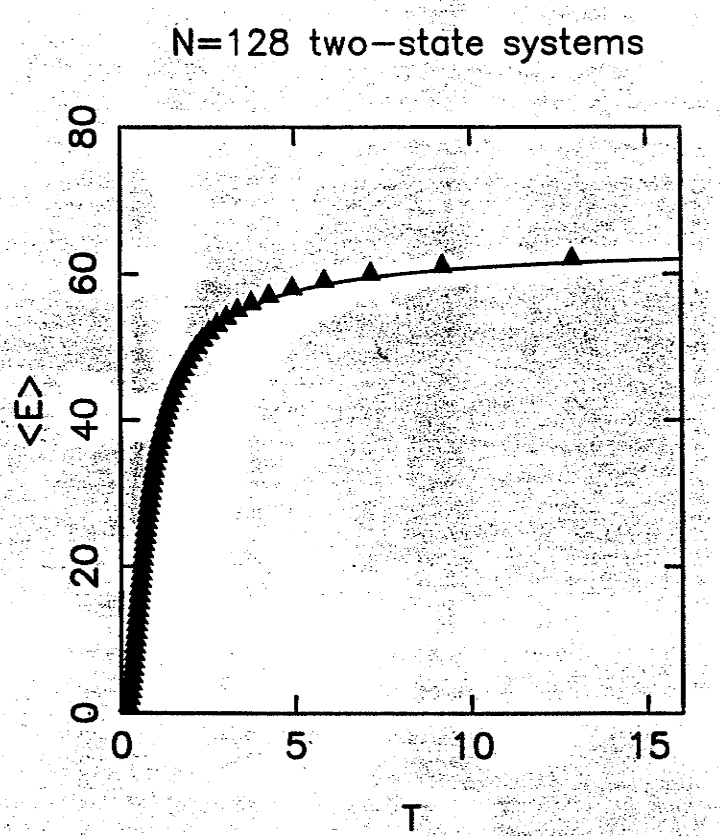
— canonical

$E = N/(e^{\beta\epsilon} + 1)$

N=128 two-state systems



4-5


N=128 two-state systems
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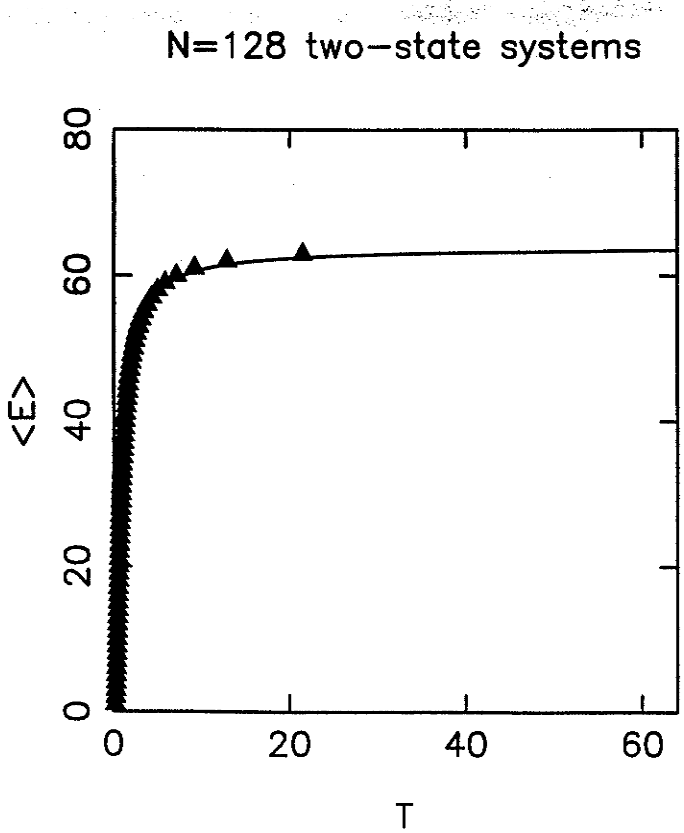
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