Multi-product expansion and higher order algorithms for solving evolution equations

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Physics and Mathematics

- Only a portion of mathematics describes physics
  → mathematical physics
- Only a subset of numerical methods is most useful for solving physical problems
  → physics-preserving numerical methods
- For example, a necessary condition for a classical dynamic algorithm to be stable is for it to be phase-space volume preserving.

Physic-Preserving algorithms

- How to derive classical algorithms that exactly conserve phase volume (Liouville's theorem) or energy? Symplectic integrators
- How to derive algorithms for solving time - irreversible problems? Forward algorithms
- How to derive algorithms for solving periodic or quantum trace problems? Corrector/Process algorithms.
- How to derive gauge-invariant algorithms for solving electromagnetic field problems?

Exponential Splitting

Many physical evolution equations (Hamilton, Schrödinger, Maxwell, etc.) of the form

$$\frac{\partial w}{\partial t} = (T + V)w$$

have operator solution $w(t+\epsilon) = \mathrm{e}^{\epsilon(T+V)} w(t)$

A single product approximation,

$$\mathrm{e}^{\varepsilon(T+V)} \approx \prod_{i=1}^{N} \mathrm{e}^{t_i \varepsilon T} \mathrm{e}^{v_i \varepsilon V}$$

→ "Algebraic-tization" of algorithm development (symplectic, unitary, etc.)

Poisson bracket dynamics

Classical dynamics is evolved by the Poisson bracket:

$$\frac{\partial W}{\partial t} = \frac{\partial W}{\partial q_i}\frac{\partial q_i}{\partial t} + \frac{\partial W}{\partial p_i}\frac{\partial p_i}{\partial t} = \frac{\partial W}{\partial q_i}\frac{\partial H}{\partial p_i} - \frac{\partial W}{\partial p_i}\frac{\partial H}{\partial q_i} \equiv \{W, H\}$$

$$= \left(\frac{\partial H}{\partial p_i}\frac{\partial}{\partial q_i} - \frac{\partial H}{\partial q_i}\frac{\partial}{\partial p_i}\right)W = \left(\frac{p_i}{m}\frac{\partial}{\partial q_i} + F_i\frac{\partial}{\partial p_i}\right)W = (T+V)W$$

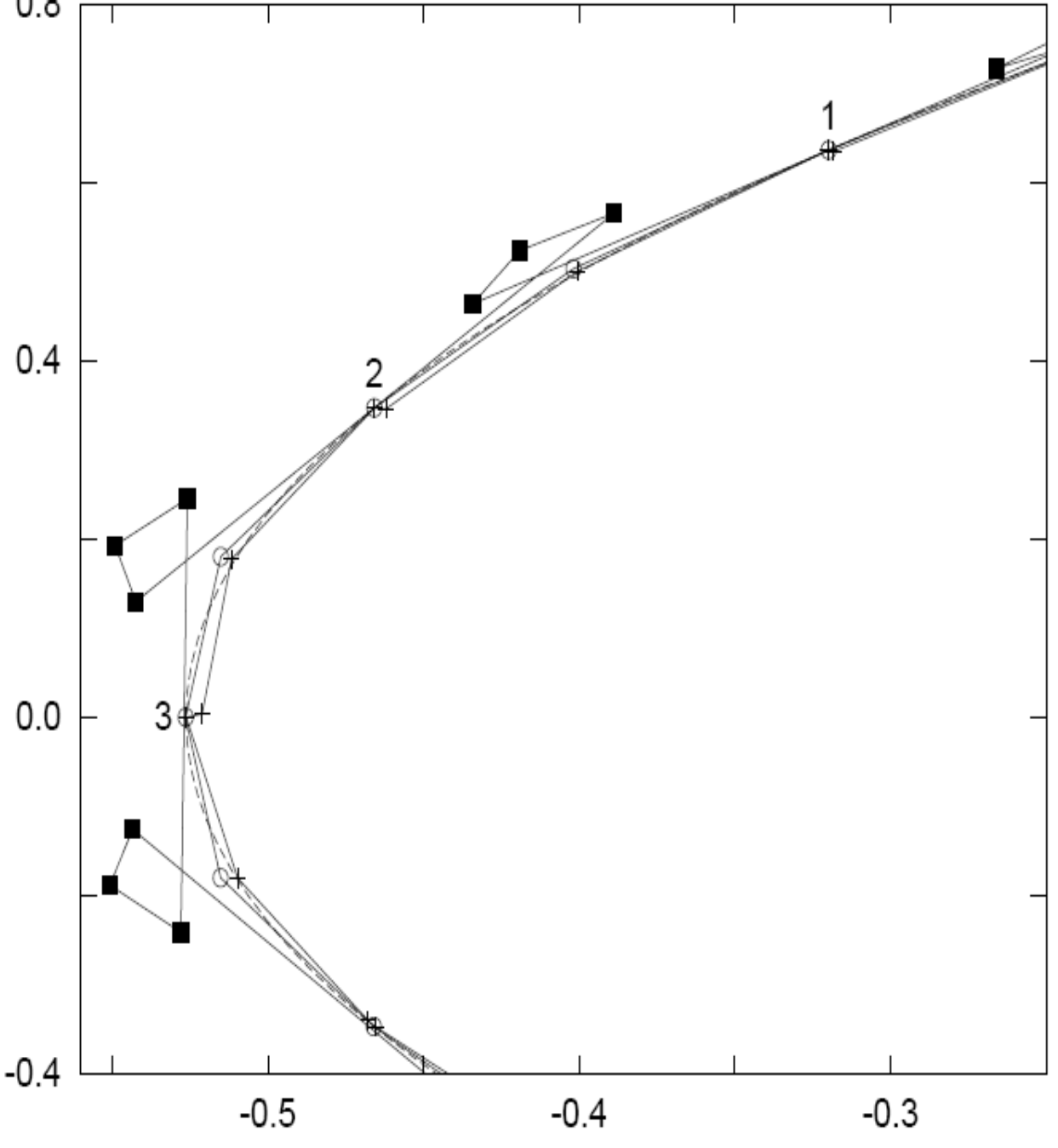
The factorization of $\mathrm{e}^{\varepsilon(T+V)} \approx \prod_{i=1}^{N} \mathrm{e}^{t_i \varepsilon T}\mathrm{e}^{v_i \varepsilon V}$ then yields symplectic integrators which automatically obey Liouville's theorem and conserve all Poincare invariants (e.g. angular momentum).

Forward and non-forward splittings

The coefficients $\{t_i , v_i\}$ correspond to time steps. Physically, $\{t_i , v_i\} > 0$.

Mathematically, for time-reversible systems, can allow intermediate $\{t_i , v_i\} < 0$.

However , these non-forward integrators evaluate the force very off the exact trajectory! Need much smaller time steps to reproduce the “physical” trajectory.

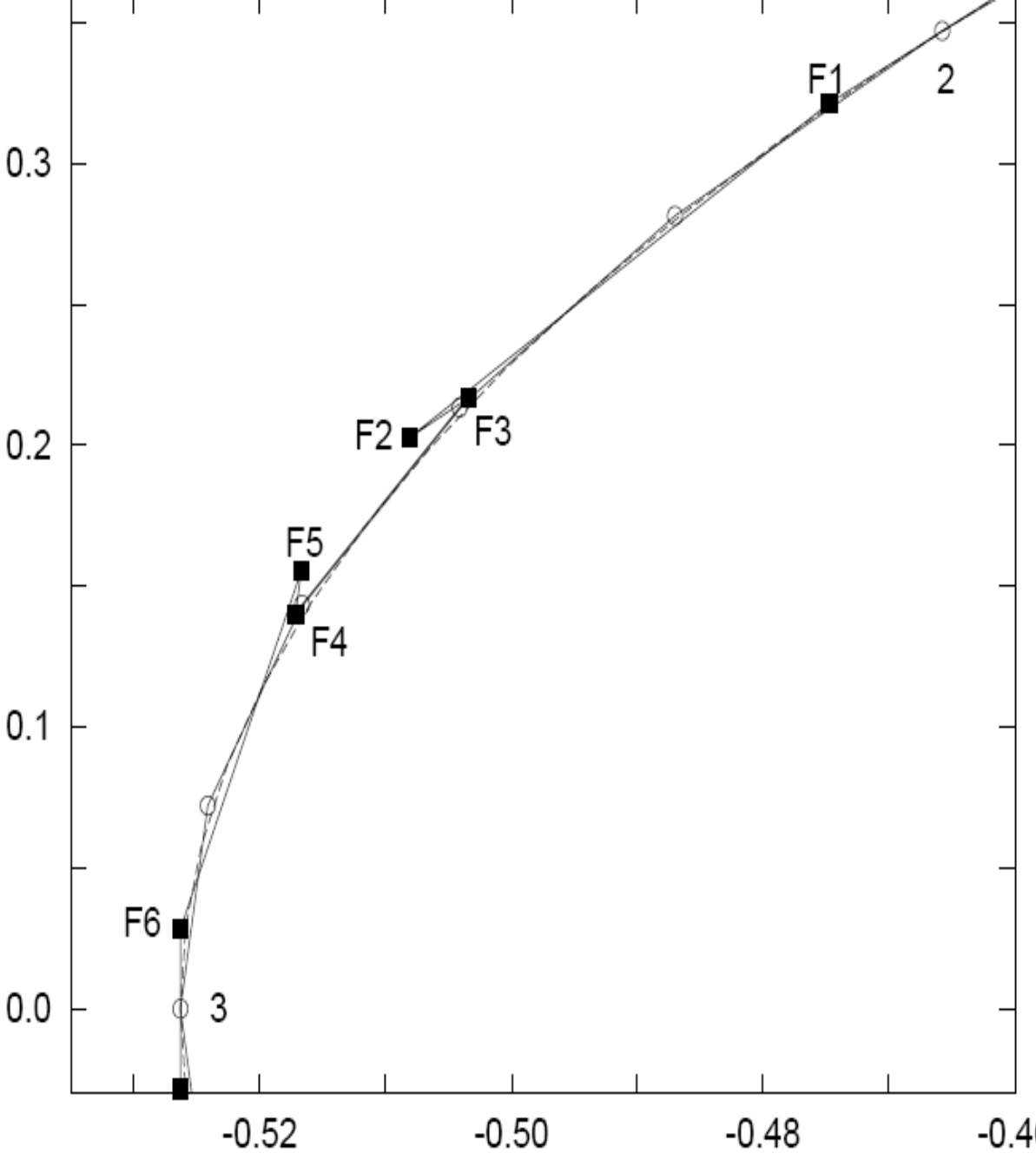


Fourth-order algorithms in solving the Kepler orbit.

Solid squares =Forest-Ruth (90)

Plus sign =MPE=RKN

Circles = forward A4 Chin(97)

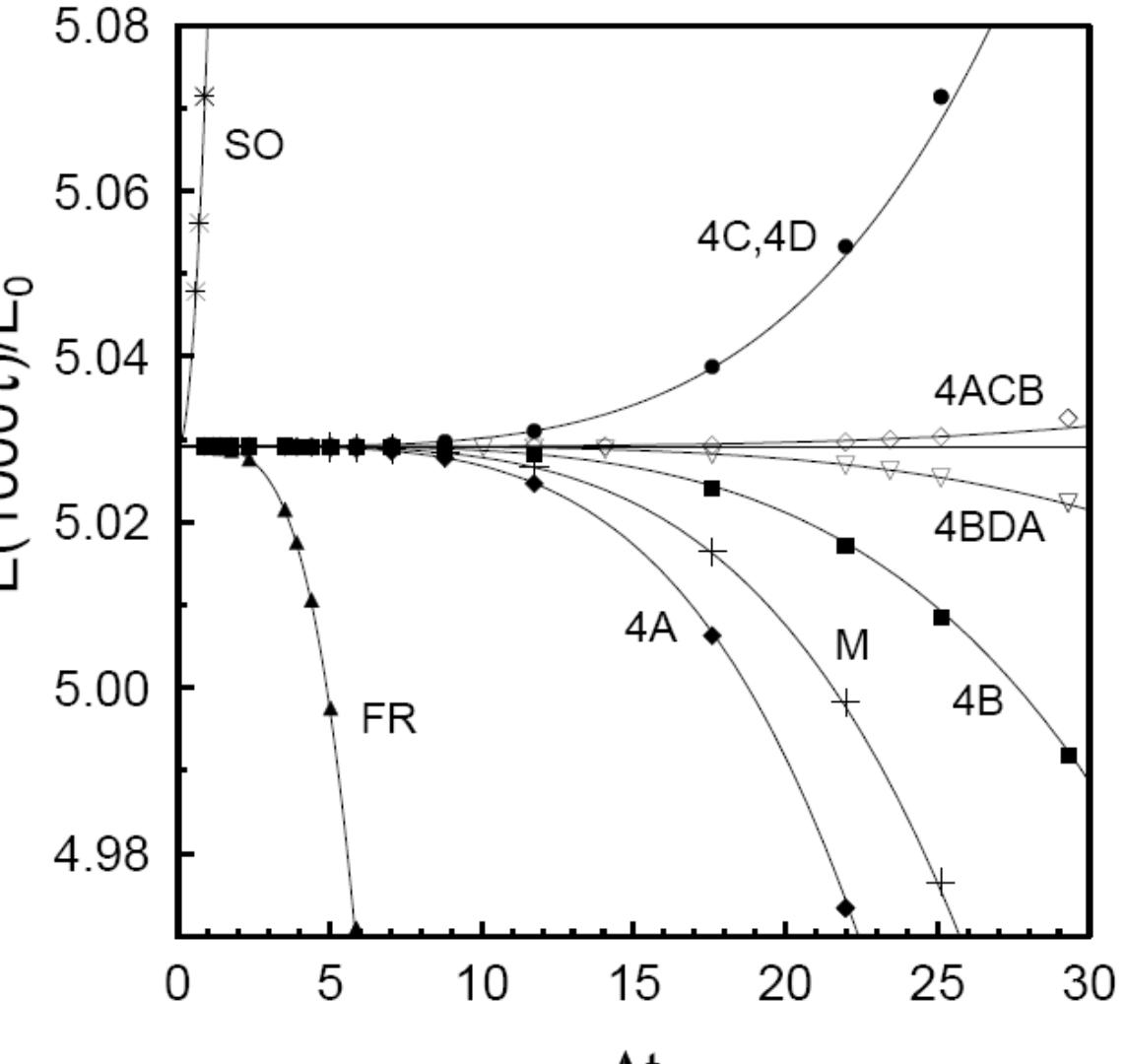


Fourth-order algorithms with six force-evaluations

Solid square: Blanes-Moan(02)

Circles: forward A6 Chin(07)

Real time Schrödinger Equation



Walker-Preston model of laser-atom interaction Chen and Chin (02)

SO = Second-order

FR=Forest-Ruth

M=McLachlan(95)

Time-irreversible systems

$\{t_i , v_i\} > 0$ essential for solving diffusion-type equations.

Sheng(89)-Suzuki(91) Theorem: Beyond second-order, you can't have $\{t_i , v_i\} > 0$!

$$\prod_{i=1}^{N} e^{t_i \varepsilon T} e^{v_i \varepsilon V} = \exp \varepsilon \left(e_T T + e_V V + \varepsilon e_{TV} [T,V] + \varepsilon^2 e_{TTV} [T,[T,V]] + \varepsilon^2 e_{VTV} [V,[T,V]] + \cdots \right)$$

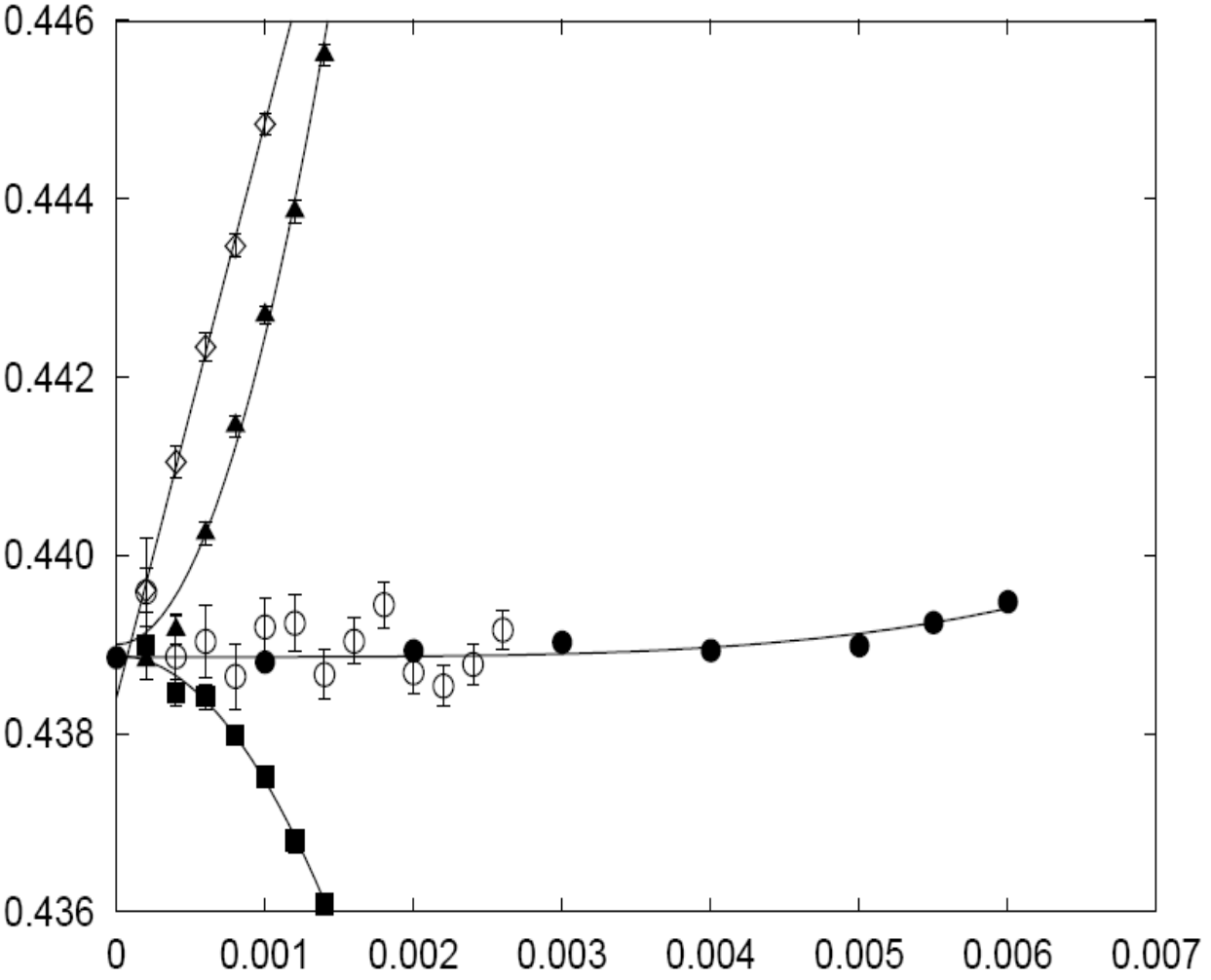
where $e_T = \sum_{i=1}^{N} t_i$ and $e_V = \sum_{i=1}^{N} v_i$, etc., are functions of $\{t_i , v_i\}$.

Can't force e_{TTV} and e_{VTV} both to be zero with $\{t_i , v_i\} > 0$.

Solution: Force $e_{TTV} = 0$ but keep the operator [V,[T,V]].

Suzuki(96), Chin(97)

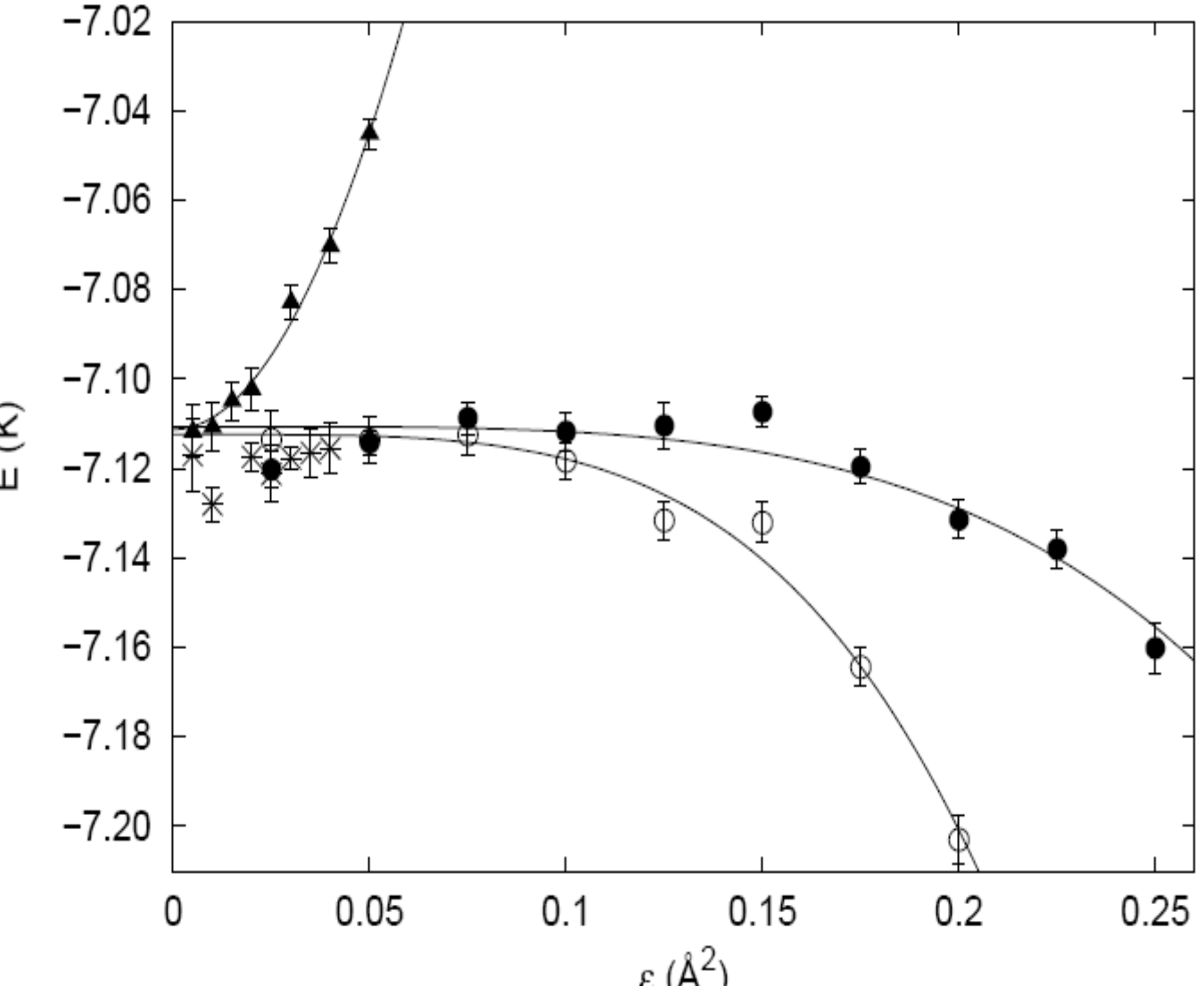
4^{th} order Langevin Algorithm



121 particles in 2D with Yukawa interaction.

Forbert and Chin (01)

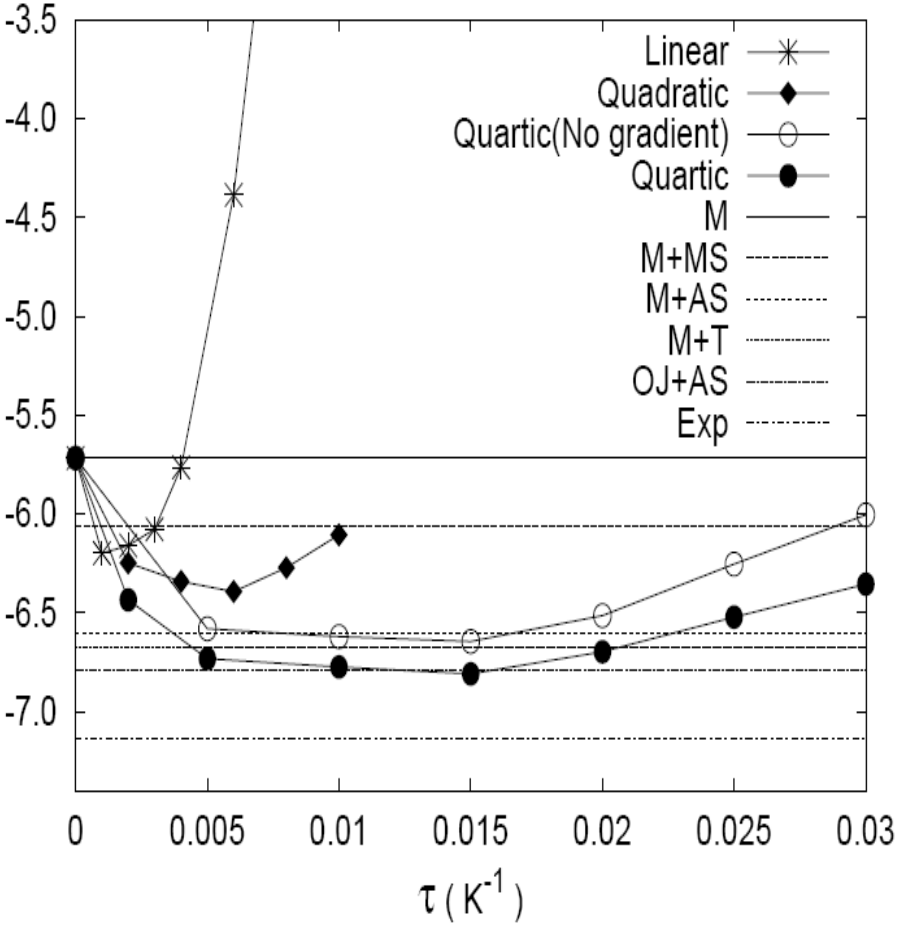
4th order Diffuson Monte Carlo

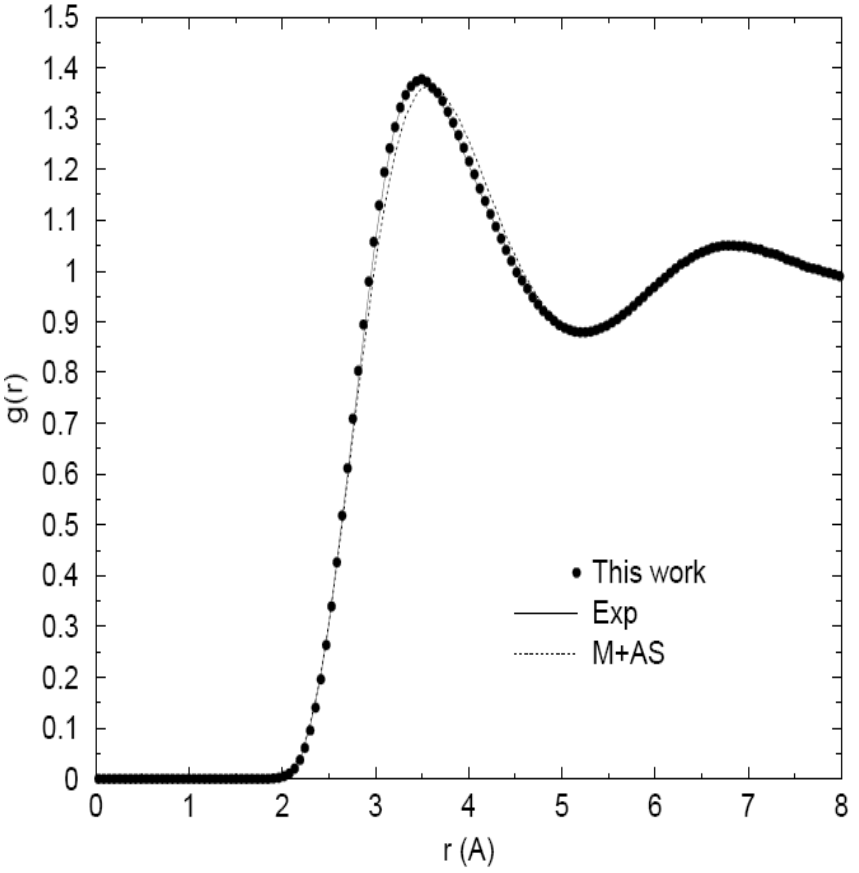


Liquid Helium

Forbert and Chin (01)

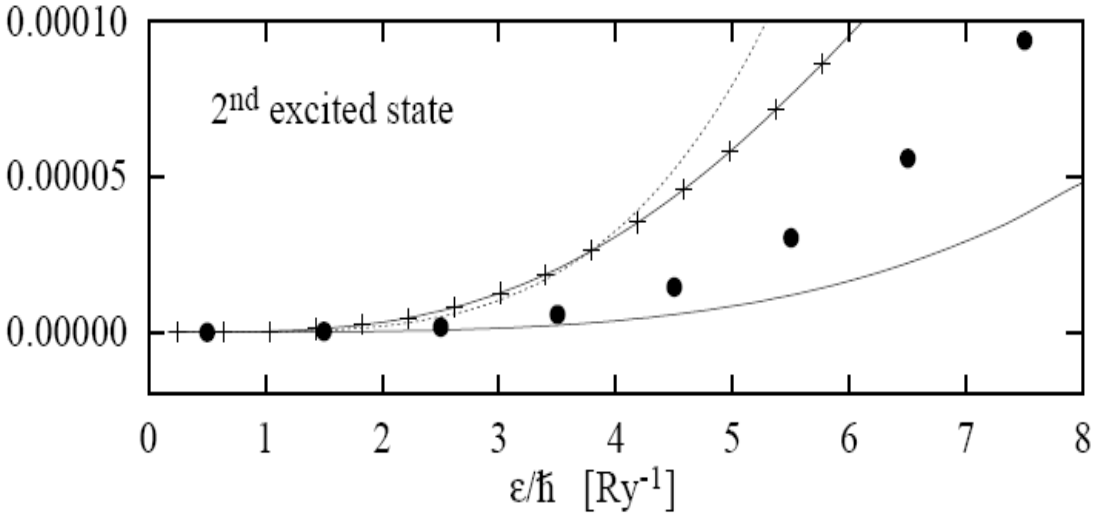
4^{th} order variational wave function

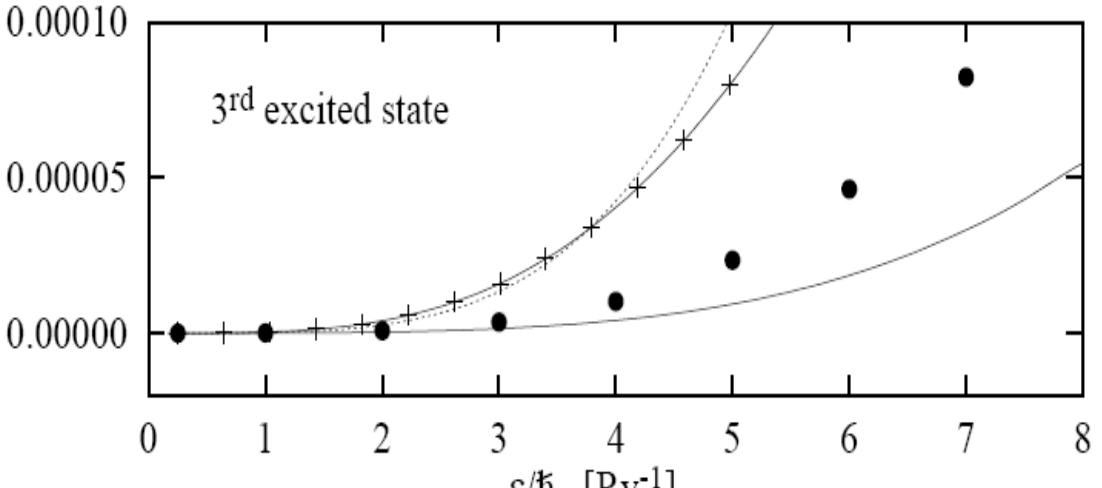




Liquid Helium, Ciftja and Chin(03)

4th order imaginary time Schrödinger equation for excited states

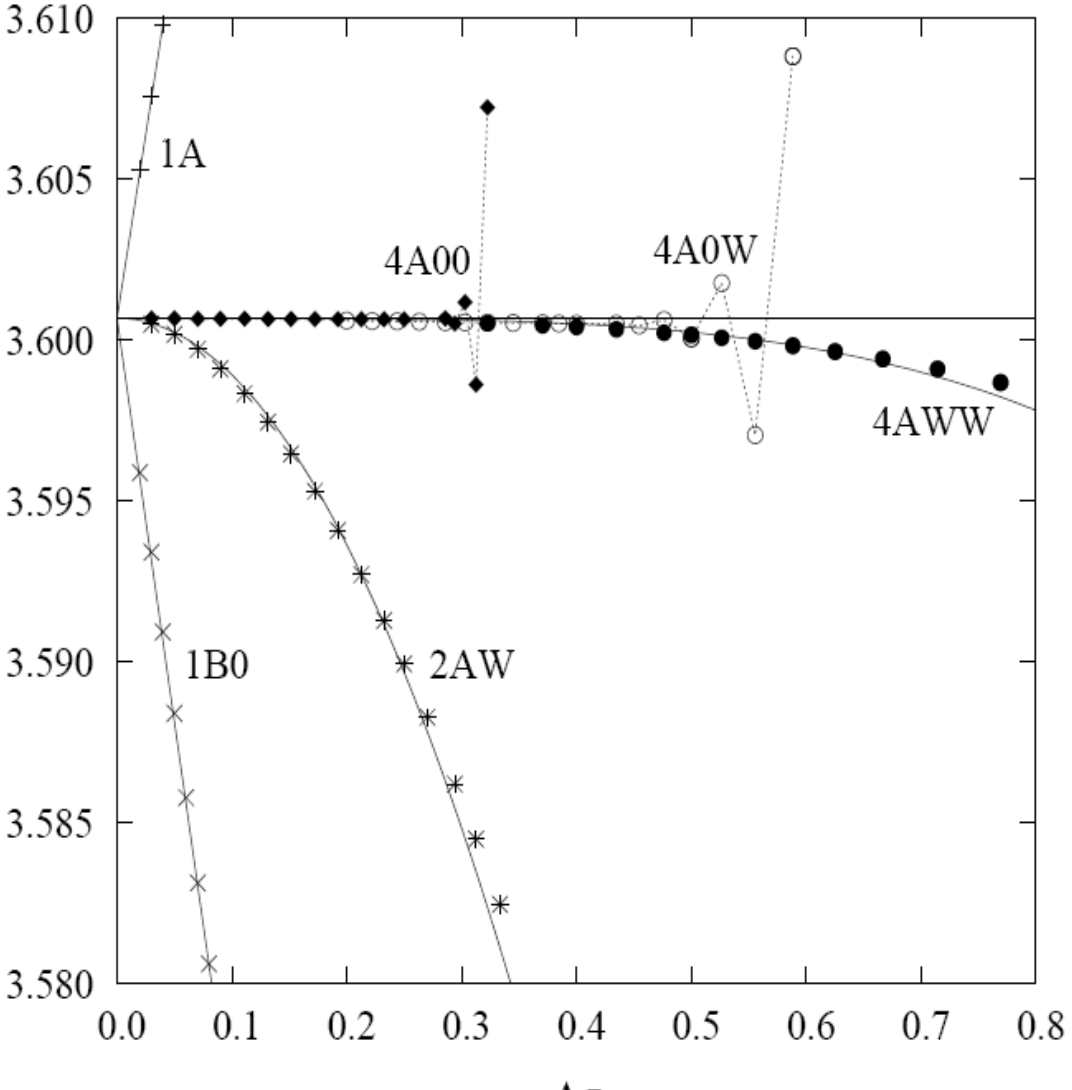




20 electrons Jellium –cluster in 3D

Auer, Krotscheck and Chin (01)

4th order algorithms for solving the imaginary time Gross-Pitaevskii equation



BEC in a rotating trap – vortices nucleation.

Chin and Krotscheck (05)

Path Integral MC and Periodic Motion

Let $$\rho_A = \prod_{i=1}^{N} \mathrm{e}^{t_i \varepsilon T} \mathrm{e}^{v_i \varepsilon V} = \mathrm{e}^{\varepsilon H_A}$$

with $$H_A = T + V + \varepsilon(e_{TV}[T,V]) + \varepsilon^2(e_{TTV}[T,[T,V]] + e_{VTV}[V,[T,V]]) + ..$$

The trace of ρ_A is invariant under the transformation

$\tilde{\rho}_A = S\rho_A S^{-1} = \mathrm{e}^{\varepsilon(SH_AS^{-1})} = \mathrm{e}^{\varepsilon \widetilde{H}_A}$ and $S = \exp[\varepsilon C]$ gives

$$\widetilde{H}_A = e^{\varepsilon C} H_A \mathrm{e}^{-\varepsilon C} = H_A + \varepsilon[C,H_A] + \frac{1}{2!}\varepsilon^2[C,[C,H_A]] + \ldots$$

$$= T + V + \varepsilon^2(e_{TTV}[T,[T,V]] + e_{VTV}[V,[T,V]]) + \varepsilon[C,T+V] + \cdots$$

If $e_{TTV} = e_{VTV}$ then

$C = \varepsilon e_{TTV}[T,V]$ will cancel ε^2 errors!

Symplectic corrector or process algorithms

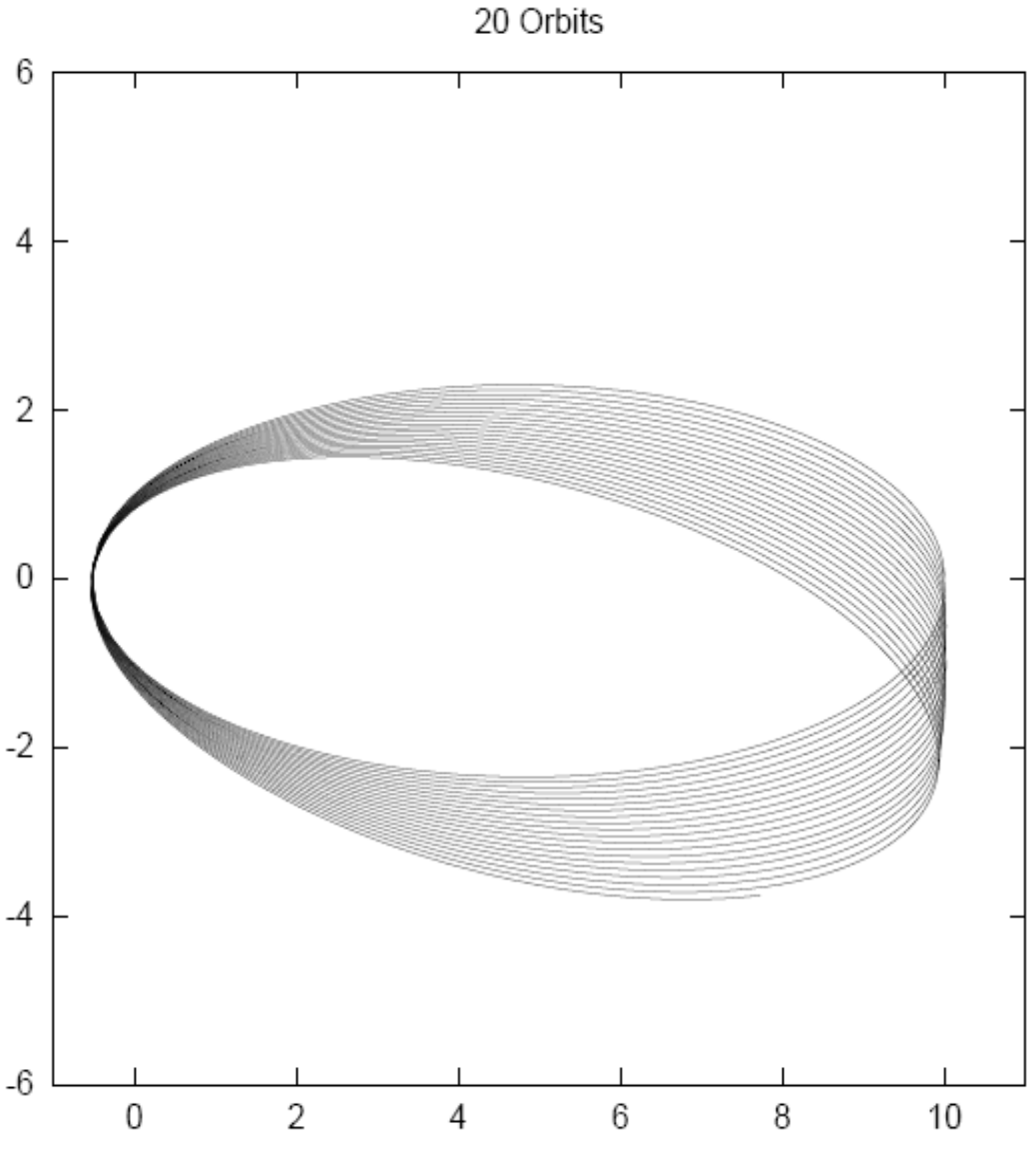
Higher order error terms are of the form [T,Q] and [V,Q]. For periodic orbits or quantum traces, the error terms don't have to vanish, only need to be pair-wise equal : $e_{TQ} = e_{VQ}$

In classical dynamics, these are corrector or process algorithms (Wisdom, et al. (96), Blanes, Casas & Ros (99))
Are there process algorithms $> 2^{nd}$ order with only $\{t_i , v_i\} > 0$? (Needed for PIMC)

NO! Chin(04), Blanes & Casas(05). The fourth order Takahashi-Imada propagator again requires [V,[T,V]].

This generalizes Sheng-Suzuki.

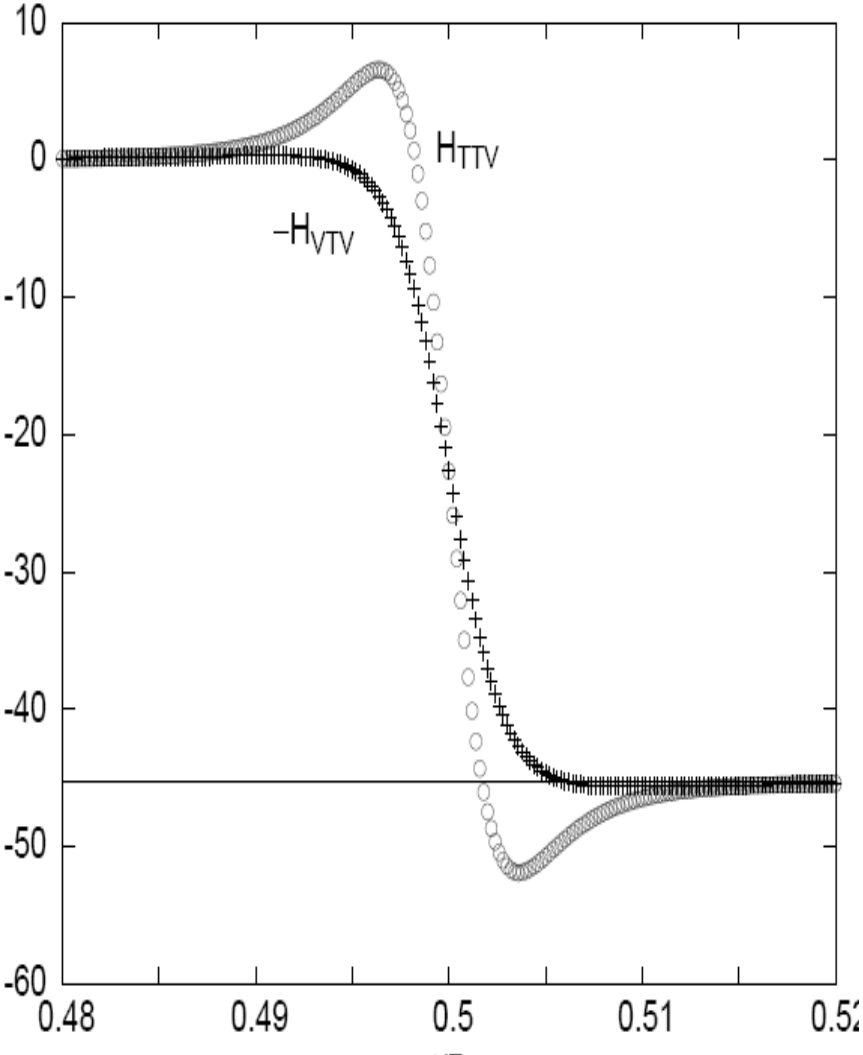
Precession error of Kepler's orbit

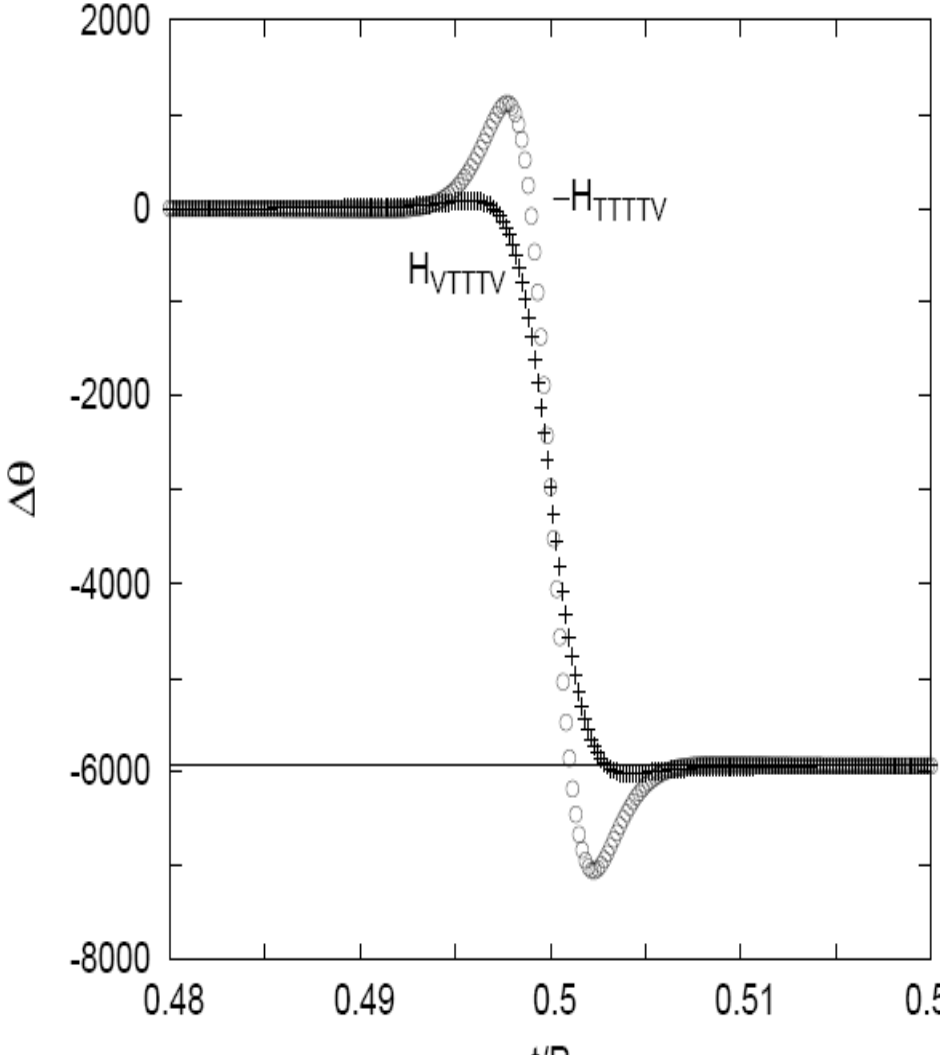


Precession error (advance of the perihelion of planets) of an high eccentricity orbit (e=0.9) when the time step size is not small enough.

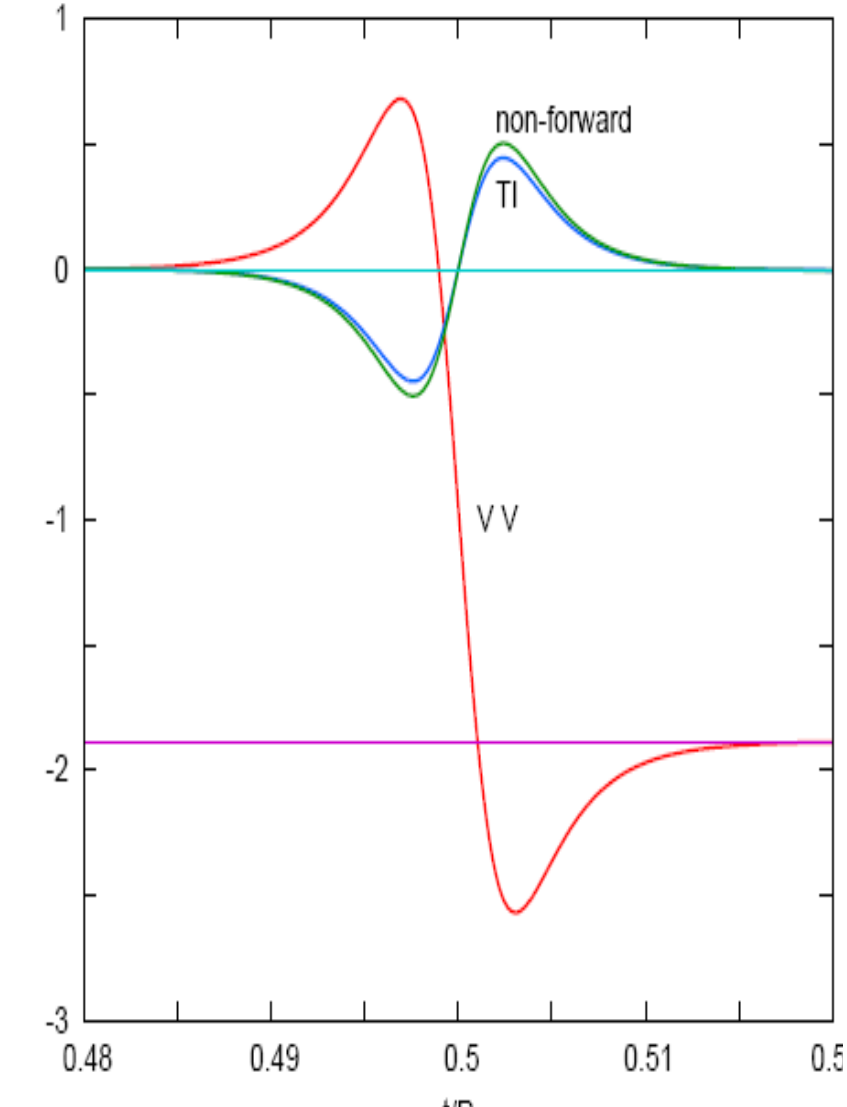
Caused by the error terms in H_A and can be computed analytically .

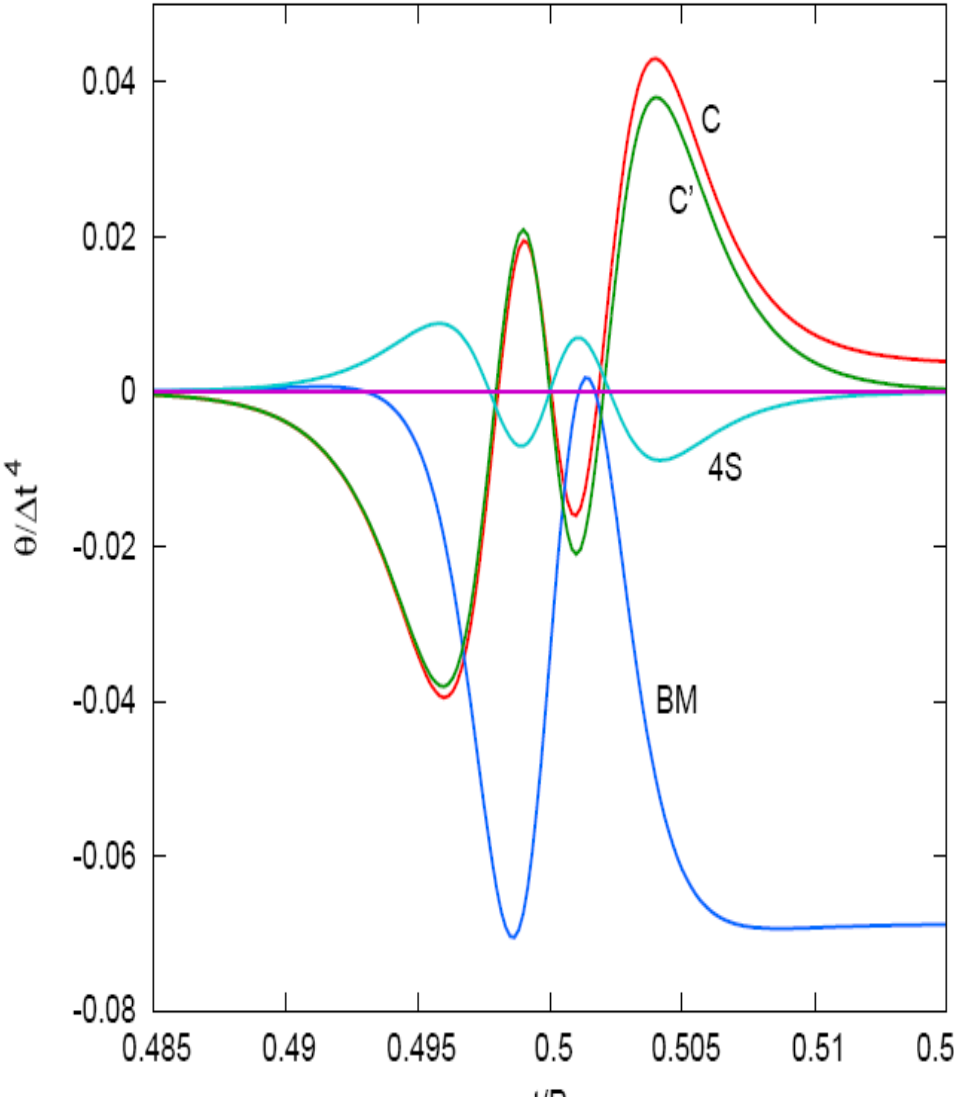
Paired error terms produces opposite precession errors. Chin (07)





4^{th} and 6^{th} order corrector algorithms





4^{th} and 6^{th} order PIMC algorithms?

- Fourth-order PIMC algorithms? YES, by incorporating error operator H_{VTV} =[V,[T,V]]. Many explicit fourth-order algorithms beside Takahashi-Imada.

- Sixth-order PIMC algorithm? Must incorporate the error operator H_{VTTTV}=[V,[T,[T,[T,V]]]] . Chin(05), Chin(07). No practical quantum algorithm.

- Jordi and his group have developed special sixth order methods.

A fundamental theorem Chin (06)

For $\sum_i t_i = 1, \sum_i v_i = 1, t_1 = 0$ and $\{t_{i>1}\} > 0$

$$\prod_{i=1}^{N} \mathrm{e}^{t_i \varepsilon T} \mathrm{e}^{v_i \varepsilon V} = \exp\Big[\varepsilon (T + V + \varepsilon e_{TV}[T,V] + \varepsilon^2 e_{TTV}[T,[T,V]] + \varepsilon^2 e_{VTV}[V,[T,V]] + ..)\Big]$$

The first three error coefficients are related by

$$\mathrm{e}_{VTV} + \frac{1}{2} e_{TV}^2 - e_{TTV} \leq -\frac{1}{24}\delta g - \frac{6}{1-\delta g}(e_{TTV} - \frac{1}{12}\delta g)^2$$

where $\delta g = \sum_{i=1}^{N} t_i^3 > 0$

Implications of the theorem

$$e_{VTV} + \frac{1}{2}e_{TV}^2 - e_{TTV} \leq -\frac{1}{24}\delta g - \frac{6}{1-\delta g}(e_{TTV} - \frac{1}{12}\delta g)^2$$

- The first three error coefficients cannot all vanish for $t_1=0$, $t_i>0$. → Sheng-Suzuki.
- The right-hand-side cannot be zero → no process algorithm beyond second order→ Chin, Blanes-Casas.
- All three error coefficients can vanish only if δg=0 → least one t_k <0, Goodman-Kaper (96)
- All known fourth-order forward algorithms can be derived by saturating the upper bound:

$$e_{VTV} = -\frac{1}{24}\frac{\delta g}{1-\delta g}$$

Solving classical magnetic field problems Chin(08)

In the canonical formalism, the Lorentz force law

$$m\frac{d\mathbf{v}}{dt} = q\mathbf{v} \times \mathbf{B}(\mathbf{r}) \qquad (1)$$

is derived from a *non-separable* Hamiltonian

$$H = \frac{1}{2m}(\mathbf{p} - q\mathbf{A}(\mathbf{r}))^2$$

To derive symplectic integrators, one must do a gauge transformation to disentangle A(r) from p and split *H* in each direction.

Alternatively, one can use a *non-canonical* formulation by directly integrating (1) holding B(r) fixed

→ Exact energy conserving algorithms

Energy conserving algorithms

Directly using the Lorentz force law gives

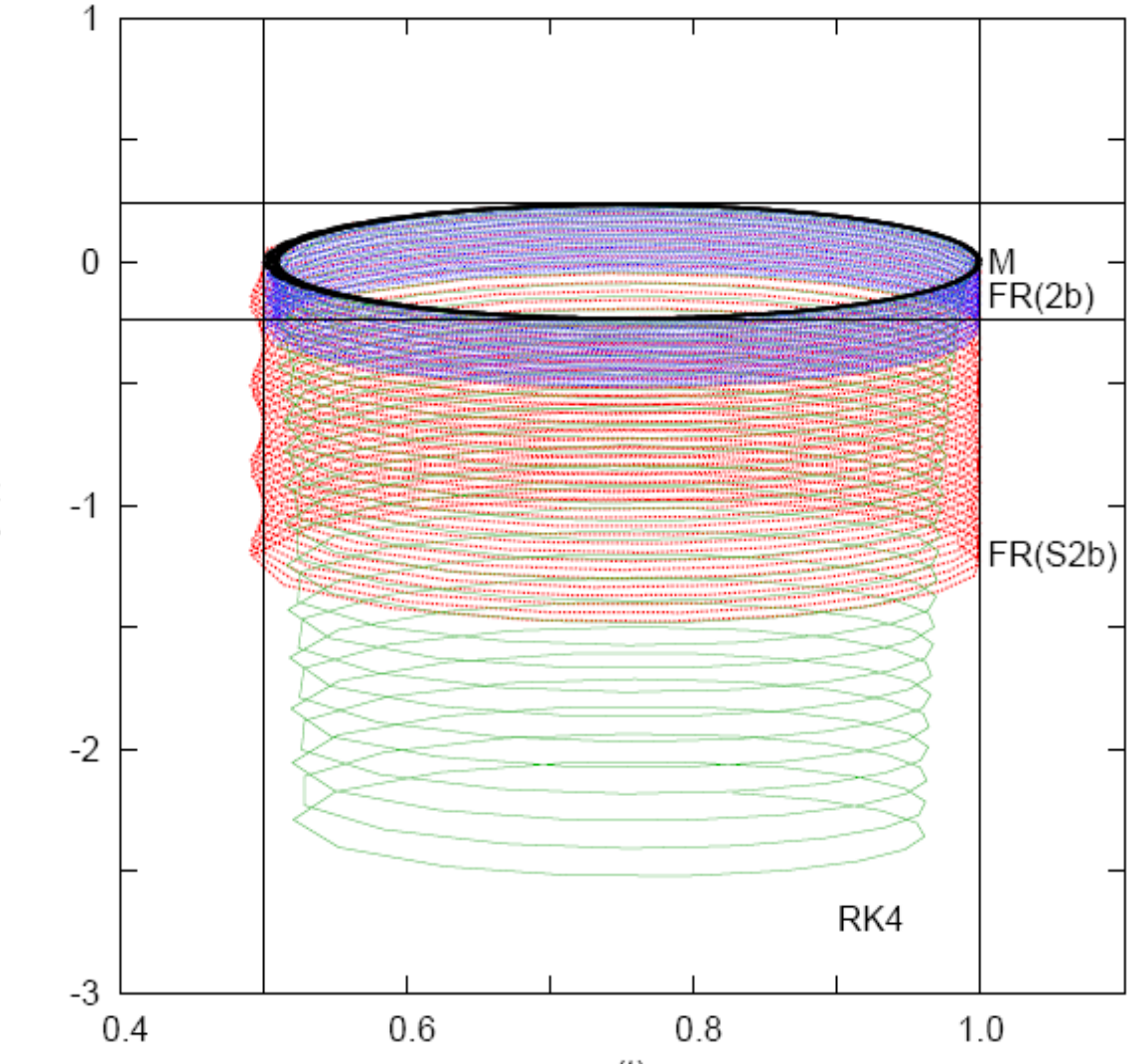
$$\begin{aligned}\frac{dW}{dt} &= \frac{\partial W}{\partial \mathbf{r}} \cdot \frac{d\mathbf{r}}{dt} + \frac{\partial W}{\partial \mathbf{v}} \cdot \frac{d\mathbf{v}}{dt} \\ &= \left(\mathbf{v} \cdot \frac{\partial}{\partial \mathbf{r}} + \omega(\hat{\mathbf{B}} \times \mathbf{v}) \cdot \frac{\partial}{\partial \mathbf{v}}\right) W\end{aligned}$$

Since $e^{\varepsilon T} v^2 = v^2$ and $e^{\varepsilon V} v^2 = v^2$, then

$$\left(\prod_{i=1}^{N} e^{t_i \varepsilon T} e^{v_i \varepsilon V} \right) v^2 = v^2$$

All such splitting algorithms exactly conserve energy for magnetic field trajectory problems.

Symplectic and energy conserving algorithms



Trajectories in a magnetic field $B(x)=(1/x^2)z$

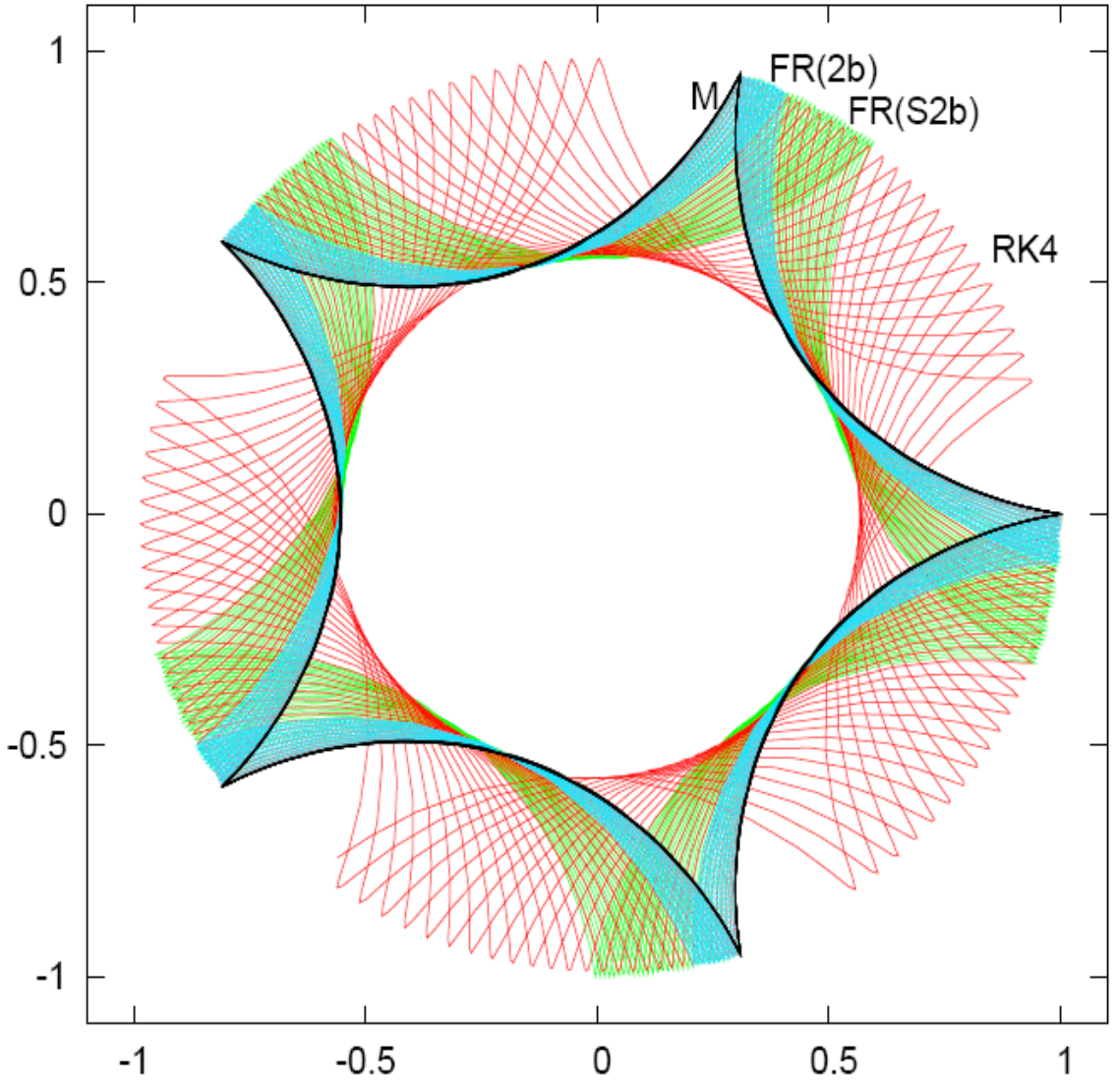
Upward drift velocity removed

S2b=symplectic second-order

2b=energy-conserving second order

M, FR, RK, fourth-order algorithms

Trajectories in a combined E & M field



Trajectories in a magnetic field $B(r)=(1/r)z$ and a 2D HO force field.

S2b-symplectic 2^{nd} order

2b- exponential splitting 2^{nd} order

M, FR, RK, 4^{th} order

Quantum magnetic algorithms

- For classical magnetic field problems, there are two distinct types of gauge invariant algorithms: symplectic and energy-conserving, based on the canonical and non-canonical Hamiltonian formulation respectively.

- For quantum problems, only the canonical formulation based on the gauge potential A(r) is known. (See Stefan Janecek's work.) Are there corresponding non-canonical algorithms for solving quantum magnetic field problems?

Higher order algorithms

For a single product decomposition:

$$\mathrm{e}^{\varepsilon(T+V)} \approx \prod_{i=1}^{N} \mathrm{e}^{t_i \varepsilon T} \mathrm{e}^{v_i \varepsilon V}$$

- No general forward algorithms beyond the 4^{th} order.
- Higher order non-forward splitting algorithms require exponentially growing number of operators. Order 4, 6, 8, 10 requires 3, 7, 15 and 31 force-evaluations or FFT respectively.
- A dead-end for high order algorithms ?

Multi-product decomposition

There's tremendous freedom in the more general multi-product decomposition:

$$\mathrm{e}^{\varepsilon(A+B)} = \sum_k c_k \prod_i \mathrm{e}^{a_{k,i}\varepsilon A}\mathrm{e}^{b_{k,i}\varepsilon B}$$

However, if we require $\{a_{k,i}, b_{k,I}\}>0$, then by Sheng-Suzuki, *each* product can only be second-order. The simplest would be the symmetric, time-reversible

$$\mathcal{T}_2(\varepsilon) = \mathrm{e}^{\frac{1}{2}\varepsilon B}\mathrm{e}^{\varepsilon A}\mathrm{e}^{\frac{1}{2}\varepsilon B} = \exp(\varepsilon(A+B) + \varepsilon^3 E_3 + \varepsilon^5 E_5 + \cdots)$$

Its powers $\mathcal{T}_2^k\left(\frac{\varepsilon}{k}\right) = \exp(\varepsilon(A+B) + k^{-2}\varepsilon^3 E_3 + k^{-4}\varepsilon^5 E_5 + \cdots)$ can form a basis spanning the space of all second-order algorithms.

Multi-product expansion Chin(08)

For any set of n integers $\{k_1, k_2, \ldots k_n\}$, one can form a $2n^{th}$ order expansion:

$$e^{\varepsilon(A+B)} = \sum_{i=1}^{n} c_i \mathcal{T}_2^{k_i}\left(\frac{\varepsilon}{k_i}\right) + e_{2n+1}(\varepsilon^{2n+1} E_{2n+1})$$

with closed form expressions for the expansion and error coefficients

$$c_i = \prod_{j=1(\neq i)}^{n} \frac{k_i^2}{k_i^2 - k_j^2} \qquad e_{2n+1} = (-1)^{n-1} \prod_{i=1}^{n} \frac{1}{k_i^2}$$

Minimal expansion

For the harmonic sequence $\{k_i\}=\{1,2,3,\ldots n\}$, one has

$$\mathcal{T}_4(\varepsilon) = -\frac{1}{3}\mathcal{T}_2(\varepsilon) + \frac{4}{3}\mathcal{T}_2^2\left(\frac{\varepsilon}{2}\right)$$

$$\mathcal{T}_6(\varepsilon) = \frac{1}{24}\mathcal{T}_2(\varepsilon) - \frac{16}{15}\mathcal{T}_2^2\left(\frac{\varepsilon}{2}\right) + \frac{81}{40}\mathcal{T}_2^3\left(\frac{\varepsilon}{3}\right)$$

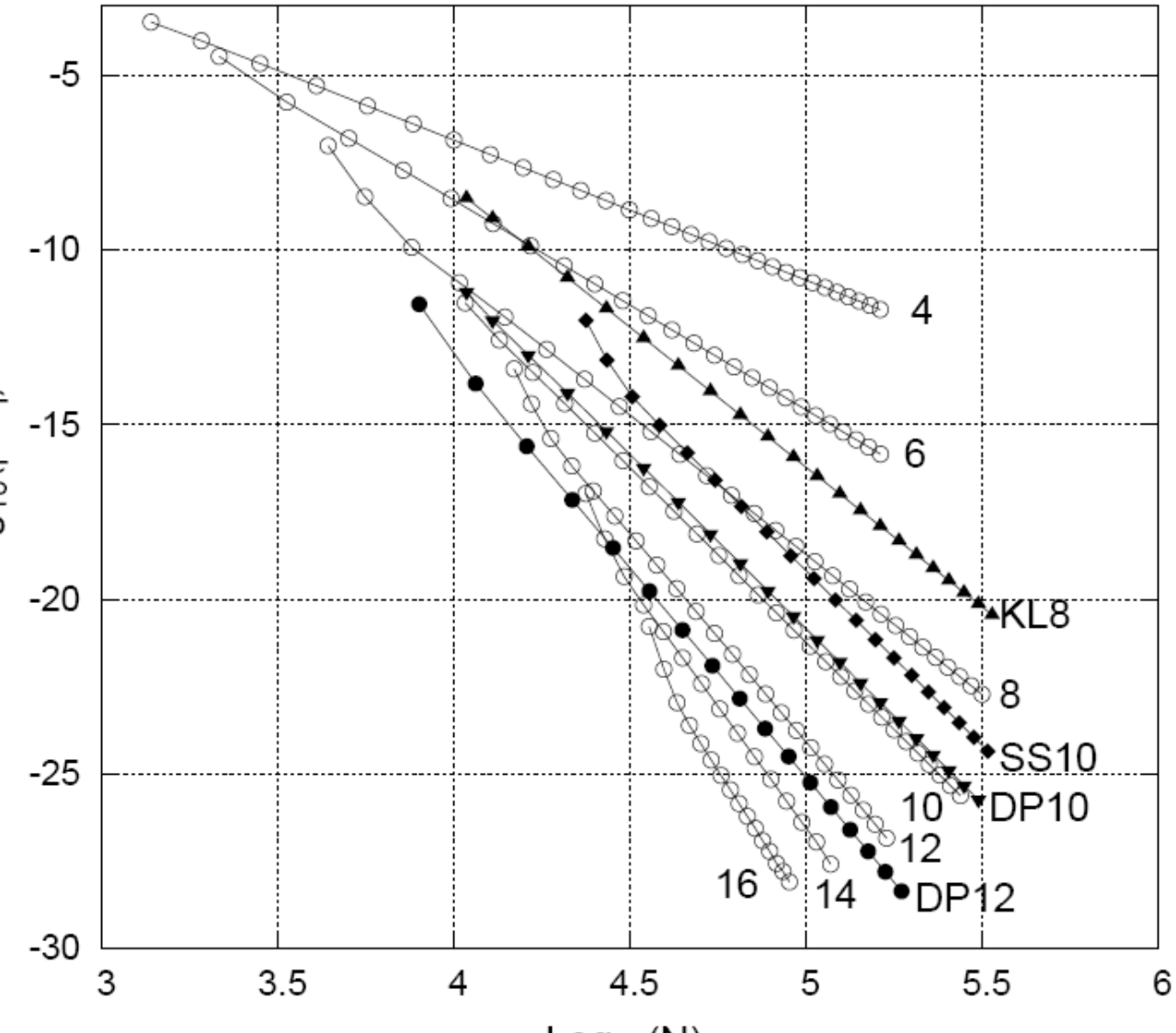
$$\mathcal{T}_8(\varepsilon) = -\frac{1}{360}\mathcal{T}_2(\varepsilon) + \frac{16}{45}\mathcal{T}_2^2\left(\frac{\varepsilon}{2}\right) - \frac{729}{280}\mathcal{T}_2^3\left(\frac{\varepsilon}{3}\right) + \frac{1024}{315}\mathcal{T}_2^4\left(\frac{\varepsilon}{4}\right)$$

$$\mathcal{T}_{10}(\varepsilon) = \frac{1}{8640}\mathcal{T}_2(\varepsilon) - \frac{64}{945}\mathcal{T}_2^2\left(\frac{\varepsilon}{2}\right) + \frac{6561}{4480}\mathcal{T}_2^3\left(\frac{\varepsilon}{3}\right) - \frac{16384}{2835}\mathcal{T}_2^4\left(\frac{\varepsilon}{4}\right) + \frac{390625}{72576}\mathcal{T}_2^5\left(\frac{\varepsilon}{5}\right)$$

The resulting algorithms are no longer symplectic, but surprisingly, correspond to RKN-type integrators.

The number force-evaluations or FFT now only grow as n(n+1)/2.

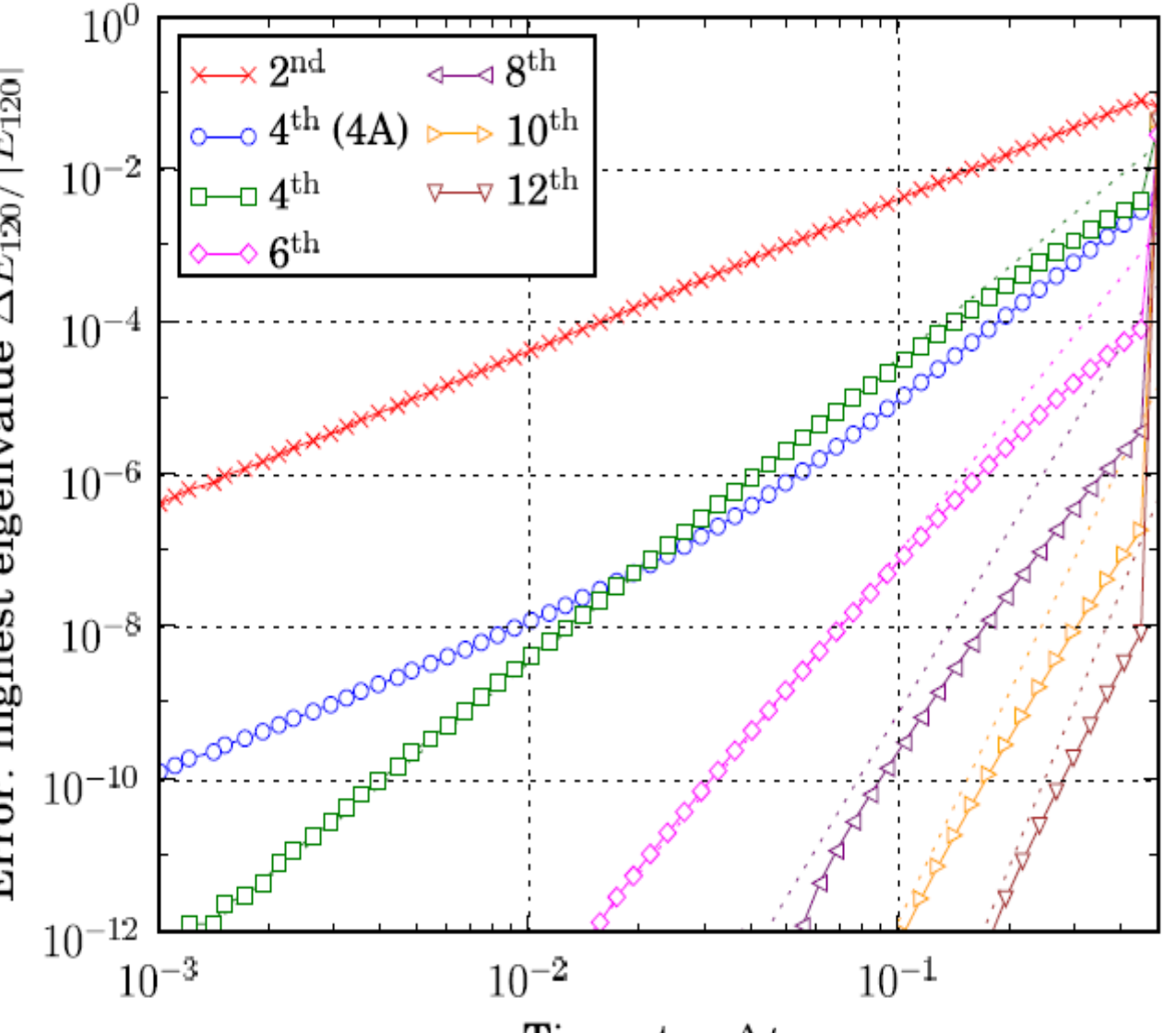
MPE for solving classical dynamics



The orbital precession error in the Kepler problem. Chin(08)

DP12=Dormand and Prince's 12^{th} – order Integrator.

MPE for solving quantum states



Solving for the 120th state of a model C60 molecule.

Chin, Janecek and Krotscheck (09)

MPE for solving time-dependent problems

By relabeling the radial Schrödinger equation

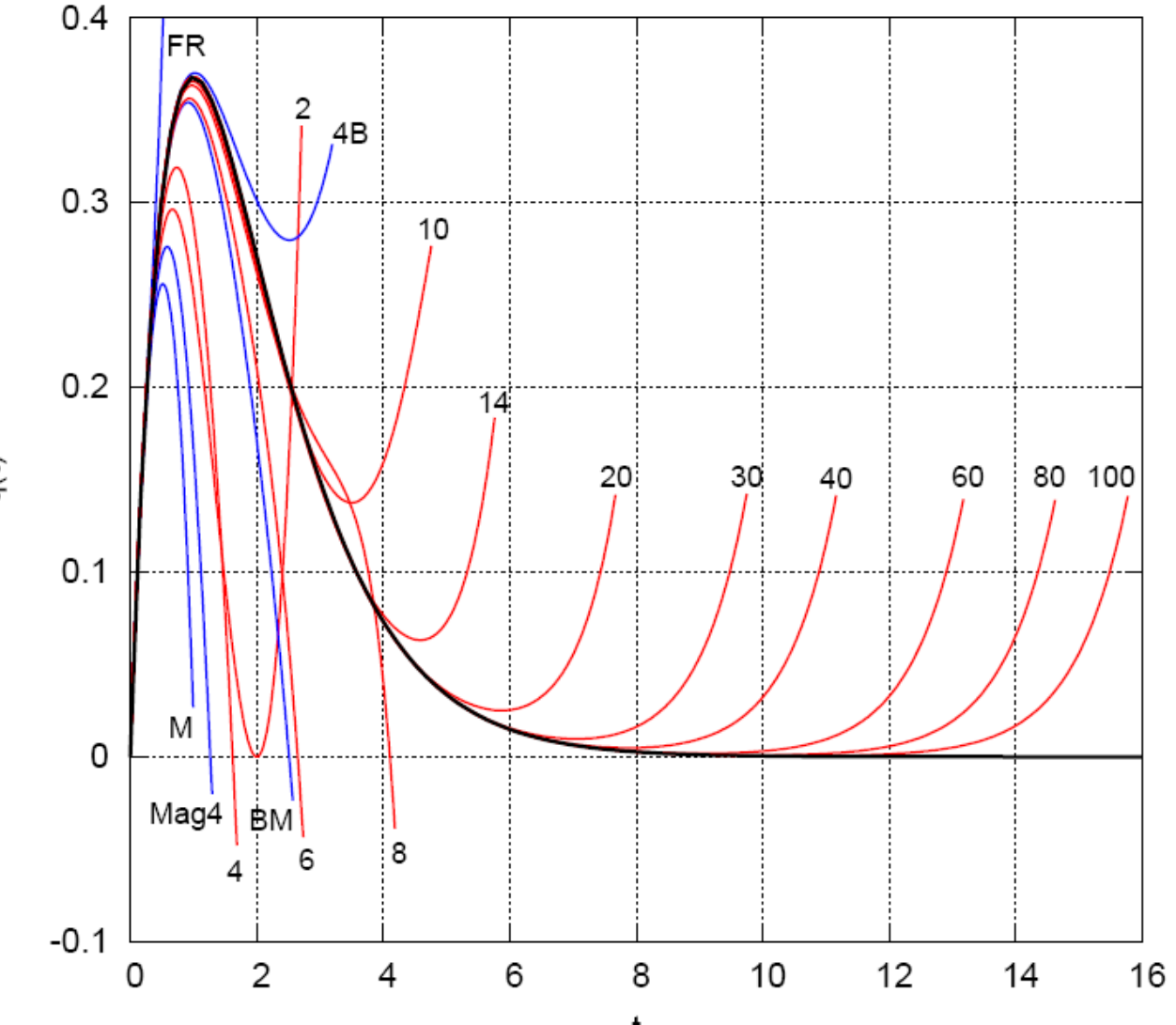
$$\frac{\partial^2 u}{\partial r^2} = f(r,E)u(r) \quad \text{with} \quad f(r,E) = 2V(r) - 2E + \frac{l(l+1)}{r^2}$$

via $r \longrightarrow t$ and $u(r) \longrightarrow q(t)$, it can be solved as a classical harmonic oscillator with a time-dependent spring constant. The ground state wave function of hydrogen is then the trajectory for $d^2q/dt^2=(1-2/t)q(t)$ with $(q_0,p_0)=(0,1)$.

This can be solved using MPE and adopting Suzuki's rule for the time-ordered exponential.

(Juergen Geiser will talk more about this.)

Solving for the Coulomb ground state



Integrating out from t=0.
The time-step size is just t!

FR=Forest-Ruth
BM=Blanes-Moan
M=McLachlan
Mag4=Magnus
4B=forward B

MPE, up to the **100th order!**

Chin and Geiser (09)

Conclusions

The decomposition of $e^{\varepsilon(A+B)}$ is the "holy grail" of algorithm development . (The exact Zassenhaus formula is not practical.) The multi-product expansion, while not symplectic/unitary (but can be energy conserving), is an extremely simple way of achieving high-order accuracy.

Hope that it is also useful in your own field of study!

I thank all my collaborators, but specially Eckhard, for many years of fruitful collaboration. I am specially indebted to Jordi for making this conference possible.