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"Path integral ground state method"

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PATH INTEGRAL GROUND STATE METHOD (PIGS)

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Idea is not New — At least 10 years old — But Few Implementations

Ceperley in his 1995 Review called it Variational Path Integral, but didn't implement it.

Standard PIMC calculates

$$\frac{\mathrm{tr}\left[\mathcal{O}\, e^{-\beta H}\right]}{\mathrm{tr}\, e^{-\beta H}} = \frac{\sum_n e^{-\beta E_n} \langle n|\mathcal{O}|n\rangle}{\sum_n e^{-\beta E_n}}$$

and we have heard some methods to expand $e^{-\beta H}$.

PIGS uses same technique to calculate

$$\mathcal{O}\left(\frac{\tau}{2}\right) = \frac{\langle \Psi_T | e^{-H\tau/2}\, \mathcal{O}\, e^{-H\tau/2} | \Psi_T \rangle}{\langle \Psi_T | e^{-H\tau} | \Psi_T \rangle}$$

$$|\Psi_T\rangle = \sum_n c_n |n\rangle$$

$$\mathcal{O}(\tau/2) \longrightarrow \langle 0|\mathcal{O}|0\rangle \quad \text{for } \tau \to \infty$$

An alternative way of thinking of PIGS, is to write PIMC as

$$\sum_{P} \int \prod_{i=1}^{M-1} dR_i \, \langle R_1 | e^{-H\Delta\beta} | R_2 \rangle \langle R_2 | e^{-H\Delta\beta} \cdots$$

$$\cdots | R_{M-1} \rangle \langle R_{M-1} | e^{-H\Delta\beta} | R_{1,Perm} \rangle$$

↑ permutations for Bosons

$$\Delta\beta = \beta / M$$

For $\Delta\beta$ small enough, we have good approximations to $\langle R | e^{-H\Delta\beta} | R' \rangle$ the density matrix.

If I replace one of the links with an approximate "ground state density matrix"

$$\rho(\beta \to \infty) \simeq \langle R | \Psi_0 \rangle \langle \Psi_0 | R' \rangle$$

$$\approx \Psi_T(R) \Psi_T(R')$$

↑ trial function

I GET PIGS

The method is easy To apply if you can already do PIMC. You need a good approximation to $e^{-H\Delta\beta}$.

We use pair product form as developed by Pollock & Ceperley.

The pair product form is like the virial expansion. If only pairs of particles interact at any time, it is exact, and the errors $\longrightarrow 0$ as $\Delta\beta \longrightarrow 0$.

$$\rho_0(R, R'; \beta) \equiv \langle R | e^{-H_0 \beta} | R' \rangle$$

with $H_0 = \sum_i \frac{p_i^2}{2m}$ Free gas Hamiltonian

$\Rightarrow$ ρ_0 is the usual Gaussian From R to R'; A product of N gaussians, one for each particle.

$$\rho_0^{(2)}(\vec{r}_1, \vec{r}_2, \vec{r}_1', \vec{r}_2'; \beta) = \langle \vec{r}_1, \vec{r}_2 | e^{-H_0^{(2)} \beta} | \vec{r}_1', \vec{r}_2' \rangle$$

$$H_0^{(2)} = \frac{p_1^2}{2m} + \frac{p_2^2}{2m}$$

This 2-body density matrix is just the product of 2 gaussians:

$$\frac{1}{(4\pi D \beta)^{3/2}} e^{-|\vec{r}_1 - \vec{r}_1'|^2 / (4D\beta)}$$

The exact density matrix can be written as

$$\rho(R,R';\beta) = \rho_0(R,R';\beta)\, e^{-U(R,R';\beta)}$$

The simple primitive approximation is the choice:

$$U(R,R';\beta) = \frac{\beta}{2}\left[V(R)+V(R')\right]$$

This corresponds to the break up

$$H = T + V$$

$$e^{-\beta H} \cong e^{-\beta V/2}\, e^{-\beta T}\, e^{-\beta V/2}$$

For pair wise potentials,

$$V(R) = \sum_{i<j} u(|\vec{r}_i - \vec{r}_j|) \equiv \sum_{i<j} v_{ij}$$

The pair product form is given by choosing the exact U for 2 particles

$$\rho^{(2)}(\vec{r}_1, \vec{r}_2, \vec{r}_1', \vec{r}_2'; \beta) = \rho_0(\vec{r}_1, \vec{r}_2, \vec{r}_1', \vec{r}_2'; \beta) \times e^{-\beta u(\vec{r}_{12}, \vec{r}_{12}', \beta)}$$

Where I have assumed that the two body H is translationally invariant

$$H^{(2)} = \frac{-\hbar^2}{2m}\nabla_1^2 - \frac{\hbar^2}{2m}\nabla_2^2 + v(|r_1 - r_2|)$$

The pair product form is then

$$U_{P\text{-}P}(R, R', \beta) = \sum_{i<j} u(\vec{r}_{ij}, \vec{r}_{ij}', \beta)$$

Additional corrections are given by Caperley and Pollock

$$\delta U = -\frac{D}{3} \sum_i \left[\left(\sum_{j \neq i} \vec{\nabla}_i u(\vec{\pi}_{ij}, \vec{\pi}'_{ij}, \beta) \right)^2 - \sum_{j \neq i} \left(\vec{\nabla}_i u(\vec{\pi}_{ij}, \vec{\pi}'_{ij}; \beta) \right)^2 \right] + O(\beta^4)$$

But I will not discuss these further. You simply plug into the definition of ρ and perform approximate averaging.

The improvement over pair product is useful but small.

Calculating $u(\vec{r}_{12}, \vec{r}_{12}'; \beta)$

Accurately. I like to calculate these at high enough accuracy [so] that I do not need to worry later.

Method that I use (Michel Lee + KES)
Phys. Rev. E 51, 5495 (1995).

Takes a few minutes to calculate u.
[Others use matrix squaring — Hermite Integ.]
We start with Trotter Formula

$$e^{-\tau H} = \lim_{n \to \infty} \left[e^{-\tau T/N} e^{-\tau V/N} \right]^N$$

T = Kinetic energy
V = potential " $\tau = \beta$

Define $\Delta\tau = \tau/N$

For numerical problems N is finite

$$e^{-\Delta\tau H} \cong e^{-\Delta\tau T} e^{-\Delta\tau V} + O(\Delta\tau^2)$$

$\Rightarrow$ error $\frac{1}{N}$ in entire prop.

Feynman used:

$$e^{-\Delta\tau H} \cong e^{-\Delta\tau/2 V} e^{-\Delta\tau T} e^{-\Delta\tau/2 V}$$

$$\equiv U_s(\Delta\tau)$$

↑ symmetrized.

Error $\mathcal{O}(\Delta\tau^3)$. $\Rightarrow$ error $O(\frac{1}{N^2})$ in entire prop.

The error structure of these breakups can be made to contain only even order errors in $\frac{1}{N}$.

Hatano + Suzuki

To have even order errors, the breakup will be invariant under $N \to -N$.

$$\left[U(T/N)\right]^N = \left[U\left(\frac{-T}{N}\right)\right]^{-N}$$

This will be true if the propagators U are reversible

$$U(\Delta T)\, U(-\Delta T) = 1$$

For the real time propagators

$\Rightarrow$ U unitary.

The break up $e^{-\Delta T T} e^{-\Delta T V}$ fails this test.

The break up $e^{-\frac{\Delta T}{2} V} e^{-\Delta T T} e^{-\frac{\Delta T}{2} V}$ passes.

So does $(1-\frac{\Delta T}{2}H)/(1+\frac{\Delta T}{2}H)$ $\leftarrow$ Crank Nicholson

So not only does the symmetrized break up have higher order errors, it leads to only <u>even</u> order errors in the entire propagator.

The equivalent analysis for trapezoidal integration allows us to extrapolate away the error term to give Simpson's and higher rules with the error reduced by $\frac{1}{N^2}$ for each extrapolation ⇒ Romberg Integration.

$$e^{-\tau H} \approx \left[4 U_S\left(\frac{\tau}{2N}\right)^{2N} - U_S\left(\frac{\tau}{N}\right)^{N} \right] / 3$$

⇒ 3 times computations of ⌐⌐
2 " storage of ⌐
errors is now $1/N^4$ not $1/N^2$.

You can continue this to get very high order accuracy.

Let's calculate ρ_2. Initially this has 12 coordinates plus β. The center of mass can be separated, leaving 6 coordinates. The equation for this relative coordinate 2-body density matrix is:

$$\left[\frac{-\hbar^2}{2m}\nabla^2 + U(r)\right]\rho(\vec{r},\vec{r}',\beta) = -\frac{\partial}{\partial\beta}\rho(\vec{r},\vec{r}',\beta)$$

m: reduced mass

We partial wave expand (r, r': distances)

$$\rho(\vec{r},\vec{r}',\beta) = \sum_{l=0}^{\infty} \frac{(2l+1)\rho_l(r,r',\beta)}{4\pi r r'} P_l(\hat{r}\cdot\hat{r}')$$

P_l: Legendre polynomial

The partial wave ρ_ℓ satisfy

$$\left(\frac{-\hbar^2}{2m}\left[\frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{r^2}\right] + v(r)\right)\rho_\ell(r,r',\beta)$$

$$= -\frac{\partial}{\partial\beta}\rho_\ell(r,r',\beta)$$

We now apply the Trotter breakup with extrapolation To this equation.

We take $T = \frac{-\hbar^2}{2m}\frac{d^2}{dr^2}$

$$V = \frac{\hbar^2}{2m}\frac{\ell(\ell+1)}{r^2} + v(r)$$

Unlike Monte Carlo, we want a set of grid points in the spatial coordinates.

We choose a uniform grid, the j th grid point is at $j\Delta r$, and

$1 < j \leq M-1$ and $M\Delta r$ is large enough so $\rho \to 0$ there.

An <u>incorrect</u> method is to evaluate a short time propagator (continuous space) at the grid points. If you take the symmetrized form, the $e^{-\Delta\tau T}$ goes to the usual gaussian. However evaluating this at the grid points does not give a reversible propagator on the grid points, even though it is reversible in continuous space.

To construct a discrete reversible propagator, we use a Fourier Trorsform.

Since the V terms are diagonal in r space, they will give a reversible propagator. We insert a plane wave basis of discrete k points

$|k_n\rangle$ $\quad\quad$ $|j\rangle$

↑ $\quad\quad$ ↑

k-space basis $\quad\quad$ real space basis

$$\langle j|k_n\rangle = \sin\left(\frac{\pi n j}{M}\right)\sqrt{\frac{2}{M}}$$

with $k_n r_j = \frac{\pi n j}{M}$

The discrete propagator that is reversible is:

$$U_{jm} = \sum_n \langle j| e^{-\frac{\Delta T}{2}V(r_j)} |k_n\rangle$$

$$\times e^{-\Delta T \frac{\hbar^2 k_n^2}{2m}} \langle k_n| e^{-\frac{\Delta T}{2}V(r_m)} |m\rangle$$

As $\tau \to 0$,

$$U_{jm} = \delta_{jm}$$

We start with

$$\rho_2(i,j,0) = \frac{\delta_{ij}}{\Delta r}$$

Multiply by $e^{-\frac{\Delta\tau}{2}V(r_m)}$ at each grid point.

Fourier sine transform (FFT) which gives ρ in terms of k grid.

Multiply by $e^{-\Delta\tau \frac{\hbar^2 k_n^2}{2m}}$

Fourier transform back to r grid and multiply by $e^{-\frac{\Delta\tau}{2}V(r_m)}$

Repeat N times.

We now extrapolate the error away by evaluating at $N = 2, 4, 6, 8, 12, 16, 24, 32$.

We usually break the entire interval into 4 equal intervals and apply the extrapolation on each.

This removes the time step error to $\simeq 10^{-9}$ i.e. $1/2$ machine precision on 64 bit machine.

On a cray with double precision we also go to $\simeq 1/2$ machine precision i.e 10^{-16}.

What about the space grid?

You might think the error in the spatial discretization is like the time error. It isn't for hard core potentials!!

Using our uniform grid and FFT is equivalent to using trapezoidal rule for all integrals.

Euler-Maclaurin formula:

$$\frac{1}{2} f(0) + f(1) + \cdots f(n-1) + \frac{1}{2} f(n) \equiv \text{trapezoidal rule}$$

$$= \int_0^n f(x)\,dx - \frac{1}{12}\left(f'(0) - f'(n)\right)$$

$$+ \frac{1}{720}\left(f^{(3)}(0) - f^{(3)}(n)\right) - \frac{1}{30240}\left(f^{(5)}(0) - f^{(5)}(n)\right)$$

$$+ \cdots \frac{B_{2m}}{(2m)!}\left(f^{(2m-1)}(0) - f^{(2m-1)}(n)\right)$$

This is an asymptotic formula, the error is less than the last term dropped if n is large enough.

For ^4He or other hard core potentials

$v \to$ very large in core region $\Rightarrow \rho \to 0$
for $r \to 0$, and all its derivatives $\to 0$ too.

at large $r \to \infty$ for fixed r', $\rho \to 0$
like a gaussian. $\Rightarrow$ all derivatives $\to 0$.

So if the range of r is large enough,
all the error terms $\longrightarrow 0$ exponentially.

Trapezoidal rule is exponentially
accurate once M is large enough.

$\Rightarrow$ Essentially exact spatial integrations.

$\ell = 0$ radial density matrix for ^4He-^4He at $\beta = \frac{1}{40K}$ for various Δr, $M\Delta r$ = range and r, r' values (Å)

r	r'	M	Δr	ρ
2.4	2.0	512	0.05	0.017 939 355
		512	0.025	0.017 939 355
		256	0.05	0.017 939 355
		128	0.10	0.017 939 355
		64	0.20	0.017 939 142
		32	0.40	0.017 907 811
2.6	3.2	512	0.05	0.357 527 511
		512	0.025	0.357 527 511
		256	0.05	0.357 527 511
		128	0.10	0.357 527 505
		64	0.20	0.357 527 500
		32	0.20	0.357 527 499

The problem is that with a 128×128 point grid and $\simeq 50$ l values, the density matrix is difficult to store and expensive to evaluate.

We follow Ceperley + Pollock and use the expansion:

$$s = |r| + |r'|$$
$$t = |r| - |r'|$$
$$w = |\vec{r} - \vec{r}'|$$

} order of Thermal wavelength, so expand in power series.

Then

$$u(\vec{r}, \vec{r}', \beta) = \frac{u_{\bullet}(\vec{r}, \vec{r}, \beta) + u_{\bullet}(\vec{r}', \vec{r}', \beta)}{2} + \sum_{n,m \geq 0} w^{2n} t^{2m} u_{nm}(s, \beta)$$

10 To 20 terms $\Rightarrow$ each is a 1-d table.

Also store derivatives this way.

The functions are calculated by least squares fit To $u(\vec{r}, \vec{r}, \beta)$.

$$\langle \mathcal{O}(\tau) \rangle = \frac{\langle \Psi_T | e^{-H(T-\tau)} \mathcal{O} e^{-H\tau} | \Psi_T \rangle}{\langle \Psi_T | e^{-HT} | \Psi_T \rangle}$$

T is the total imaginary time propagated.

τ is the "slice" where the operator $\mathcal{O}$ is evaluated.

1. If $T \to \infty$ or is large enough, for $\tau \approx T/2$, the value of $\mathcal{O}(\tau)$ is the ground-state expectation

2. For any T, $\mathcal{O}(T/2)$ is a variational estimate with wave function $e^{-HT/2} |\Psi_T\rangle$

3. If 2 slices are used, the formalism looks like Shadow wave functions of a particular form. The shadow particle part is Ψ_T. It can be quite bad!

Maybe we don't need a very good ψ_T.

4. For $T \to \infty$ or large enough,

$$\mathcal{O}(T) = \mathcal{O}(0) = \text{Mixed estimate}$$

$$= \frac{\langle \psi_T | \mathcal{O} | \psi_0 \rangle}{\langle \psi_T | \psi_0} = \langle \mathcal{O} \rangle_m$$

5. For $T \to \infty$ or large enough we can calculate time correlations

$$\langle \psi_0 | A e^{-HT} B | \psi_0 \rangle \quad \text{etc.}$$

Comparison of PIGS and GFMC

GFMC is just a different way to calculate these same integrals.

It can in principle calculate all these things

An advantage to GFMC is that T can be increased as needed without repeating previous calculations.

In practice, a good trial wave function is needed to guide the walk to get a low variance result.

The expectation value of H can be written as a mixed estimate

$$\frac{\langle \Psi_T | e^{-HT/2} H e^{-HT/2} | \Psi_T \rangle}{\langle \Psi_T | e^{-HT} | \Psi_T \rangle}$$

$$= \frac{\langle \Psi_T | H e^{-HT} | \Psi_T \rangle}{\langle \Psi_T | e^{-HT} | \Psi_T \rangle}$$

Other operators don't commute with H,

to calculate them in GFMC requires

"Forward Walking" (Kalos 1970) He atom.
⇒ Good guiding function for low variance.
To avoid this approximate extrapolation

is often used.

To calculate accurate energies when a good trial function is known, GFMC is best. For other expectations or when using a poor wave function, try PIGS.

What's Wrong with Extrapolation?

Often we approximate in GFMC

$$\langle \Psi_0 | O | \Psi_0 \rangle \cong 2\langle \Psi_T | O | \Psi_0 \rangle - \langle \Psi_T | O | \Psi_T \rangle$$

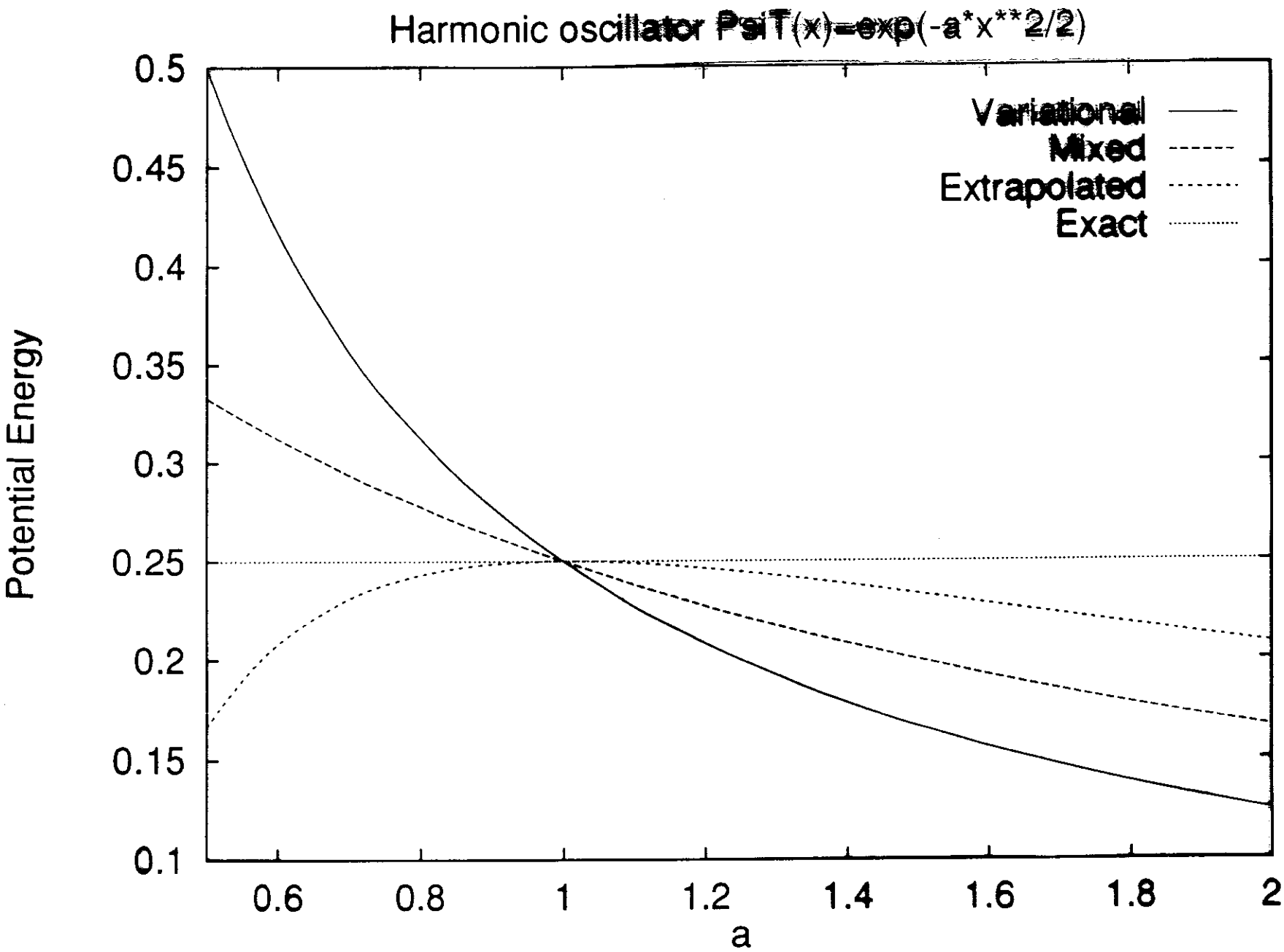
$$= 2O_m - O_v$$

LORE OF EXTRAPOLATION

1. If O_m is close to O_v, then very little extrapolation is done, and the extrapolation is accurate. ??

2. If several calculations with different trial wave functions extrapolate to the value, the extrapolation is accurate. ??

If by accurate you mean that the errors are less than those you get with the energy calculation of a variational method, then both are wrong. The error is still δ^2 ① and ② do not make δ^2 term small.


Harmonic oscillator PsiT(x)=exp(-a*x**2/2)
Variational
Mixed
Extrapolated
Exact
Potential Energy
0.5
0.45
0.4
0.35
0.3
0.25
0.2
0.15
0.1
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0.8
1
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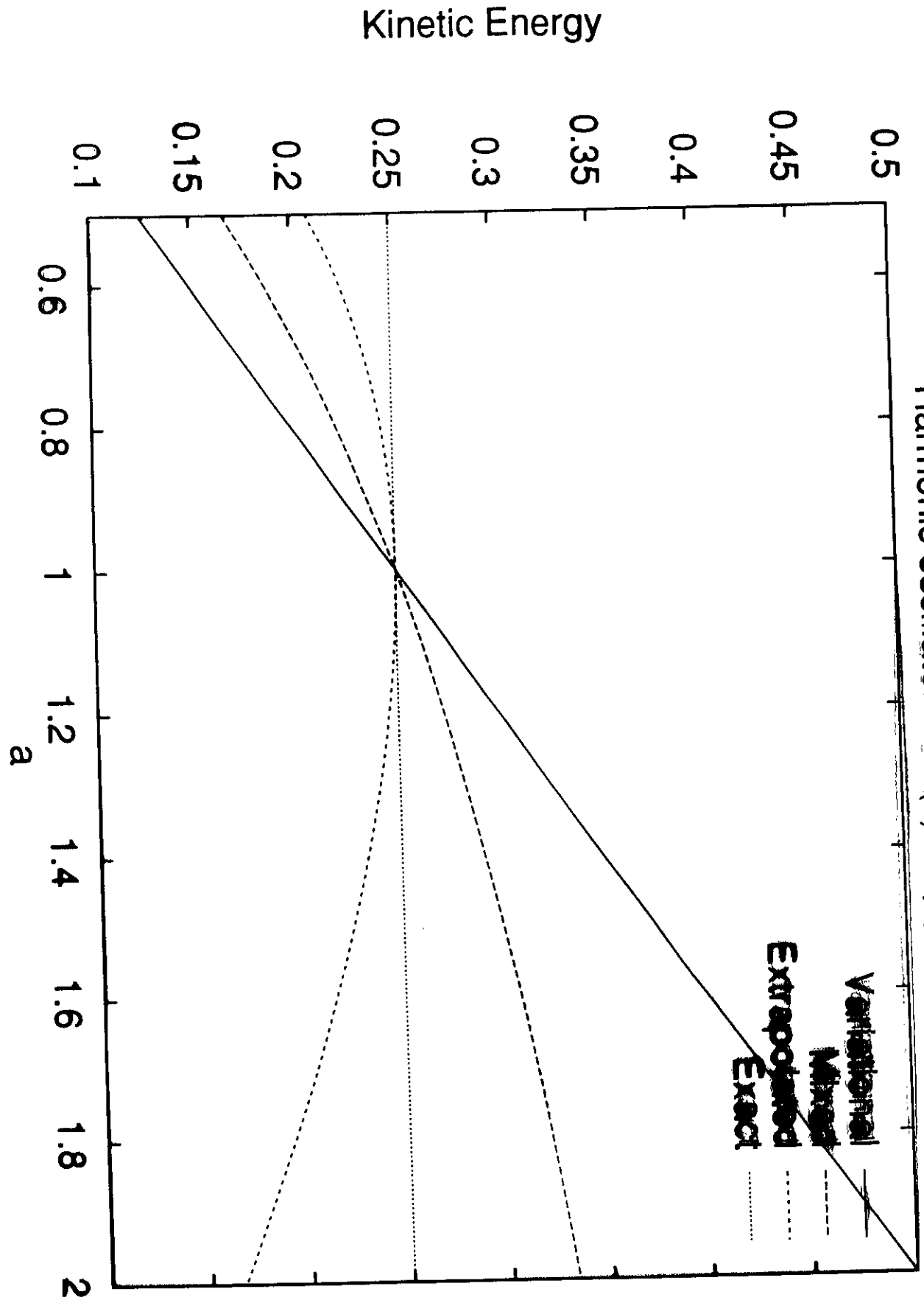
1.4
1.6
1.8
2
a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Harmonic oscillator Psi(x)=exp(-a*x**2/2)
Variational
Mixed
Extrapolated
Exact
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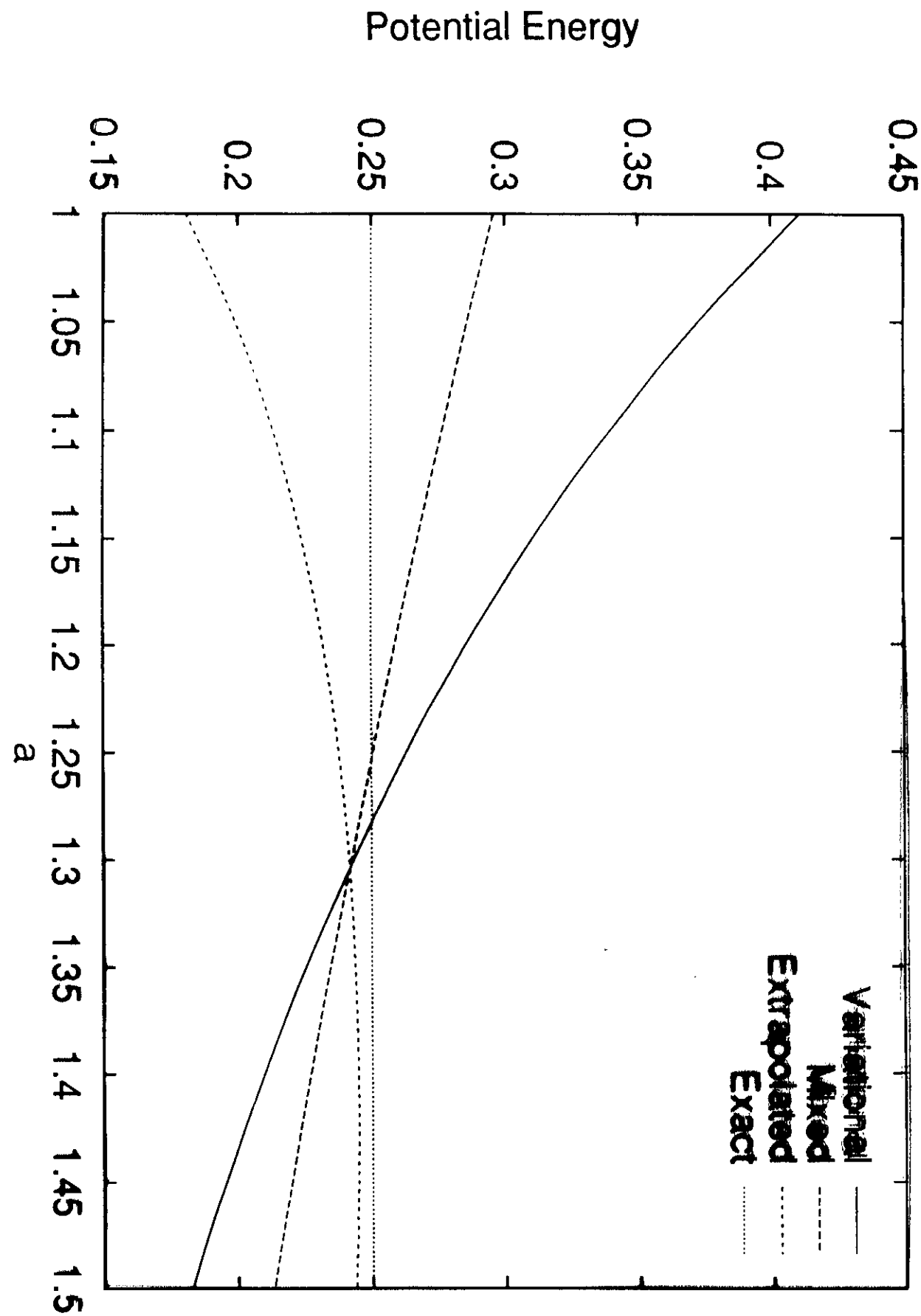
Potential Energy
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Variational
Mixed
Extrapolated
Exact
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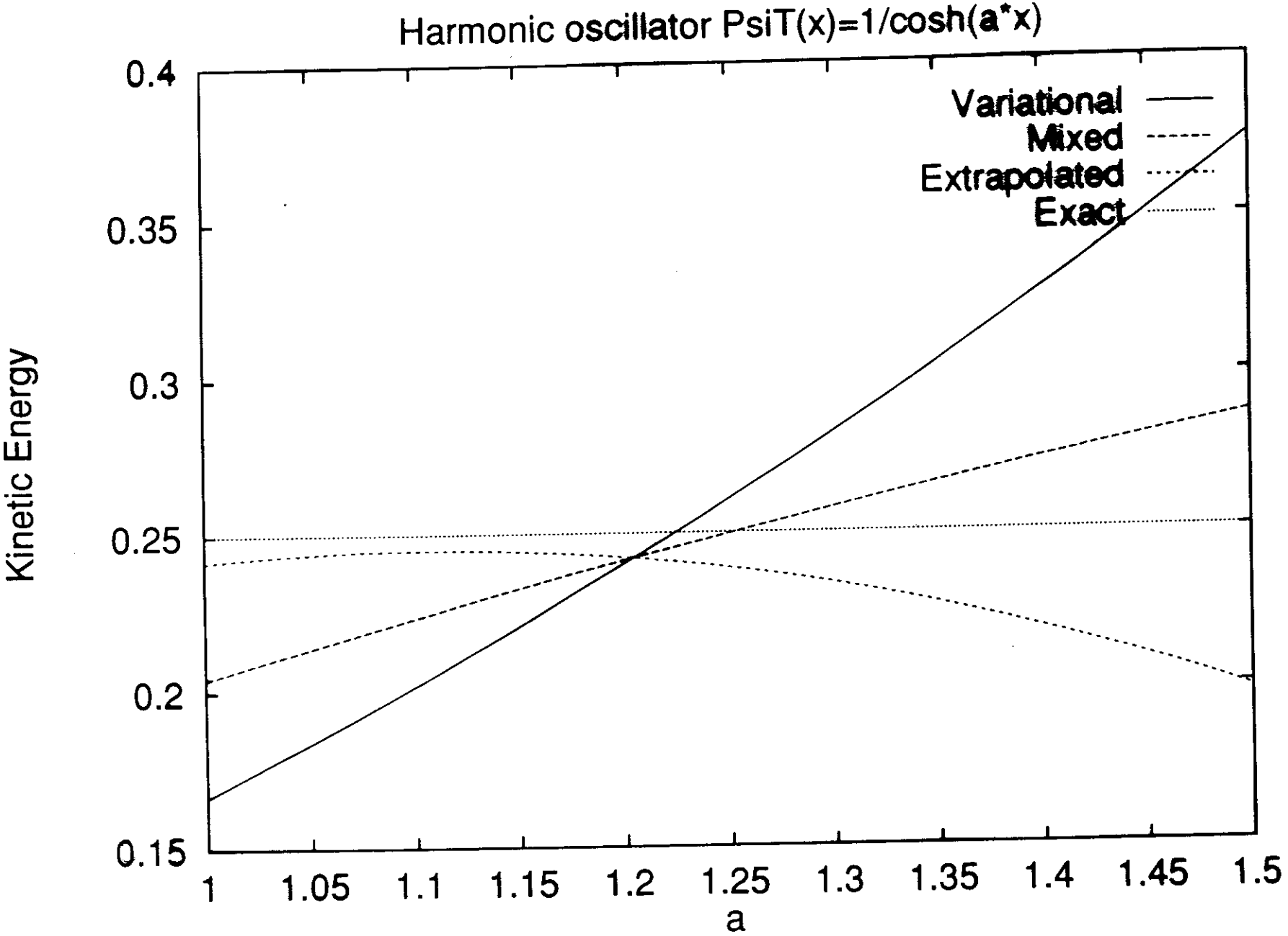
Harmonic oscillator PsiT(x)=1/cosh(a*x)
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1.15
1.2
1.25
1.3
1.35
1.4
1.45
1.5
a

Also Notice:

$$E_m = E_o = T_m + V_m$$

$$E_v = T_v + V_v$$

$$2E_o - E_v = T_{ext} + V_{ext}$$

So the sum of T_{ext} and V_{ext} for the same trial function must give a value that is below E_o by $(E_v - E_o)$.

In the literature V is often extrapolated and $T = E_o - V_{ext}$

2-body dist. → g(r) and ← momentum dist. n(k)

⇒ GFMC g(r) and n(k) if extrapolated from the same wave function must give an energy below the ground state.

Advantages of PIGS

1. Does not require a particularly good wave function.
2. Does not normally use a guiding function ⇒ higher variance, but ➡ you don't need a good one
3. No extrapolations needed i.e. expectation values of all operators are equally easy.

Advantages of GFMC

1. Gives low variance energies cheaply and easily when a good importance function is used.
2. Code is simpler
3. Easy to make GFMC exact so there is no time step error.

Some PIGS Details

1. Start with a working PIMC code (with or w/o permutation sums). Since Ψ_T has correct symmetry, Permutations change efficiency but not result.

2. Use usual PIMC bisection moves. A path segment is snipped out and a new path segment is sampled using a gaussian approximation To the density matrix. First the midpoint, then the midpoints of the remaining 1/2 segments are sampled, etc. Detailed balance gives the usual Metropolis acceptance prob.

3. Keep step 2 for segments w/o Ψ_T. For segments ending on Ψ_T, we simply move particles in a little box of side Δ as in VMC and then weave in the rest of the path.

4. If the total path length is greater than β_λ, the superfluid transition, Permutation moves speed things up.

Results

^{4}He Liquid at equilibrium density
$\rho = 0.0218\ \text{Å}^{-3}$, 64 particles, E in K.

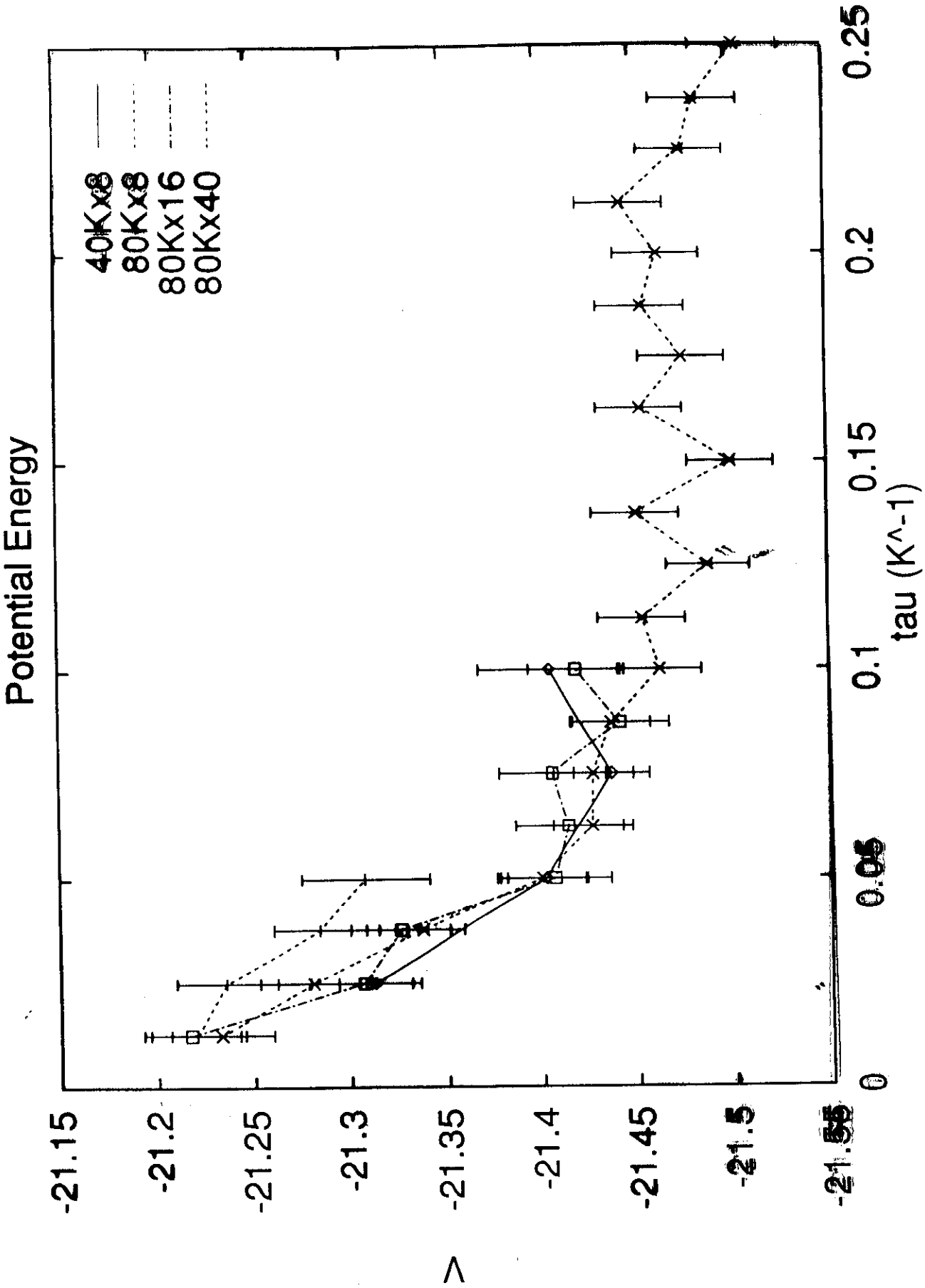
$E_{DMC} = -7.12 \pm .02$ Kalos et al.
$E_{DMC} = -7.14 \pm .01$ (KES)
$E_{DMC} = -7.145 \pm .004$ Moroni, Fantoni, Senatore

$E_{PIGS} = -7.14 \pm .01$ $\frac{1}{80K}$ per slice 16 slices

For $\frac{1}{40K}$ per slice 8 slices
$-7.18 \pm .01$ ⇒ Below correct energy because we use $\langle -\partial/\partial\tau \rangle$ instead of H.

GFMC R.B. Whitlock + Panoff $-21.59 \pm .09$
DMC Moroni et al. $-21.19 \pm .02$

PIGS PE = $-21.48 \pm .03$


Potential Energy
V
tau (K^-1)
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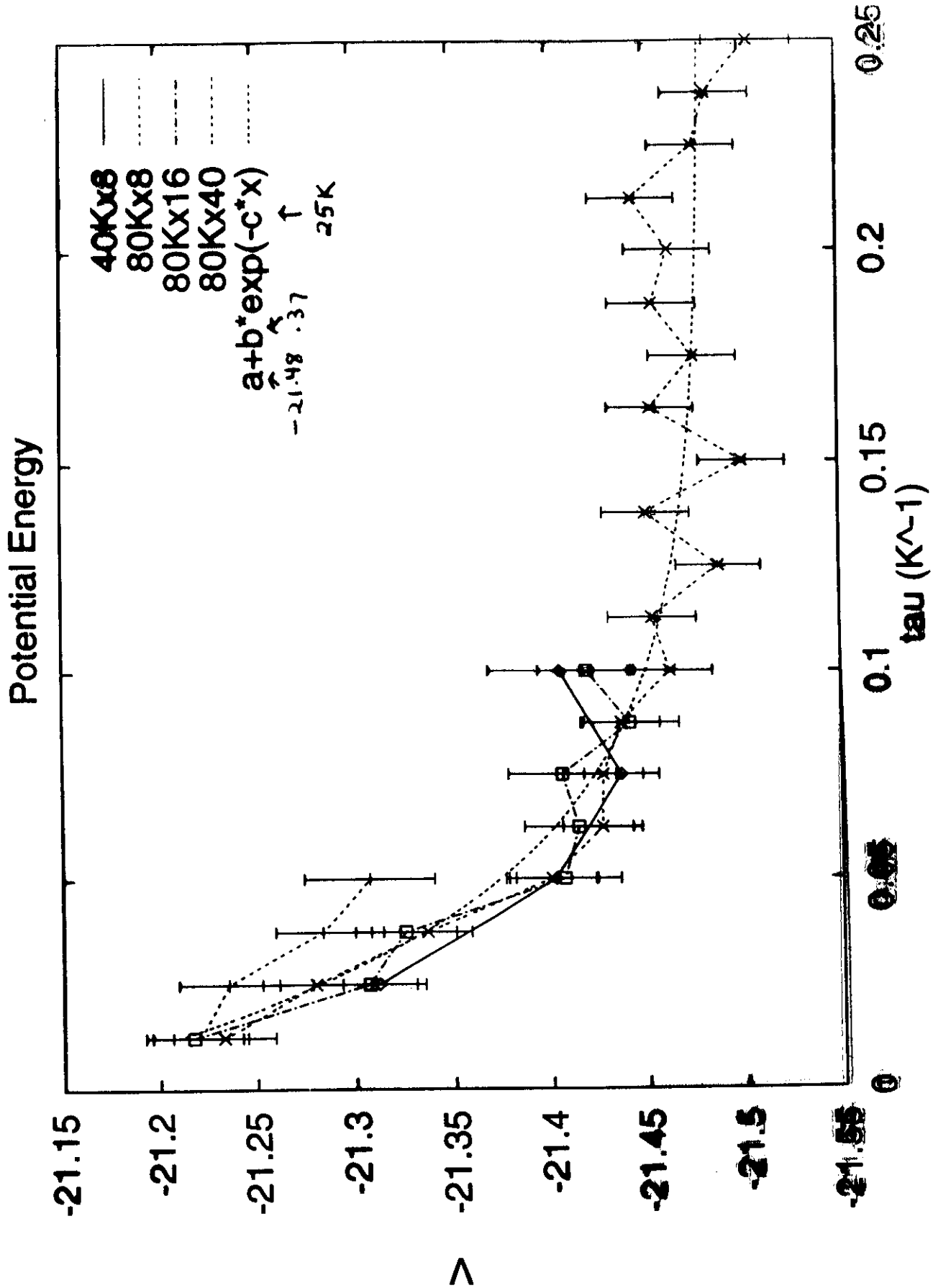
80Kx8
80Kx16
80Kx40
-21.15
-21.2
-21.25
-21.3
-21.35
-21.4
-21.45
-21.5
-21.55
0
0.1
0.15
0.2
0.25


Potential Energy
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80Kx8
80Kx16
80Kx40
a+b*exp(-c*x)
-21.48
.37
25K
V
tau (K^-1)
-21.15
-21.2
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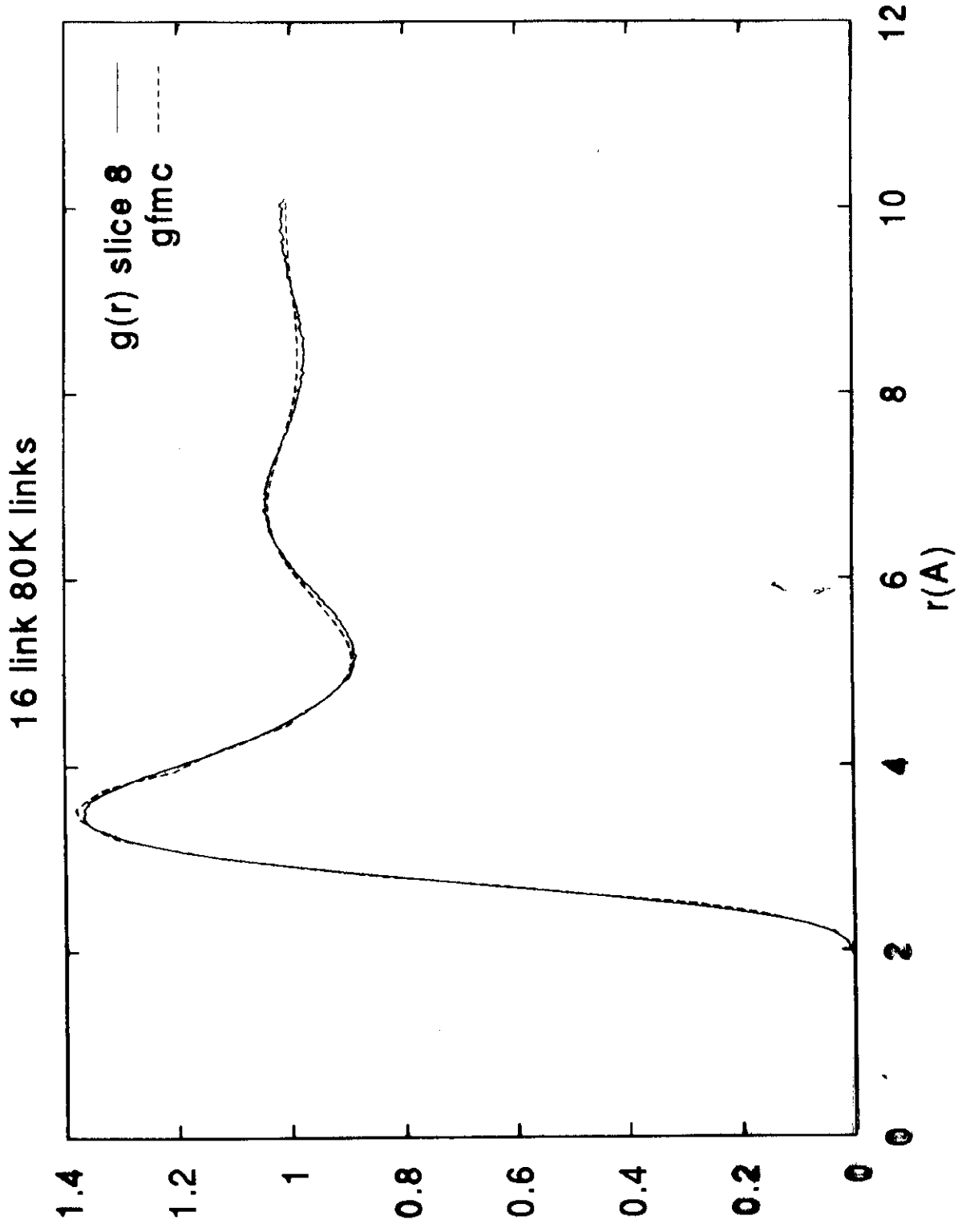
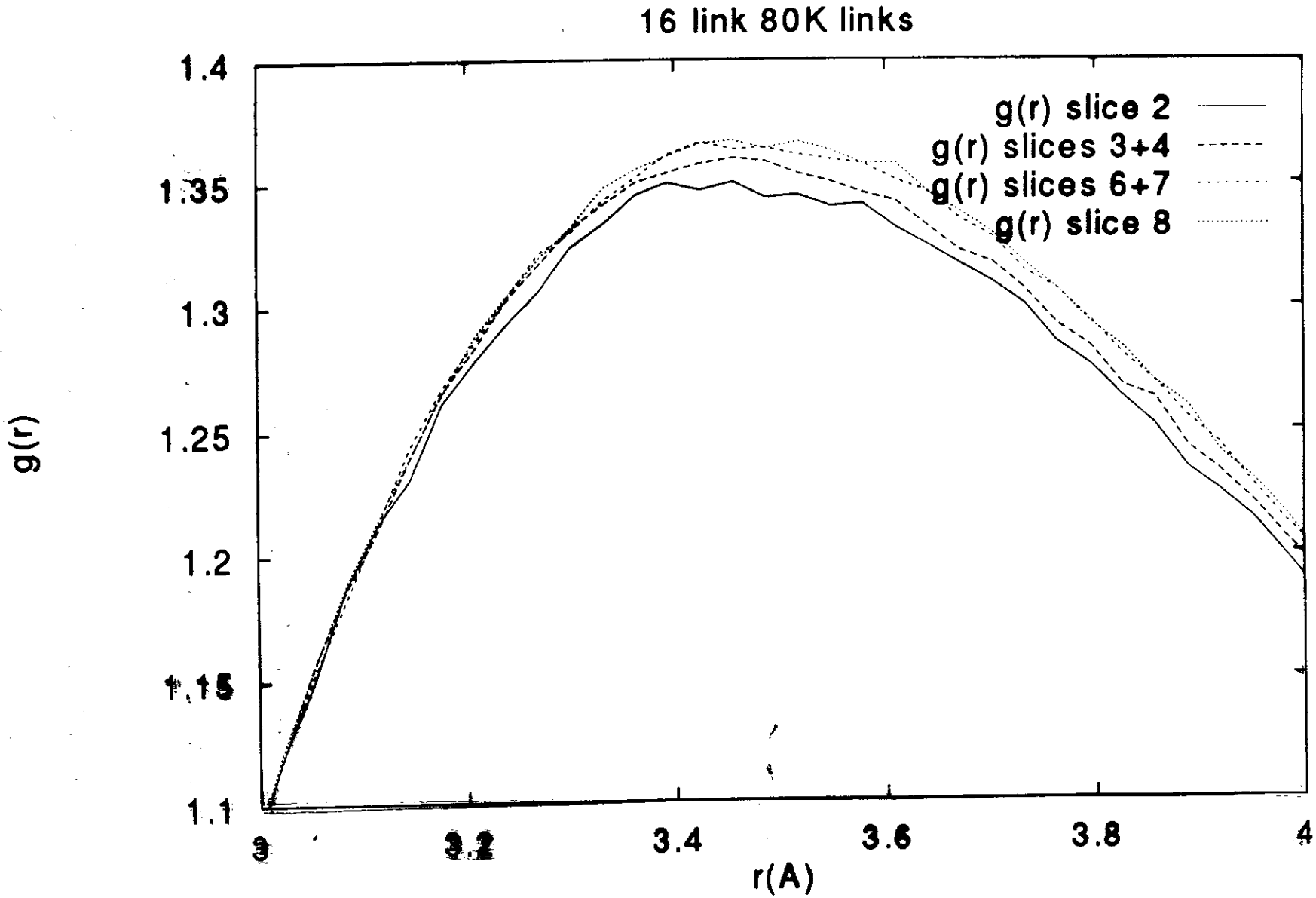

16 link 80K links
g(r) slice 8
gfmc
1.4
1.2
1
0.8
0.6
0.4
0.2
0
0
2
4
6
8
10
12
r(A)
g(r)

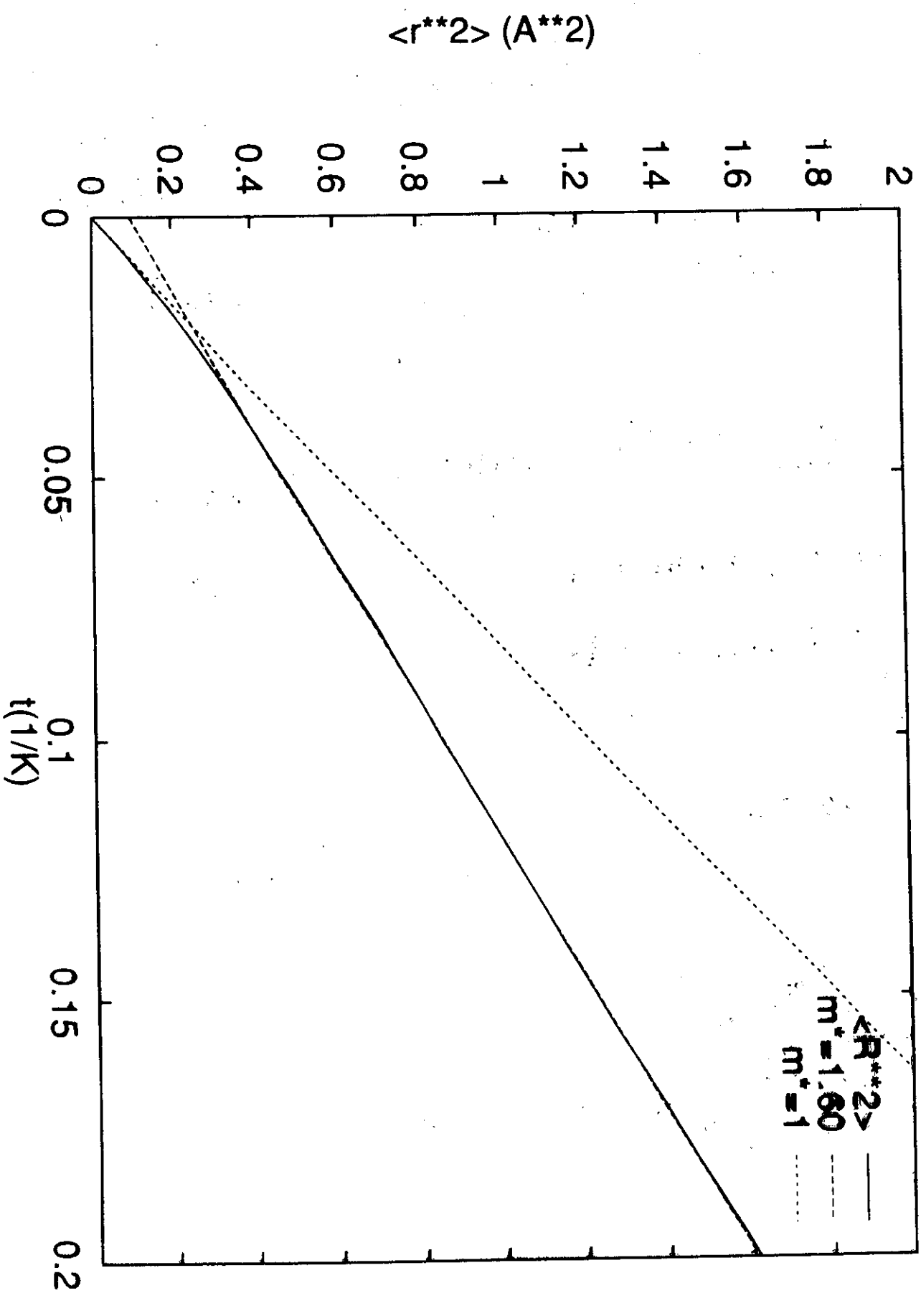

16 link 80K links
g(r) slice 2
g(r) slices 3+4
g(r) slices 6+7
g(r) slice 8
g(r)
r(A)
1.4
1.35
1.3
1.25
1.2
1.15
1.1
3
3.2
3.4
3.6
3.8
4

Convergence is good within $\frac{1}{5K}$

The decay rate is consistent with the lowest energy $P=0$ eigenvalues.

2 phonons of wavevector $\frac{2\pi}{L}$ or

2 rotons $\approx 2K$.


<r**2> (A**2)
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
2
0
0.05
0.1
0.15
0.2
t(1/K)
<R**2>
m*=1.60
m*=1

Solid ^4He 108 Particles FCC

PIGS Wave Function taken from Shadow calculations; A Jastrow that solidifies

$$E_{GFMC} = \begin{cases} -2.68 \pm .06 & \text{Kalos et al} \\ -2.70 \pm .06 & \text{Whitlock + Panoff.} \end{cases}$$

$E_{PIGS} = -2.68 \pm .03$ $\frac{1}{80K}$, 16 slices and 24 slices.

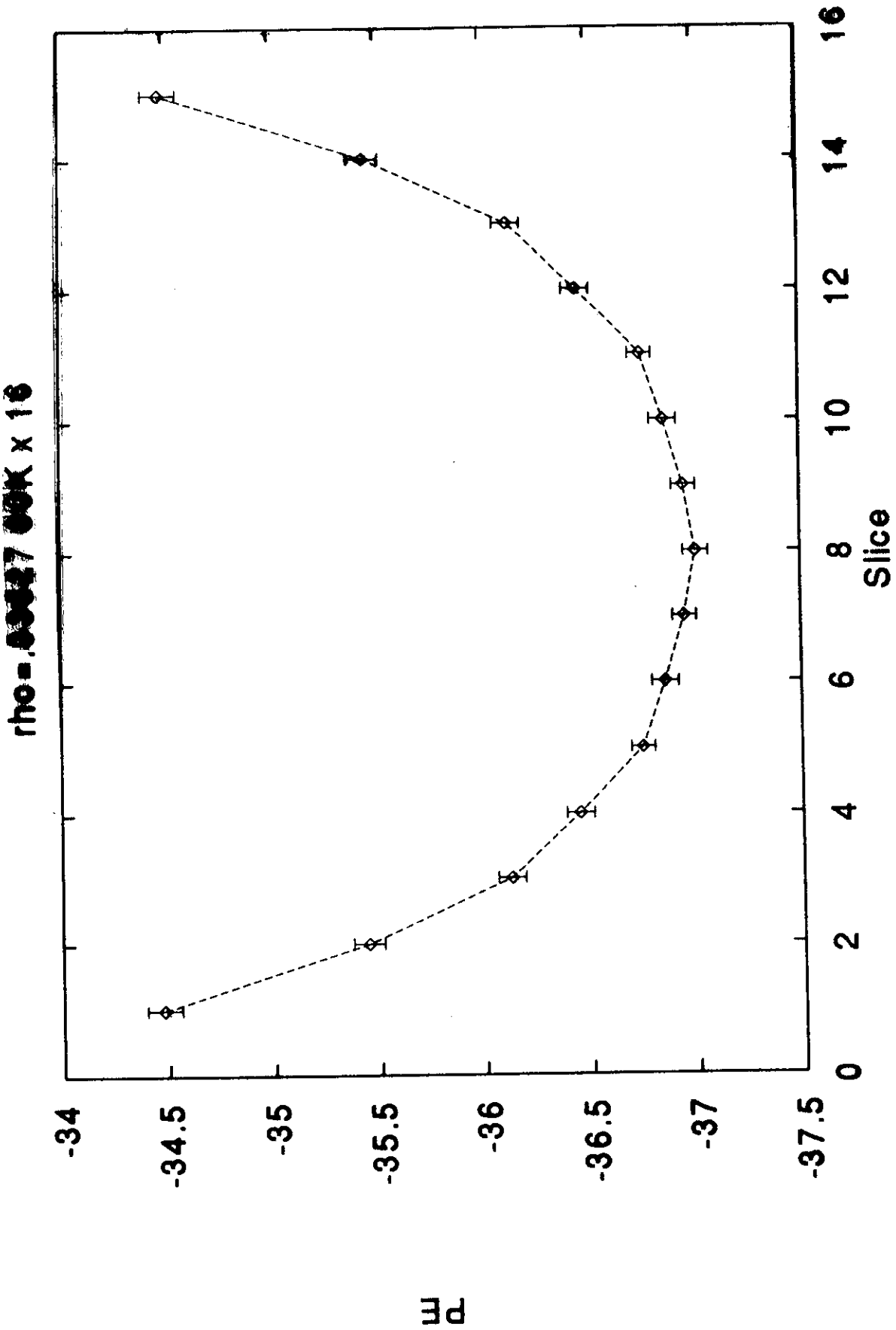
$\Psi_T = e^{-\frac{1}{2}(b/r)^m}$ $b = 2.61 \text{ Å}$, $m = 9$

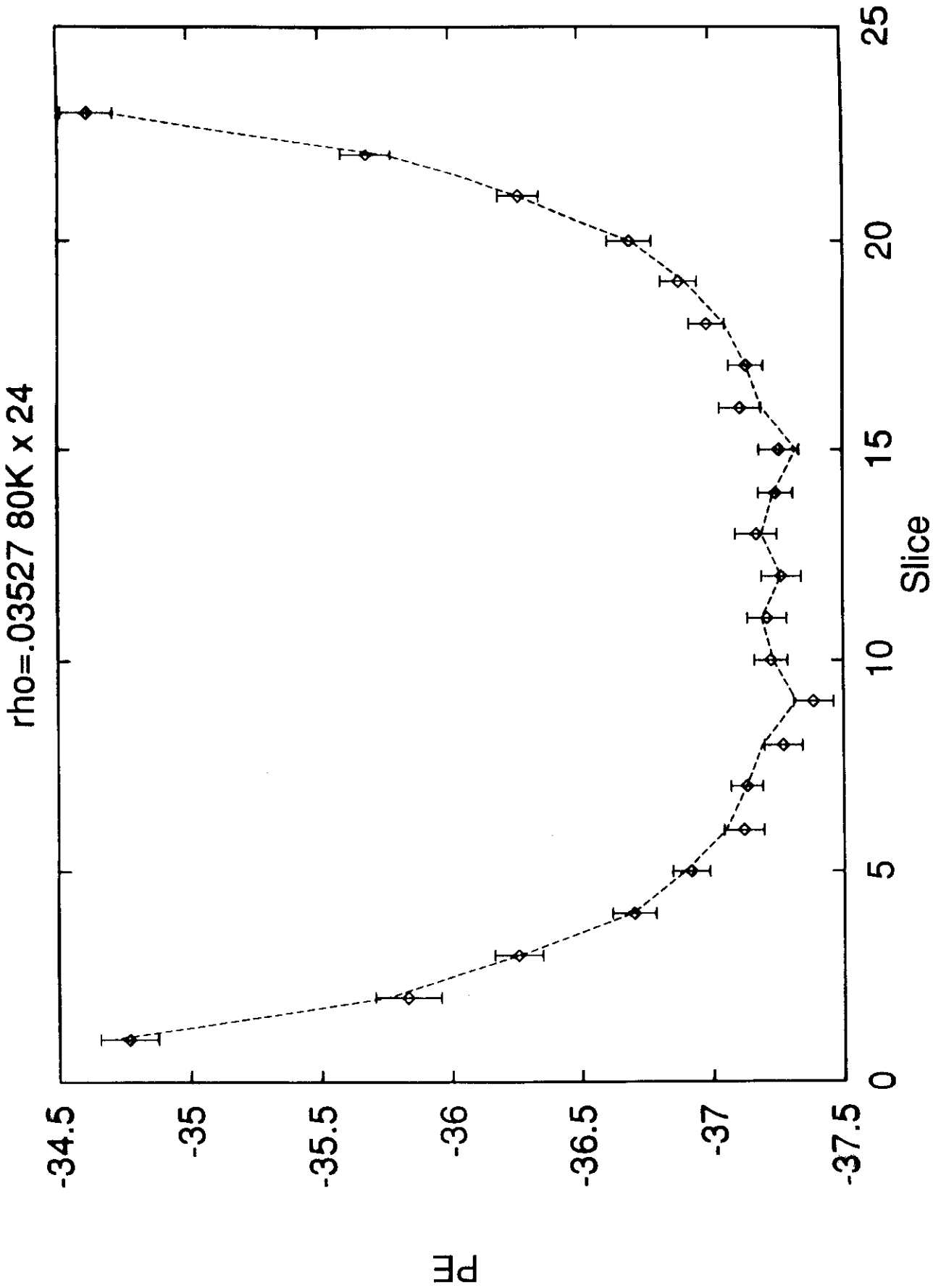
$E_V \approx 11K$ ← Very Poor Energy.

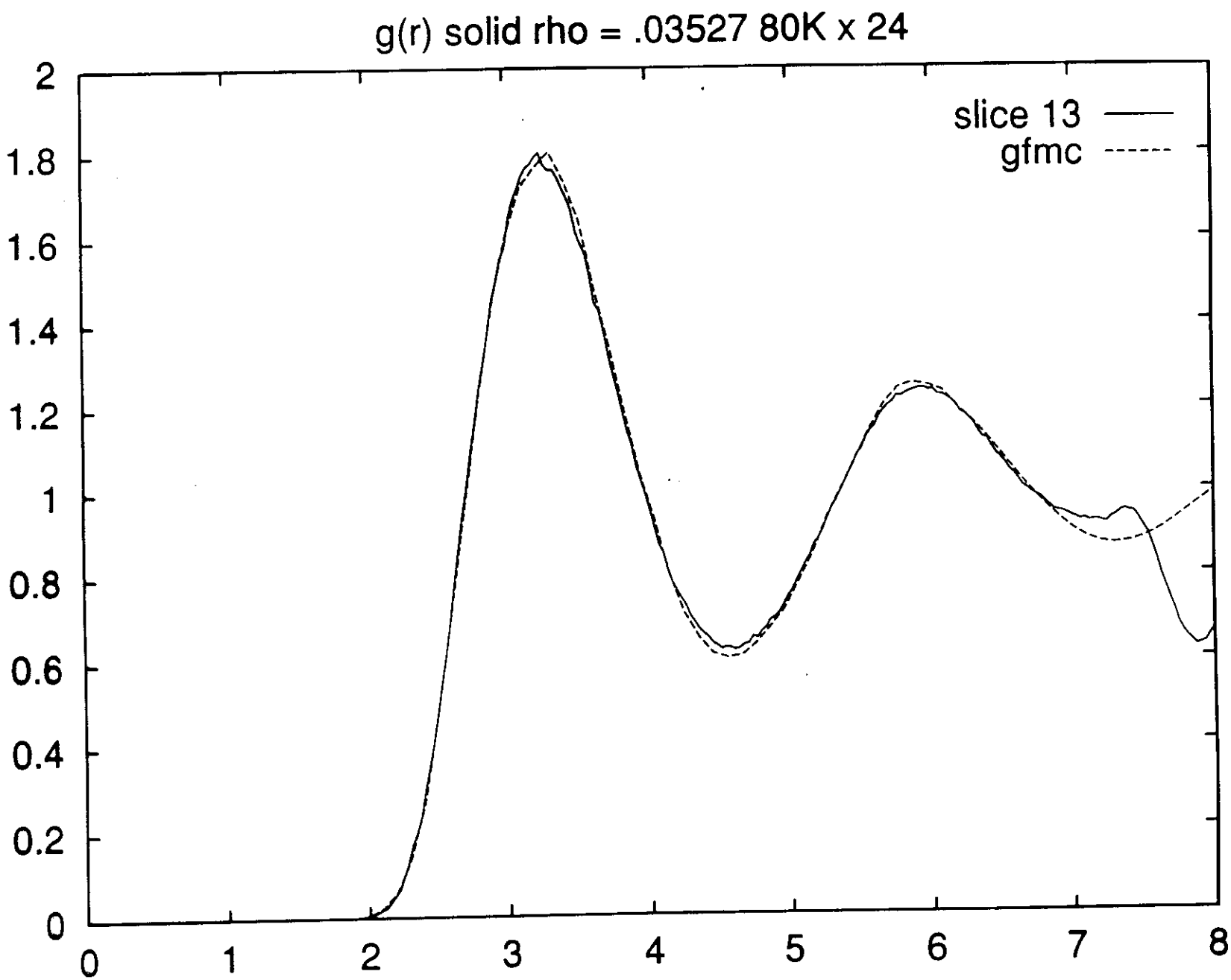
$V_{PIGS} = \frac{1}{80K}$ 24 slices $= -37.30 \pm .05$

$V_{GFMC} = -36.0 \pm .1$ ← Whitlock + Panoff (But Paula thinks the number is not correct)

$= -37.0 \pm ?.1$ ← My calculation based on gcrl from Kalos et al.


rho=.8
x 16
-34
-34.5
-35
-35.5
-36
-36.5
-37
-37.5
0
2
4
6
8
10
12
14
16
Slice
πd


rho=.03527 80K x 24
PE
Slice
-34.5
-35
-35.5
-36
-36.5
-37
-37.5
0
5
10
15
20
25


g(r) solid rho = .03527 80K x 24
slice 13
gfmc
2
1.8
1.6
1.4
1.2
1
0.8
0.6
0.4
0.2
0
0
1
2
3
4
5
6
7
8

Conclusion

1. PIGS Gives an easy way to calculate ground state expectations. Computing resources are roughly equivalent to GFMC

2. No Extrapolations

3. Crude Wave functions work, so systems like strongly bound clusters etc. [redacted] can be done without devising good variational functions.