UNITED NATIONS EDUCATIONAL, SCIENTIFIC AND CULTURAL ORGANIZATION
INTERNATIONAL ATOMIC ENERGY AGENCY
INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS
I.C.T.P., P.O. BOX 586, 34100 TRIESTE, ITALY, CABLE: CENTRATOM TRIESTE

SMR.998a - 24

Research Workshop on Condensed Matter Physics
30 June - 22 August 1997
MINIWORKSHOP ON
QUANTUM MONTE CARLO SIMULATIONS OF LIQUIDS AND SOLIDS
30 JUNE - 11 JULY 1997
and
CONFERENCE ON
QUANTUM SOLIDS AND POLARIZED SYSTEMS
3 - 5 JULY 1997

"The diffusion Monte Carlo algorithm"

S.A. CHIN
Texas A&M University
Department of Physics
College Station
TX 77843-4242
U.S.A.

These are preliminary lecture notes, intended only for distribution to participants.

The Diffusion Monte Carlo Algorithm

— A tutorial

Siu A. Chin
Center for Theoretical Physics
Department of Physics
Texas A+M University

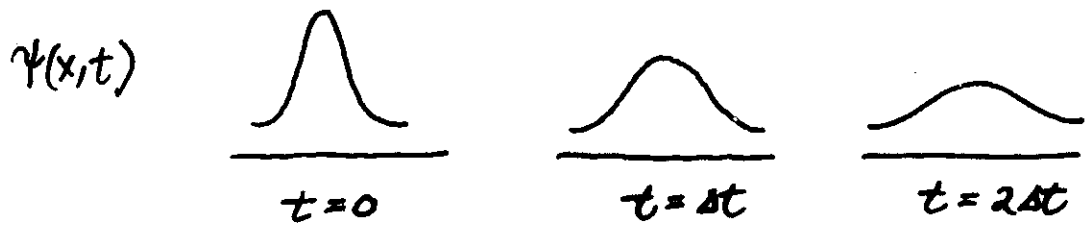
Content:

I. The Intuitive Idea – a biological analog.

Consider a "primitive" life form that can move and reproduce. Let $\psi(x,t)$ denotes its population density distribution at time t.

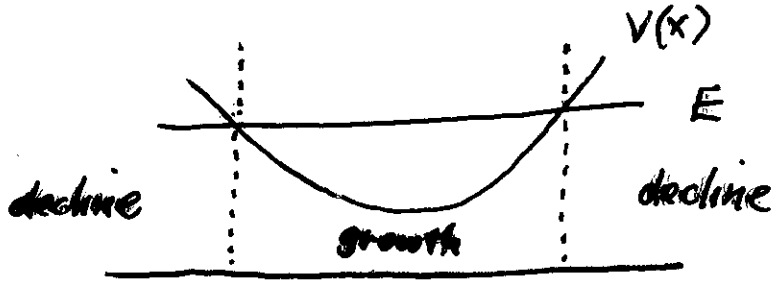
a) Mobility – aimless random walks $\Rightarrow$ diffusive motion

$$\frac{\partial}{\partial t}\psi(x,t) = \frac{1}{2}\nabla^2\psi(x,t)$$



b) Reproduction – replicate according to internal "metabolism" rate E and environmental "stress" distribution $V(x)$.

$$\frac{\partial}{\partial t}\psi(x,t) = [E - V(x)]\psi(x,t)$$



Questions: 1) For a given environment $V(x)$, for what metabolism rate E is the population sustainable over time?

2) If the population can evolve by collectively adjusting its metabolism rate E, what would be its long time population distribution?

Answers: The population evolves according to

$$\frac{\partial}{\partial t}\psi(x,t) = \frac{1}{2}\nabla^2\psi(x,t) + [E - V(x)]\psi(x,t)$$

$$= (E - H)\psi(x,t)$$

where

$$H = -\frac{1}{2}\nabla^2 + V(x)$$

The evolution in time, given that $\psi(x,0) = \phi_0(x)$, is

$$\psi(x,t) = \sum_n c_n \, e^{(E-E_n)t} \psi_n(x)$$

where $H\psi_n(x) = E_n \psi_n(x)$ and $c_n = \langle \psi_n | \phi_0 \rangle$.

$$\Rightarrow \underset{t\to\infty}{\psi(x,t)} \to c_0 e^{(E-E_0)t} \psi_0(x) + \cdots$$

Sustainable population only possible for $E = E_0$,

and $\underset{t\to\infty}{\psi(x,t)} \propto \psi_0(x)$.

Thus turning the argument around, the ground state energy E_0 and wavefunction $\psi_0(x)$ of H can be obtained by simulating the evolution of a population of "primitive life form" (point particles) with positions $\{x_1, x_2, \cdots x_N\}$:

a) Diffusion: $\frac{\partial}{\partial t}\psi(x,t) = \frac{1}{2}\nabla^2\psi(x,t)$

$$\Rightarrow \psi(x',t+\Delta t) = \int dx \frac{1}{\sqrt{2\pi\Delta t}} e^{-\frac{1}{2\Delta t}(x'-x)^2}\psi(x,t)$$

$$\Rightarrow \quad x_i \to x_i + \xi\sqrt{\Delta t}$$

ξ: Gaussian random numbers unit.

$\langle \xi \rangle = 0 \; ; \; \langle \xi^2 \rangle = 1$

b) Replication: $\frac{\partial}{\partial t}\psi(x,t) = [E - V(x)]\psi(x,t)$

$$\Rightarrow \psi(x,t+\Delta t) = \underbrace{e^{[E-V(x)]\Delta t}}_{\text{local growth factor} = m}\psi(x,t)$$

(multiplicity)

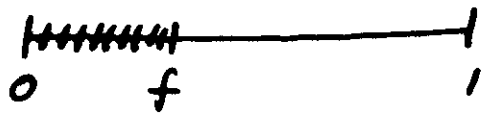
Duplicate each x_i,

$$m_i = e^{[E-V(x_i)]\Delta t} \text{ times},$$

treating the fractional part of m_i as a probability for duplication.

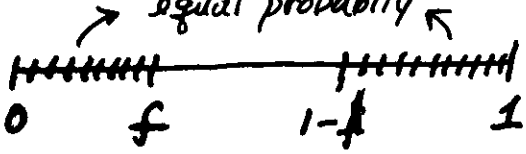
i.e., let $m = I + f$
(I: integer, f: fraction)

Roll a continuous "dice", draw r, a random number number uniformly distributed in $[0,1]$.



If $r \leq f$: replicate $I+1$ times
$r > f$: " I "

Note :



If $r \geq 1-f$: replicate $I+1$ times
$r < 1-f$: " I " } replicate $\underbrace{I + INT[f+r]}_{INT[m+r]}$ times

Replicate each $x_i \rightarrow \underbrace{x_i, x_i, \cdots x_i}_{INT[m_i+r]}$ times

Remarks : 1) A stationary state is a state of dynamic equilibrium between the competing process of diffusion and replication.

2) Distributions not constrained by $V(x)$ will "diffuse away."

c) Stablizing the population: change E so that the population is stabilized around a target value of N_T.

Assume that at $E = E_0$, the population is stable at a size N_T. If now E is changed to E_i, then the population is then changed to

$$N_i = N_T e^{(E_i - E_0)\Delta t},$$

$$\Rightarrow \quad E_0 = E_i - \frac{1}{\Delta t} \ln\left(N_i / N_T\right)$$

$$\Rightarrow \quad E_i' = E_i - \frac{1}{\Delta t} \ln\left(N_i / N_T\right)$$

$\uparrow$ new estimate for E_0

Better yet $\quad E_i' = \overline{E_i} - \frac{1}{\Delta t} \ln\left(N_i / N_T\right)$

$\uparrow$ continously averaged estimate for $E_0 = E_N$

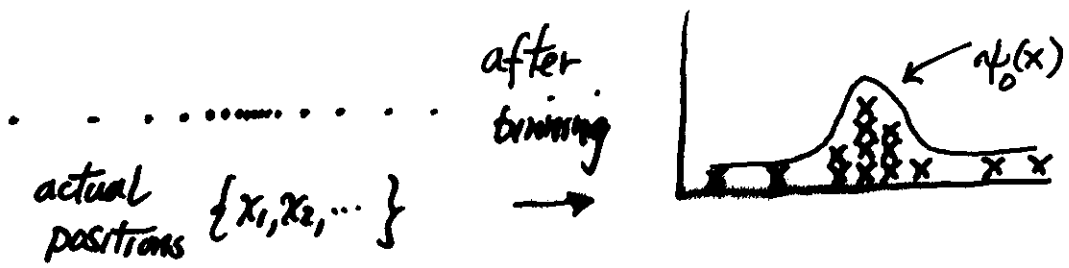
E_N = the growth or normalization estimate for E_0.

d) Ground state wavefunction

$$\psi_0(x) \approx \frac{1}{N}\sum_{i=1}^{N}\delta(x-x_i),$$

in that $\int_x^{x+\Delta x}\psi_0(x')dx' \simeq \psi_0(x)\Delta x \simeq \frac{1}{N}n_i$ ← # of particles in $[x, x+\Delta x]$

$$\Rightarrow \psi_0(x) = \frac{1}{N}\frac{n_i}{\Delta x} \leftarrow \text{normalized density}$$



The ground state energy can also be directly computed from $\psi_0(x)$ via

← some analytic trial function for the ground state

$$E_0 = \frac{\langle\phi_0|H|\psi_0\rangle}{\langle\phi_0|\psi_0\rangle}$$

$$= \frac{\langle H\phi_0|\psi_0\rangle}{\langle\phi_0|\psi_0\rangle}$$

$$\approx \frac{N\sum_i H\phi_0(x_i)}{N\sum_i \phi_0(x_i)} = E_T$$

↓ biased trial estimate of the ground state energy

I. Importance Sampling (M. Kalos)

Defects of the previous naive DMC algorithm:

1) Aimless random walk is inefficient.

2) Population fluctuation with using the bare $V(x)$ is uncontrollable with realistic potentials.

3) E_T is a biased estimator.

Remedy: Instead of simulating the evolution of $\psi(x,t)$, simulate that of $f(x,t) = \phi_0(x)\psi(x,t)$. ← trial ground state

$$\Rightarrow \underset{t\to\infty}{f(x,t)} = \phi_0(x)\psi_0(x)$$

$$E_T = \frac{\langle H\phi/\psi\rangle}{\langle\phi/\psi\rangle} = \frac{\langle \phi^{-1}H\phi/\phi\psi\rangle}{\langle\phi/\psi\rangle}$$

$$= \frac{1}{N}\Sigma_i\, \phi^{-1}H\phi(x_i) \quad \text{unbiased}$$

The evolution of $f(x,t)$ is governed now by

$$\frac{\partial f}{\partial t} = \phi\frac{\partial \psi}{\partial t} = \phi_0\left[\tfrac{1}{2}\nabla^2 + E - V(x)\right]\psi \qquad \text{since } \phi_0\nabla^2\psi = \nabla^2(\phi_0\psi) - 2\vec{\nabla}\cdot(\psi\vec{\nabla}\phi_0) + \psi\nabla^2\phi_0$$

$$= \tfrac{1}{2}\nabla^2 f - \vec{\nabla}\cdot(\vec{v}(x)f) + \left[E - \phi_0^{-1}H\phi_0(x)\right]f$$

where $v(x) = \vec{\nabla}\phi/\phi_0 = -\vec{\nabla}S$ if $\phi_0 = e^{-S}$ $\qquad \phi_0^{-1}H\phi_0 = E_L(x)$ Local energy

Replicate according to $e^{\Delta t[E - \phi_0^{-1}H\phi_0(x_i)]}$;

If $\phi_0 \to \psi$, $\phi_0^{-1}H\phi_0(x_i) \to E_0$, a constant

no population fluctuation. In general, fluctuation is reduced.

Random walks according to

$$\frac{\partial \rho}{\partial t} = \frac{1}{2}\nabla^2 \rho - \vec{\nabla}\cdot(\vec{v}(x)\rho) \qquad \text{Fokker-Planck}$$

If $\vec{v}(x)$ is interpreted as an external velocity field, then $\rho\vec{v} = \vec{J}$ is the current density. The new term

$$\frac{\partial \rho}{\partial t} = -\vec{\nabla}\cdot\vec{J}$$

is just the equation of continuity. It can be easily simulated by

$$x_i \to x_i + v(x_i)\Delta t$$

Thus Fokker-Planck give rises to

$$x_i \to x_i + \xi\sqrt{\Delta t} + v(x_i)\Delta t \qquad \text{Langevin algorithm}$$

i.e. the random walk is now guided by the trial function, being "blown" by it.

By itself, the Langevin algorithm will converge to

$$\rho(x,t) \xrightarrow[t\to\infty]{} \phi_0^2(x)$$

since $0 = \frac{1}{2}\nabla^2\rho - \vec{\nabla}\cdot(\vec{v}\rho)$

$$\frac{\vec{\nabla}\rho}{\rho} = 2\vec{v} = 2\frac{\vec{\nabla}\phi_0}{\phi_0}$$

Replication change this to

$$\rho(x,t) \to \phi_0^2(x)\,\phi_0(x)/\phi_0(x) = \phi_0(x)\psi_0(x)$$

Computing Expectation Values

Knowing only $\Psi_0\Psi_0$, for any observable other H, one can only compute the mixed expectation value $\langle\Phi_0|\Theta|\Psi_0\rangle$. However, for $\Phi_0 = \Psi_0 + \epsilon$ ← small error

$$\langle\Phi_0|\Theta|\Psi_0\rangle = \langle\Psi_0|\Theta|\Psi_0\rangle + \langle\epsilon|\Theta|\Psi_0\rangle$$

$$\langle\Phi_0|\Theta|\Phi_0\rangle = \langle\Psi_0|\Theta|\Psi_0\rangle + 2\langle\epsilon|\Theta|\Psi_0\rangle + O(\epsilon^2)$$

$$\Rightarrow \quad \langle\Psi_0|\Theta|\Psi_0\rangle = 2\langle\Phi_0|\Theta|\Psi_0\rangle - \langle\Phi_0|\Theta|\Phi_0\rangle + O(\epsilon^2)$$

This is the state of DMC as of

Reynolds, Ceperly, Alder, Lester, J. Chem. Phys. 77 (1982) 5593.
Moskowitz, Schmidt, Lee, Kalos, " " " 77 (1982) 349.

For a rephrasing,

Chin, Negele, Koonin, Ann. Phys. (N.Y.) 157 (1984) 140.

All are, however, unsatisfactory in discussing the systematic error due to the discretized step size Δt.

Consistency checks:

1) Do the variational calculation with $\phi = e^S$

$$\int \phi \nabla^2 \phi = -\int (\vec{\nabla}\phi)\cdot(\vec{\nabla}\phi)$$

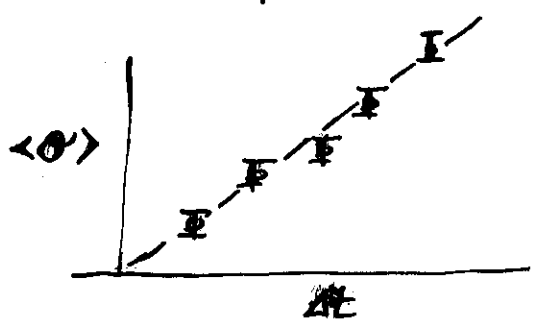
$$\Rightarrow \int [\nabla^2 S + (\vec{\nabla} S)^2]\phi^2 = -\int (\vec{\nabla} S)^2 \phi^2$$

or $$\int [\nabla^2 S]\phi^2 = -2\int (\vec{\nabla} S)^2 \phi^2$$

This equality checks various derivatives and correct Metropolis sampling.

2) Do the Langevin simulation without replication. Should converges to the variational result as $\Delta t \to 0$. This checks the gradient $\vec{\nabla} S$ calculation and the Langevin algorithm.

3) Check Δt step size convergence.



4) Check trial function sensitivity.

DMC results should not be too sensitive to the fine details of the trial function. Should de-optimize and see that DMC results are independent of the choice of variational parameters.

III) Operator form and QDMC (SAC, Phys. Rev. A 42 (1990) 6991)

The intuitive picture of evolution in continous time obscures the nature of the time step-size error and does not correspond to what one does in practice. In practice one iterates.

a) The Perron-Frobenius Thm:

$$\text{If } T > 0 \text{ then } \lim_{n\to\infty} T^n \to \lambda^n \Psi_R$$

(T: transfer matrix; λ: largest eigen value; Ψ_R: associate right eigen vector)

b) Let $T = e^{\Delta t[E-H]}$

$$\lim_{n\to\infty} T^n \longrightarrow e^{\Delta t[E-E_0]} \psi_0(x)$$

(E_0: Lowest eigen value and ψ_0: eigen state of H)

One cannot iterate T directly, but only some approximate T', i.e.

$$T' = e^{\Delta t \frac{1}{2}\nabla^2} e^{\Delta t [E - V(x)]}$$

with matrix element

$$\langle x'|T|x\rangle = \sqrt{\quad} e^{-\quad (x'-x)^2} e^{\Delta t(E - V(x))}$$

Iterating this stochastically gives the naive DMC algorithm

c) To determine the step-size error, one can reconstitute T' in the form $T' = e^{\Delta t[E - H']}$ and study the ground state and energy of H' perturbatively

$$H' = H - \underbrace{\tfrac{1}{2}\Delta t\,[H,V] + \cdots}_{\text{perturbation}}$$

CBH: $e^A e^B = e^{A+B+\frac{1}{2}[A,B]+\cdots}$

To order Δt, since by inspection

$$H' \simeq e^{\frac{1}{2}\Delta t V} H e^{-\frac{1}{2}\Delta t V}$$

if

$$H'\psi' = e^{\frac{1}{2}\Delta t V} H e^{-\frac{1}{2}\Delta t V}\psi' = e^{\frac{1}{2}\Delta t V} H \psi_0 = E_0 \psi_0'$$

$$\psi_0' \simeq e^{\frac{1}{2}\Delta t V}\psi_0 \simeq \psi_0 + \tfrac{1}{2}\Delta t\, V\psi_0$$

$$E_T \simeq E_0 + \tfrac{1}{2}\Delta t\,\frac{\langle\phi_0|\,[H,V]\,|\psi_0\rangle}{\langle\phi_0|\psi_0\rangle}$$

d) Importance sampling corresponds to the study of

$$\tilde{T} = \phi_0\, e^{\Delta t[E-H]}\phi_0^{-1}$$ Similarly transformed

$$= e^{\Delta t[E-\tilde{H}]}$$

$$\tilde{H} = \phi_0 H \phi_0^{-1} = \underbrace{\underbrace{-\tfrac{1}{2}\nabla^2}_{K} + \underbrace{\vec{\nabla}\cdot(\vec{v}\ )}_{D\ (\text{drift})}}_{L\ (\text{Langevin})} + E_L(x)$$

$$\langle x'|e^{-\Delta t D}|x\rangle = \delta(x' - x(\Delta t)) \quad \text{with} \quad \dot{x}(t) = v(x)$$

e) Linearly convergent DMC

$$\tilde{T}' = e^{-\Delta t L}\, e^{\Delta t (E - E_L)}$$

$$= \underbrace{e^{-\Delta t K}}_{\text{walk}}\ \underbrace{e^{-\Delta t D}}_{\text{drift}}\ \underbrace{e^{\Delta t (E - E_L)}}_{\text{replicate}}$$

f) Quadratically convergent DMC

$$\tilde{T}' = e^{\frac{1}{2}\Delta t (E - E_L)}\, e^{-\Delta t L}\, e^{\frac{1}{2}\Delta t (E - E_L)}$$

$$\simeq e^{\frac{1}{2}\Delta t (E - E_L)}\ \underbrace{e^{-\frac{1}{2}\Delta t K}\, e^{-\Delta t D}\, e^{-\frac{1}{2}\Delta t K}}_{\text{quadratically convergent Langevin}}\ e^{\frac{1}{2}\Delta t (E - E_L)}$$

+ other decomposition

g) Even higher order DMC ?

M. Suzuki's (1993) no-go theorem

$$e^{\frac{1}{2}\Delta t A}\, e^{\frac{1}{2}\Delta t B}\, e^{\frac{1}{2}\Delta t A} = e^{\Delta t (A + B + O(\Delta t^2))}$$

(positive coefficients on the left; these type of)

For higher order decomposition, some coefficients must be negative.

New 4th order decompositions

IV) A DMC algorithm with rejection: (Reynold et al. / Chester et al.)

Enforce detail-balance on the 1st order Langevin moves so that the algorithm exactly samples Ψ_0^2 without any Δt step-size error. (What is its effect on DMC?)

Rederiving the Metropolis algorithm (Chin) (No Markov chain!)

Basic ideas: 1) Device "artificial dynamics" so that particles will come to equilibrium at a pre-determined distribution $\rho_e(x)$.

2) The "dynamics" need not be deterministic (i.e. Newtonian) but can be probabilistic, just like quantum mechanics. Let the dynamics be described by $P(x';x)$, the prob. of moving to x', if initially at x, in unit time.

How should we choose $P(x';x)$?

Requirements on $P(x';x)$:

i) $P(x';x) \geq 0$

ii) $\int dx' \, P(x';x) = 1$

Let $\rho_n(x)$ be the prob. density distribution of particles at time step n, then

$$\rho_{n+1}(x') = \int dx \, P(x';x) \rho_n(x).$$

We want $\lim_{n \to \infty} \rho_n(x) \to \rho_e(x)$ the prescribed equilibrium dist.

$\Rightarrow$ iii) $\rho_e(x') = \int dx \, P(x';x) \rho_e(x)$ stationary condition

$\Rightarrow$
- The dynamics must leave the eq. dist. invariant
- $\rho_e(x)$ is a "fixed point" (an attractor) of the dynamic
- The dynamics corresponds to iterating the continuous matrix $P(x';x)$: $\rho_n(x_n) = \int dx_{n-1} \cdots dx_2 dx_1 \, P(x_n, x_{n-1}) \cdots P(x_2, x_1) \rho_1(x_1)$
- $P(x';x)$ is not symmetric.

ii) $\Rightarrow$ 1 is the left eigenstate of $P(x';x)$ with eigenvalue 1

$$1\ 1 = \int dx'\ 1\ P(x';x)$$

iii) $\Rightarrow$ $\rho_e(x)$ is the right eigenstate of $P(x';x)$ with eigenvalue 1

$$\int dx\ P(x';x)\rho_e(x) = 1\ \rho_e(x')$$

i.e. $$\int dx\ P(x';x)\ R_n(x) = \lambda_n R_n(x')$$

$$\int dx'\ L_n(x')P(x';x) = \lambda_n L_n(x)$$

$\Rightarrow$ $P(x';x) = \sum_n \lambda_n R_n(x')L_n(x)$ with $\int dx\ R_n(x)L_m(x) = \delta_{nm}$

All other λ_n are < 1 !

"Proof": Let C be the max of $|L_n(x)|$

$$\left|\int dx' L_n(x')P(x';x)\right| < C \int dx' P(x';x) < C$$

$\Rightarrow$ $\lambda_n |L_n(x)| < C$ for any x, choose x such that $|L_n(x)| = C$

$\lambda_n < 1$

The iteration of $P(x';x)$ converges to its largest right eigenstate, $\rho_e(x)$.

Constructing $P(x';x)$:

In general, can write

$$P(x';x) = \underbrace{\left[1 - \int dx'' W(x'';x)\right] \delta(x';x)}_{\text{Probability for NOT moving}} + \underbrace{W(x';x)}_{\text{Probability for moving to } x' \text{ from } x \text{ (transition)}}$$

stationary condition

$$\rho_e(x') = \rho_e(x') + \int dx\, W(x';x)\rho_e(x) - \int dx'' W(x'';x')\rho_e(x')$$

$$= \rho_e(x') + \underbrace{\int dx \left[W(x';x)\rho_e(x) - W(x,x')\rho_e(x') \right]}_{\text{whole integral must vanish}}$$

Choose $W(x';x)$ such that the intergrand vanishes:

$$W(x';x)\rho_e(x) = W(x,x')\rho_e(x')$$

detail-balance condition >> stationary condition.

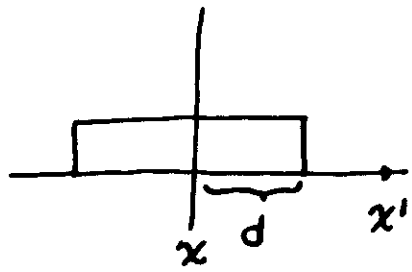
Choose $W(x';x)$ in the following way:

$$W(x';x) = A(x';x)\,T(x';x)$$

transition prob. — acceptance prob. ≤ 1 — trial move prob. $\int T(x';x)\,dx' = 1$

Take $T(x';x)$ to be symmetric $T(x';x) = T(x,x')$

(Box : $T(x';x) = \frac{1}{2d}$ if $|x'-x| < d$



or Gaussian : $T(x';x) = \frac{1}{\sqrt{2\pi\Delta t}} e^{-\frac{1}{2\Delta t}(x'-x)^2}$)

and let $P_e(x) = e^{-S(x)}$, detail-balance $\Rightarrow$
(S = action)

$$A(x';x)\, e^{-S(x)} = A(x,x')\, e^{-S(x')}$$

$$A(x';x) = A(x,x')\, e^{-\Delta S} \qquad \Delta S = S(x') - S(x)$$

Let $A(x';x)$ be a function of x', x only thru ΔS.

$$A(\Delta S) = A(-\Delta S)\, e^{-\Delta S}$$

or $$A(\Delta S)\, e^{\frac{1}{2}\Delta S} = A(-\Delta S)\, e^{-\frac{1}{2}\Delta S}$$

Detail-balance implies that

$$F(\Delta S) \equiv A(\Delta S)\, e^{\frac{1}{2}\Delta S}$$ must be even in ΔS!

i.e. the acceptance must be as

$$A(\Delta S) = e^{-\frac{1}{2}\Delta S} F(\Delta S) \leq 1 \qquad \text{with } F(\Delta S) \text{ even in } \Delta S$$

when $\underline{\Delta S < 0}$, $e^{-\frac{1}{2}\Delta S} > 1$, max. acceptance then requires

$$F(\Delta S) = e^{\frac{1}{2}\Delta S}$$

Since $F(\Delta S)$ must be even, an obvious choice is to take

$$F(\Delta S) = e^{-\frac{1}{2}|\Delta S|} \qquad \text{Metropolis derived}$$

This gives

$$A(\Delta S) = e^{-\frac{1}{2}(\Delta S + |\Delta S|)}$$

$$= \begin{cases} 1 & \text{if } \Delta S < 0 \\ e^{-\Delta S} & \text{if } \Delta S > 0 \end{cases}$$

$$= \frac{\rho_e(x')}{\rho_e(x)} < 1$$

$$= \min\left(1, \frac{\rho_e(x')}{\rho_e(x)}\right)$$

Other (less acceptance) choices for $F(\Delta S)$:

$$F(\Delta S) = \frac{1}{e^{\frac{1}{2}\Delta S} + e^{-\frac{1}{2}\Delta S}}, \quad \text{etc.}$$

Generalized Metropolis

For the case where $T(x';x)$ is NOT symmetric, such as the random walk + drift step in the Langevin algorithm:

$$T(x';x) = \frac{1}{\sqrt{2\pi\Delta t}}\, e^{-\frac{1}{2\sigma t}(x' - x - v(x)\Delta t)^2},$$

the imposition of detail-balance would make $T(x';x)$ exactly sample ϕ_0^2 for any value of Δt.

In this case

$$T(x';x)\,A(x';x) = T(x,x')\,A(x,x')\,e^{-\Delta S}$$

$$A(x';x) = A(x,x')\,\underbrace{\frac{T(x,x')}{T(x';x)}\,e^{-\Delta S}}_{e^{-\Delta U} \text{ defines } \Delta U}$$

$$A(x';x) = A(x,x')\,e^{-\Delta \tilde{S}} \qquad \Delta\tilde{S} \equiv \Delta S + \Delta U$$

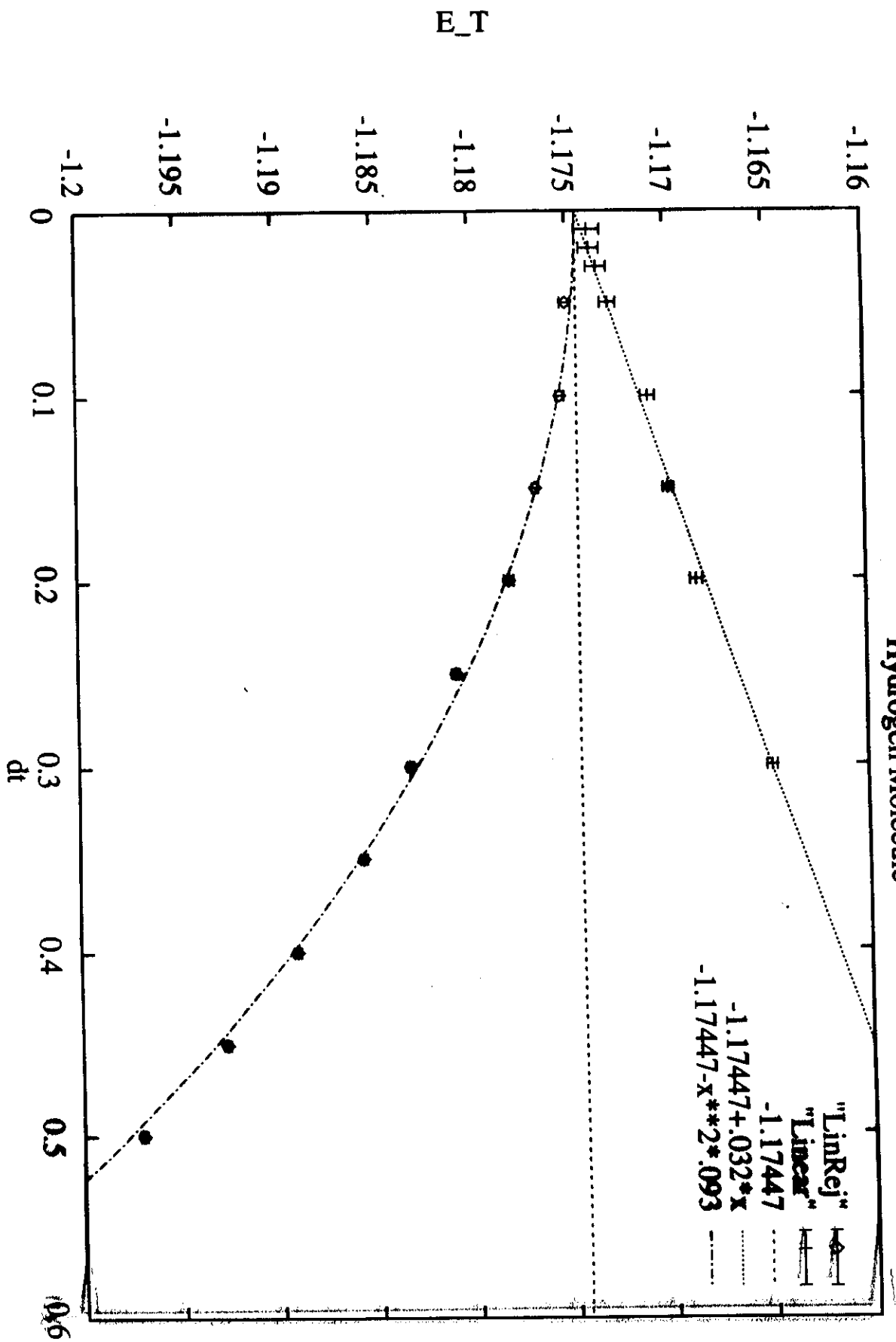
change in the effective action

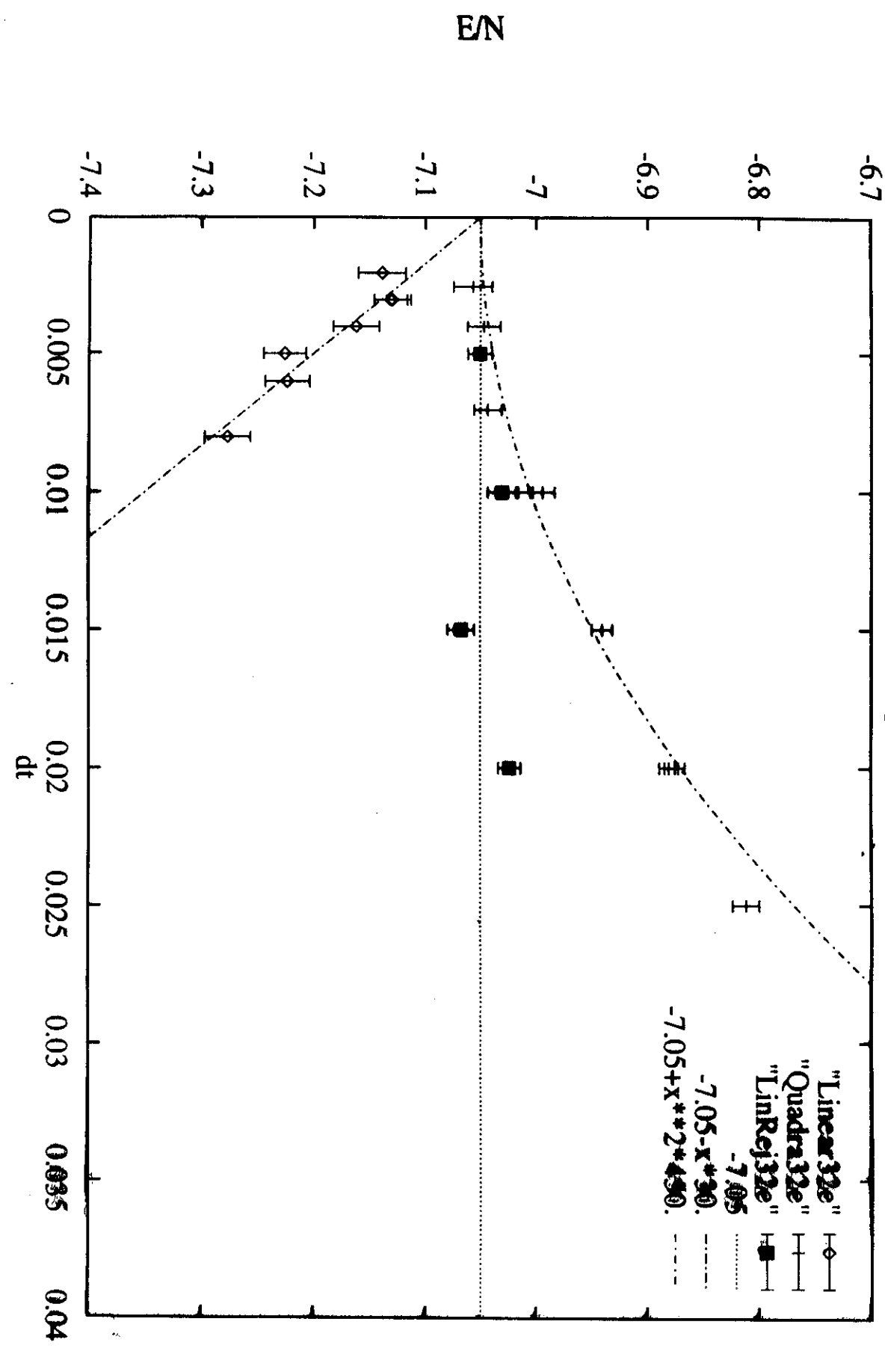
Exactly as before, gives

$$A(\Delta\tilde{S}) = e^{-\frac{1}{2}(\Delta\tilde{S} + |\Delta\tilde{S}|)}$$

$$= \min\left(1, \frac{T(x,x')\,\phi_0^2(x')}{T(x';x)\,\phi_0^2(x)}\right)$$

Some Langevin moves would then be rejected.


E_T
Hydrogen Molecule
"LinRej"
"Linear"
-1.17447
-1.17447+.032*x
-1.17447-x**2*.093
-1.16
-1.165
-1.17
-1.175
-1.18
-1.185
-1.19
-1.195
-1.2
0
0.1
0.2
0.3
0.4
0.5
0.6
dt



with only 32 particles.

17c

with only 32 particles

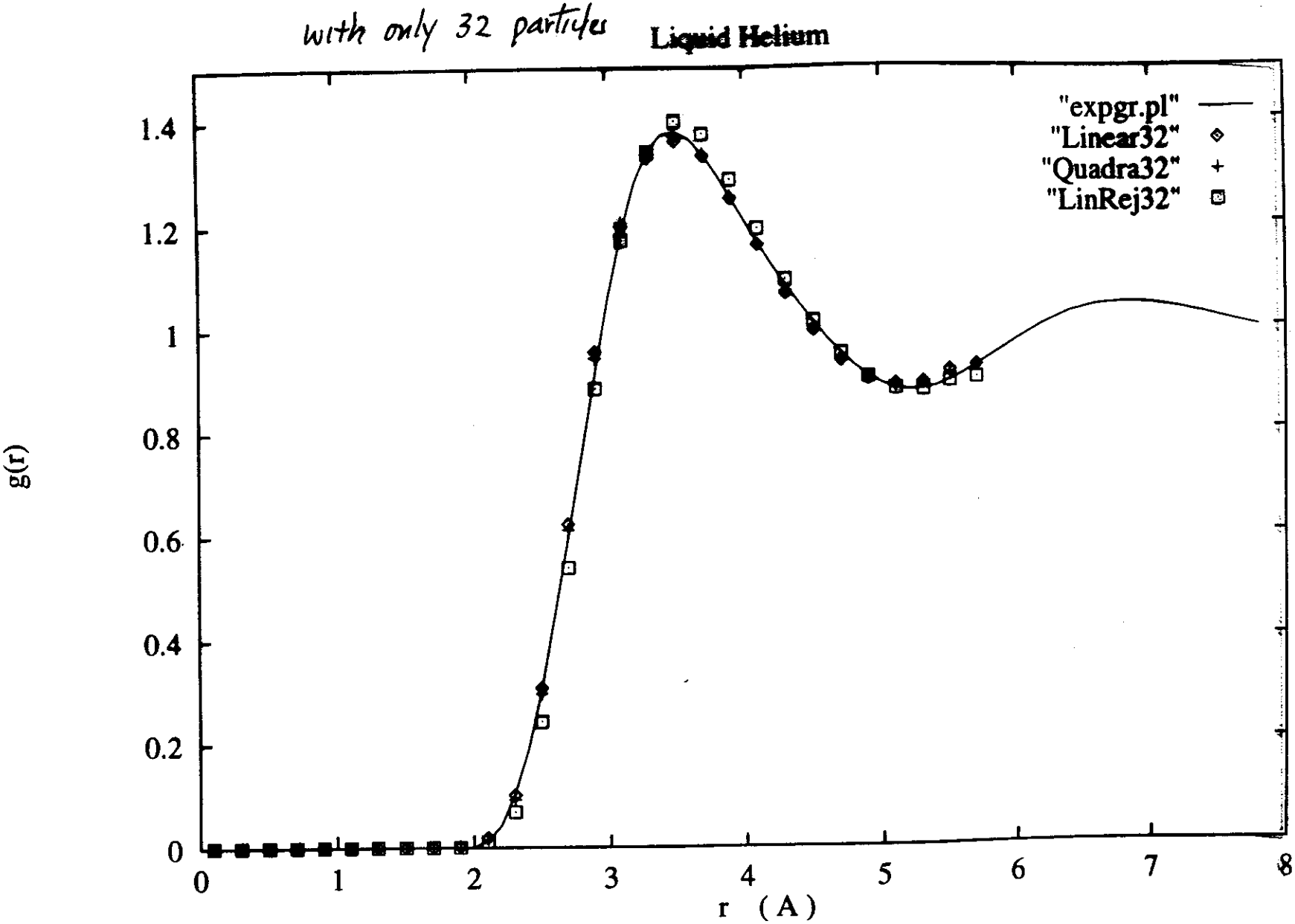
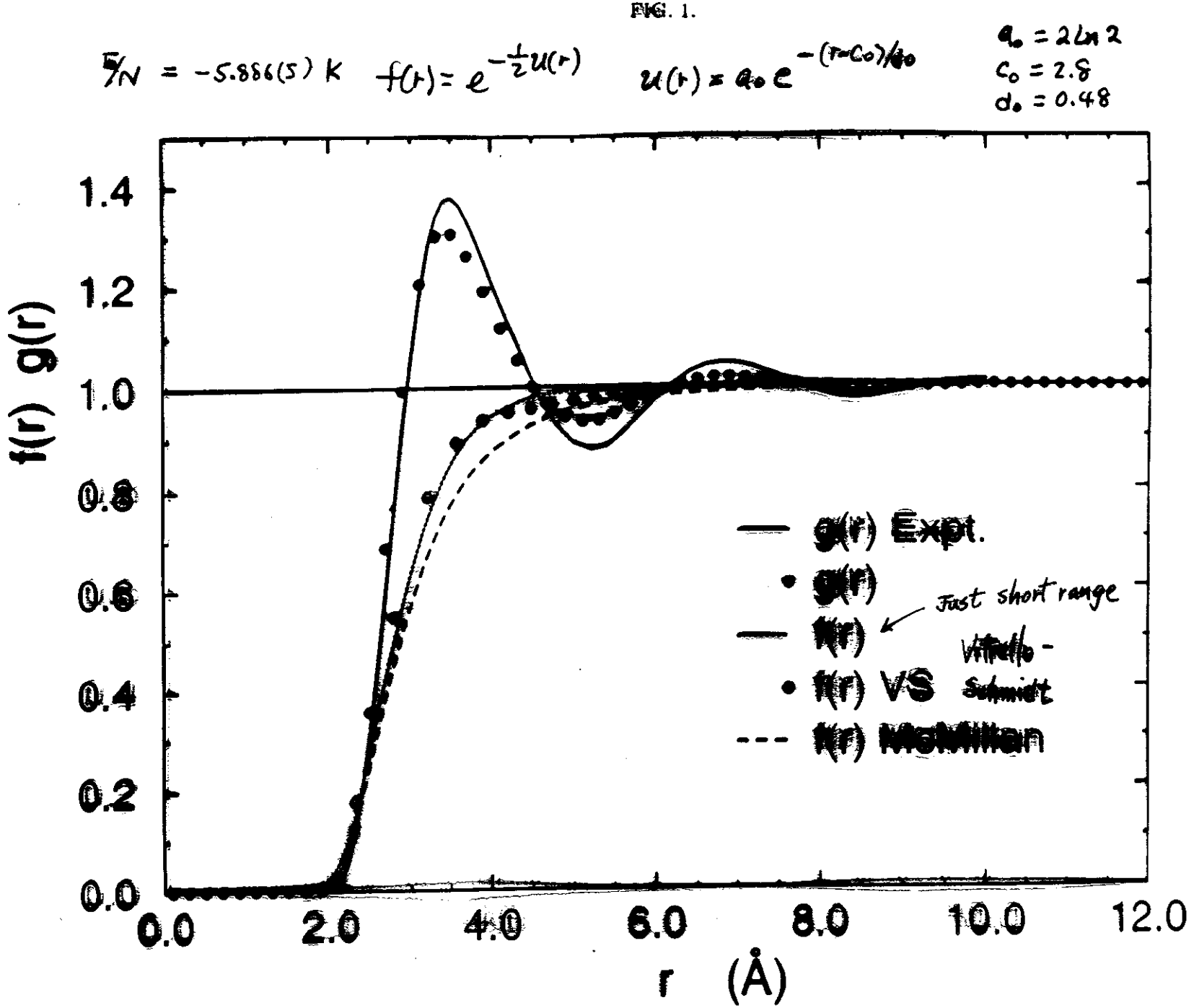


FIG. 1.


E/N = −5.886(5) K
f(r) = e^{−½u(r)}
u(r) = a₀ e^{−(r−c₀)/d₀}
a₀ = 2 ln 2
c₀ = 2.8
d₀ = 0.48
f(r) g(r)
r (Å)
0.0
2.0
4.0
6.0
8.0
10.0
12.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
g(r) Expt.
g(r)
f(r)
Fast short range
f(r) VS Schmidt
f(r) Metiu
Vitiello -

PL1

FIG. 2.

$$u(r) = a_0 e^{-(r-c_0)/d_0} + \sum_{i=1}^{2} a_i e^{-\frac{1}{2}\left(\frac{r-c_i}{d_i}\right)^2} \qquad E/N = -5.968(8)\ k$$

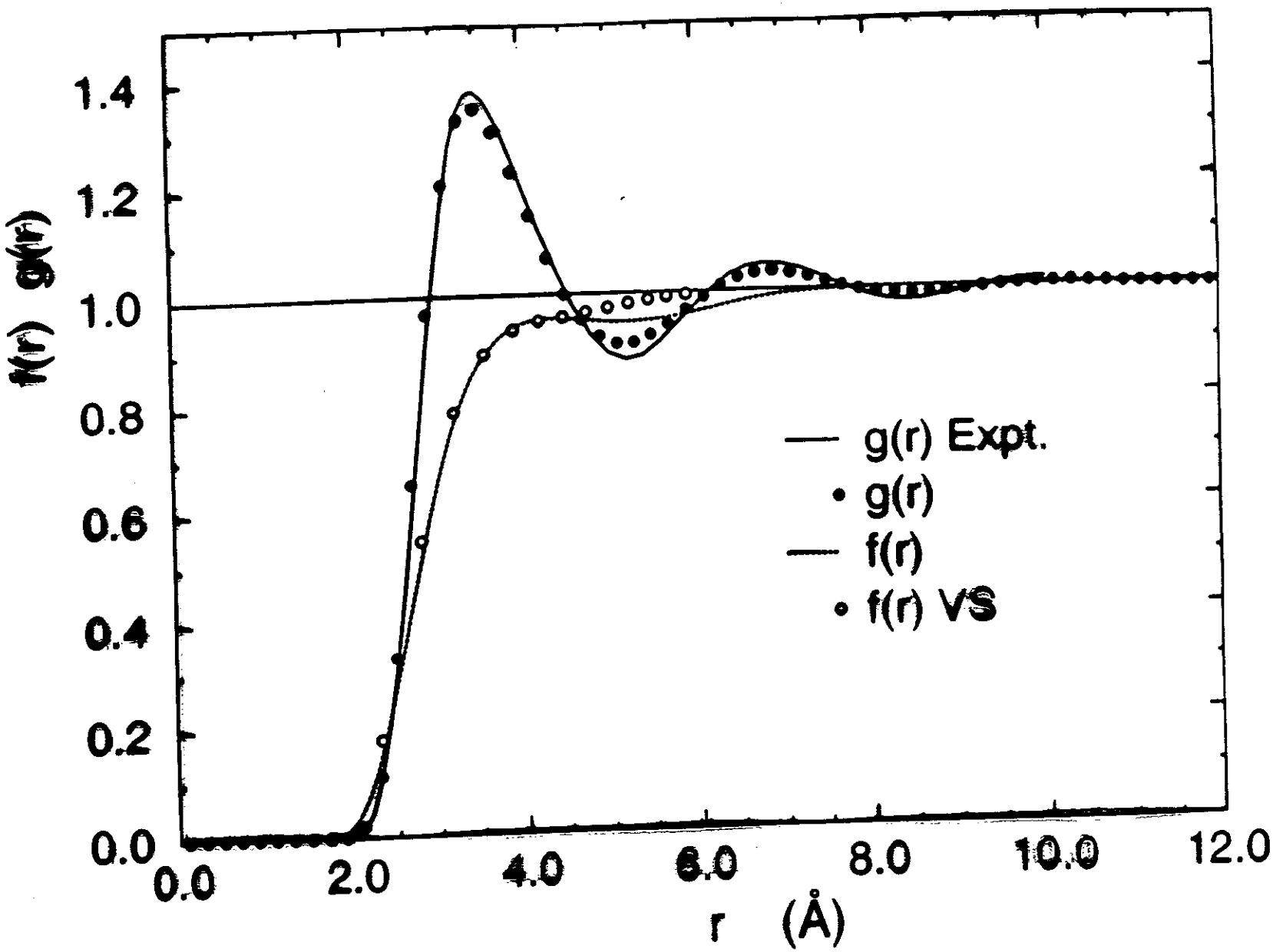
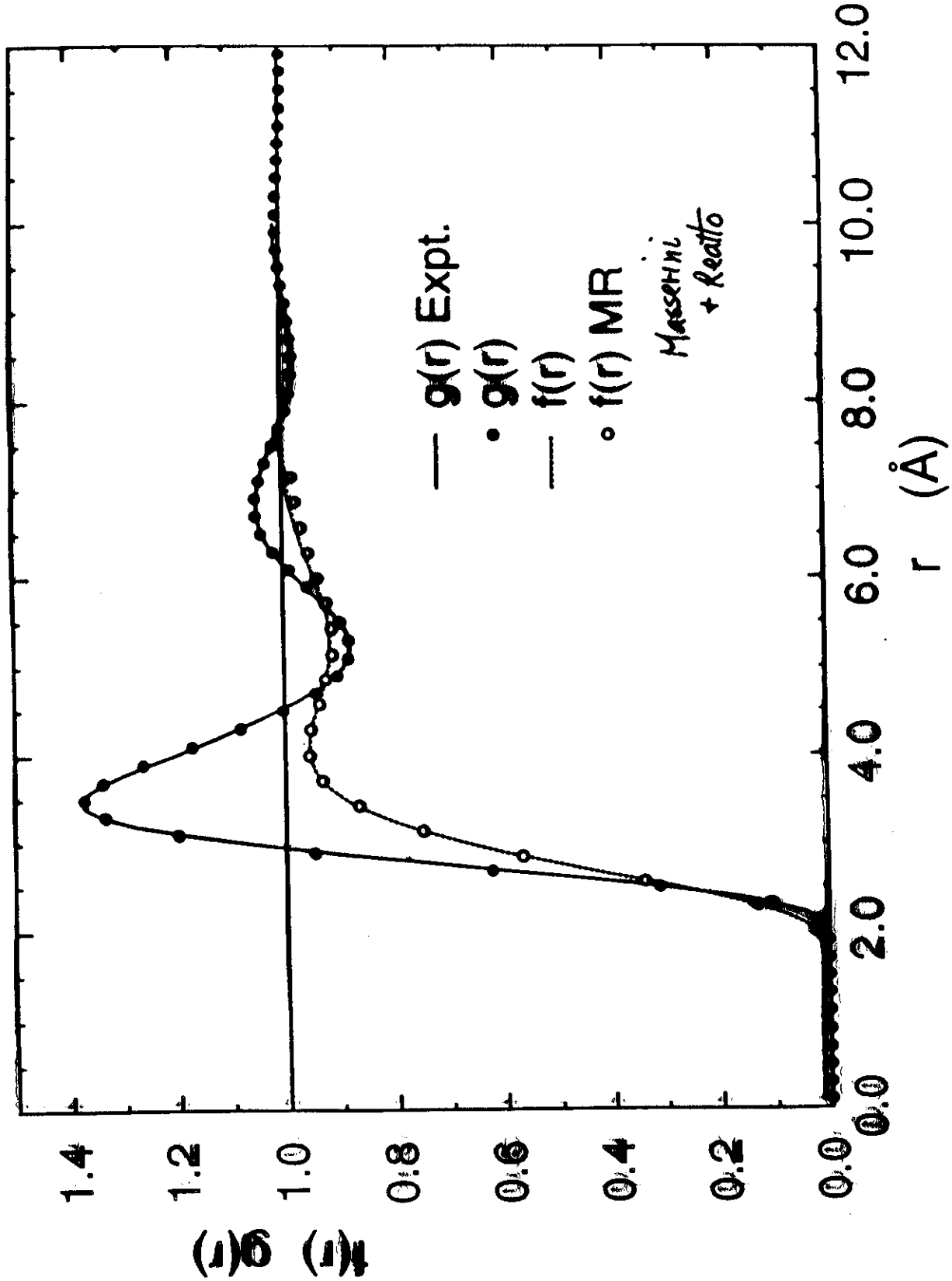


FIG. 3.


Can fit g(r); max. overlap E/N = -5.862(7) K
— g(r) Expt.
• g(r)
— f(r)
° f(r) MR
Massimi + Reatto
f(r) g(r)
r (Å)
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
2.0
4.0
6.0
8.0
10.0
12.0

V) Higher Order Algorithms

Every factorization of

$T^{DHC} = e^{\epsilon(T+V)} \Rightarrow$ algorithms for solving quantum and classical mechanical problems

↳ symplective integrators

Let

$$T^{(2)}_{(\epsilon)} = e^{\frac{1}{2}\epsilon V} e^{\epsilon T} e^{\frac{1}{2}\epsilon V}$$
$$= T(\epsilon) + C\epsilon^3 + D\epsilon^5 \quad \text{odd powers only}$$

Consider (Creutz - Gocksch, Yosida)

$$T^{(2)}(\tilde{\epsilon}) T^{(2)}(-s\tilde{\epsilon}) T^{(2)}(\tilde{\epsilon}) = T(2\tilde{\epsilon} - s\tilde{\epsilon})$$

($\tilde{\epsilon}$: backward; $-s\tilde{\epsilon}$: forward)

$$+ C(2 - s^3)\tilde{\epsilon}^3 + O(\tilde{\epsilon}^5)$$

Correct to 4th order

if $s = 2^{1/3}$

Restore $\epsilon = (2-s)\tilde{\epsilon}$

negative

$$T^{(4)}(\epsilon) = T^{(2)}\left(\frac{\epsilon}{2-s}\right) T^{(2)}\left(-\frac{s}{2-s}\epsilon\right) T^{(2)}\left(\frac{\epsilon}{2-s}\right)$$

($\Rightarrow$ Forest-Ruth symplective algorithm)

Generalization to arbitrarily high order

$$T^{(2n)}(\epsilon) = T(\epsilon) + C\epsilon^{2n+1}$$

$$T^{(2n)}(\tilde{\epsilon})\, T^{(2n)}(-s\tilde{\epsilon})\, T^{(2n)}(\tilde{\epsilon})$$

$$= T(2\tilde{\epsilon} - s\tilde{\epsilon}) + C(2 - s^{2n+1})\tilde{\epsilon}^{3} + \cdots$$

Correct to $2n+2$ order if $s = 2^{\frac{1}{2n+1}}$

$$T^{(2n+2)} = T^{(2n)}\left(\frac{\epsilon}{2-s}\right) T^{(2n)}\left(-\frac{s}{2-s}\epsilon\right) T^{(2n)}\left(\frac{\epsilon}{2-s}\right)$$

↑ negative

For quantum problems

negative coefficients

$\Rightarrow e^{+C(x'-x)^2}$ not normalizable

can't simulate!

always there if only $T+V$ are used to factorize $e^{\epsilon(T+V)}$ (M. Suzuki)

Positive Coefficient factorization

Baker-Campell-Hausdorff formula

$$e^{\epsilon T} e^{\epsilon V} = \exp\left\{ \epsilon(T+V) + \frac{1}{2}\epsilon^2 [T,V] - \frac{1}{12}\epsilon^3 [T,[V,T]] - \frac{1}{12}\epsilon^3 [V,[T,V]] + \cdots \right\}$$

for $T = -\frac{1}{2}\sum_i \nabla_i^2$

$[V,[T,V]] = \sum_i |\nabla_i V|^2$ is still "potential-like"

$\Rightarrow$ factorize $e^{\epsilon(T+V)}$ into products of $e^{\alpha T} e^{\beta V}$ and $e^{\gamma [V,[T,V]]}$

(H. Suzuki)

Three new 4th order factorizations (Chin, Phys. Lett. A226 (1997) 344)

$$e^{\epsilon(T+V)} = e^{\frac{1}{6}\epsilon V} e^{\frac{1}{2}\epsilon T} e^{\frac{2}{3}\epsilon \tilde{V}} e^{\frac{1}{2}\epsilon T} e^{\frac{1}{6}\epsilon V} \quad (A)$$

$$= e^{\alpha\epsilon T} e^{\frac{1}{2}\epsilon V'} e^{\beta\epsilon T} e^{\frac{1}{2}\epsilon V'} e^{\alpha\epsilon T} \quad (B)$$

$$= e^{\frac{1}{6}\epsilon T} e^{\frac{3}{8}\epsilon V} e^{\frac{1}{3}\epsilon T} e^{\frac{1}{4}\epsilon \tilde{V}} e^{\frac{1}{3}\epsilon T} e^{\frac{3}{8}\epsilon V} e^{\frac{1}{6}\epsilon T} \quad (C)$$

where $\tilde{V} = V + \frac{1}{48}\epsilon^2 [V,[T,V]]$

$V' = V + \frac{1}{24}(2-\sqrt{3})\epsilon^2 [V,[T,V]]$

$\alpha = \frac{1}{2}(1-\frac{1}{\sqrt{3}})$; $\beta = \frac{1}{\sqrt{3}}$

Algorithm A

By direct computation:

$$e^{\epsilon C_2 V} e^{\epsilon C_1 T} e^{\epsilon C_0 V} e^{\epsilon C_1 T} e^{\epsilon C_2 V} = e^{\epsilon W}$$

$$W = 2C_1 \epsilon T + (C_0 + 2C_2)\epsilon V$$

$$- \tfrac{1}{6} C_1 (C_0^2 - 2C_0 C_2 - 2C_2^2) \epsilon^3 [V,[T,V]]$$

$$+ \tfrac{1}{6} C_1^2 (C_0 - 4C_2) \epsilon^3 [T,[V,T]] + O(\epsilon^5)$$

In order for W to reproduce $\epsilon(T+V)$, we must

choose: $C_1 = \frac{1}{2}$; $C_0 + 2C_2 = 1$

Since $[T,[V,T]]$ is undesirable, eliminate it by

$$C_0 = 4C_2 \quad \Rightarrow C_0 = \tfrac{2}{3} \; ; \; C_2 = \tfrac{1}{6}$$

$$W = \epsilon(T+V) - \underbrace{\tfrac{1}{72} \epsilon^3 [V,[T,V]]}_{\text{move back to other side; evenly split or center it on the central } V} + O(\epsilon^5)$$

For B, exchange $T \leftrightarrow V$ and determine different coefficients.