Real-Time Lattice Simulations

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Outline

Origin - Grigoriev and Rubakov 1987

Foundation - Aarts and Smit 1997

Classical theory on the lattice

Applications
- Color-Glass-Condensate

Beyond the classical approximation

Grigoriev and Rubakov: Soliton Pair Physics

In 1987: „*Soliton pair creation at finite temperatures*“
D. Yu. Grigoriev and V.A. Rubakov, *Nucl. Physics B299 (1988) 67-78*

Model: Real scalar field ϕ with spontanous symmetry breaking in (1+1) dimensional space-time

$$\mathcal{L} = \frac{1}{2}\partial_\mu\phi\partial^\mu\phi - \frac{\lambda}{4}\left(\phi^2 - c^2\right)^2,$$

with c the vacuum expectation value.

$\Rightarrow$ For a weakly coupled theory one has $c \gg 1$.
$\Rightarrow$ The mass of an elementary excitation is $m = c\sqrt{\lambda}$.

Solitons

Topological solutions of various models of quantum field theory, that have a non-trivial vacuum structure.

At the classical level localized particle-like, smooth solutions of the classical field equations.

When quantizing the theory one fixes such a soliton solution, obtaining composite particles with form-factors determined by the classical field configurations.
$\Rightarrow$ In weakly coupled ϕ^4 theory they appear as „kink“ solutions at the classical level.

$\Rightarrow$ They are extended objects that can be assigned a soliton mass M_s and a size r_s.

Non-trivial classical soliton („kink“) solution for the given model

$$\phi_c(x) = c\tanh\left(c\sqrt{\frac{1}{2}\lambda}x\right),$$

with soliton mass $M_s = \sqrt{\frac{8}{9}\lambda}c^3$ and size $r_s \sim \frac{1}{c\sqrt{\lambda}} = \frac{1}{m}$.

Note: The soliton is much heavier than an elementary excitation $M_s/m \sim c^2 \gg 1$.

Classicality

Statement of Grigoriev and Rubakov:

The thermal creation of kink-antikink pairs is described by classical field theory, provided that the elementary excitations at the kink scale obey classical statistics, i.e.

$$\text{Excitation energy:} \quad \omega_k = \sqrt{k^2 + m^2} \ll T \quad \text{at} \quad k \sim r_s^{-1}.$$

Combining this and $r_s \sim m^{-1}$ leads to some kind of classicality condition

$$T \gg m = c\sqrt{\lambda}.$$

Especially: Temperatures of order $T \sim \sqrt{\lambda}c^3 \sim M_s$ satisfy this condition and the number of kink-antikink pairs becomes unsuppressed by the Boltzmann factor $\sim e^{-\frac{M_s}{T}}$.

Quantum effects become relevant at $\omega_k \geq T$, in particular the UV cut-off of the Rayleigh-Jeans distribution emerges at the spatial scale $r_0 \sim 1/T \ll r_s$.

$\Rightarrow$ Physical scale of the thermal production process is located in the IR of the field theory, making it possible to describe it classically. Quantum effects on the UV scale are suppressed.

First conclusion

What we can conclude at this point:

- The infrared of a weakly coupled quantum theory at large temperatures

$$T \gg m,$$

  behaves as a classical theory at leading order.
- Instead of solving the complete quantum theory, the expense is significantly reduced to solving classical field equations.

  $\Rightarrow$ The field equations of motion keep real time, no Wick rotation is involved.
- The approximation is quickly extended to Yang-Mills theory, by investigating electroweak sphaleron transitions in hot $SU(2)$ Yang-Mills theory with a doublet Higgs field, see e.g.

  „Lattice simulations of electroweak sphaleron transitions in real time"
  J. Ambjorn, T. Askgaard, H. Porter, M.E. Shaposhnikov, *Physics Letters B , Vol 244 (1990), p. 479*

But beware: The classical theory is Rayleigh-Jeans divergent $\Rightarrow$ UV-Cutoff required.

Aarts and Smit: Systematic study in scalar ϕ^4 theory

$\Rightarrow$ Yet: Validity of the approximation only based on an argumentation involving the physical scales of a hot and weakly coupled bosonic system.

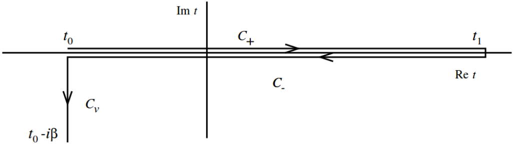
In 1997: *„Classical approximation for time-dependent quantum field theory: Diagrammatic analysis for hot scalar fields"*

Gert Aarts and Jan Smit, *Nucl. Phys. B 511 (1998) p. 451-478*

Systematic study of a (3+1) dimensional $\lambda\phi^4$ scalar model in real time formalism with (renormalized) action

$$S = -\int_{\mathcal{C}} dt \int d^3x \left(\frac{1}{2}\partial_\mu \phi \partial^\mu \phi + \frac{1}{2}\bar{m}^2\phi^2 + \frac{\bar{\lambda}}{4!}\phi^4 + \text{c.t.} \right).$$

$\Rightarrow$ Evaluation on the real time Keldysh contour $\mathcal{C}$ ($\beta = 1/T$)



Perturbative diagrammatic analysis

$\Rightarrow$ Perturbative analysis of self energy corrections (one-loop, setting sun, tadpole) and the four point function (zero- and one-loop) in quantum and classical theory.

Quantum Theory

- Propagators $G(x-y)$ live on the Keldysh contour.
  $\Rightarrow$ Matrix valued propagators.
- System completely described by retarded and advanced propagators $G^{R/A}(x-y)$ and the statistical function $F(x-y) = \frac{1}{2}\langle\{\phi(x),\phi(y)\}\rangle$.
- „Standard“ procedure of perturbation theory in QFT: Calculate the free propagators, vertex functions and the Feynman diagrams afterwards.

Classical Theory

- Hamiltonian as starting point

$$H = \int d^3x \left(\frac{1}{2}\pi^2 + \frac{1}{2}(\nabla\phi)^2 + \frac{\nu^2}{2}\phi^2 + \frac{\lambda}{4!}\phi^4 + \epsilon \right),$$

- Parameters ν, λ, ϵ need to be determined by a matching to the quantum theory, using the classical two-point function

$$S(x-y) = \frac{\int D\pi D\phi e^{-\beta H(\pi,\phi)}\phi(x)\phi(y)}{\int D\pi D\phi e^{-\beta H(\pi,\phi)}}$$

- Classical counterpart of ret/adv, involving Poisson-brackets

$$G^R_{cl}(x-y) = G^A_{cl} = -\theta(x_0 - y_0)\langle\{\phi(x),\phi(y)\}\rangle_{cl}.$$

Results

Exemplary: Setting sun diagram

Quantum theory:

$$\Sigma_R^{sun}(p) = -\frac{\bar{\lambda}^2}{2}\int \frac{d^4k_1}{(2\pi)^4}\frac{d^4k_2}{(2\pi)^4}\left[\underbrace{F_0(k_1)F_0(k_2)G_0^R(p-k_1-k_2)}_{\mathcal{O}(T^2)} - \frac{1}{12}\underbrace{G_0^R(k_1)G_0^R(k_2)G_0^R(p-k_1-k_2)}_{\mathcal{O}(T^0)}\right]$$

Classical Theory:

$$\Sigma_{R,cl}^{sun}(p) \sim -\frac{\lambda^2}{2}\int \frac{d^4k_1}{(2\pi)^4}\frac{d^4k_2}{(2\pi)^4}\underbrace{S_0(k_1)S_0(k_2)G_0^R(p-k_1-k_2)}_{\mathcal{O}(T^2)} + \text{finite}$$

$\Rightarrow$ Both expressions are similar when replacing the (bare) statistical propagator with the free classical two-point function $F_0 \to S_0$.

$\Rightarrow$ The additional contribution in the quantum case is of $\mathcal{O}(T^0)$ and suppressed compared to leading order $\mathcal{O}(T^2)$ for large T and small coupling.

$\Rightarrow$ Similar results are obtained analyzing the tadpole diagram and the four-point function.

Conclusion

⇒ Aarts and Smit have systematically shown, that the classical theory approximates a bosonic quantum theory for weak coupling and high temperatures.

⇒ In a generalized manner, in thermal real time QFT, temperature appears as the replacement of the vacuum zero point fluctuation amplitude, with the thermal fluctuation amplitude

$$\text{zero point fluctuation} \quad \sim \quad \frac{1}{2} \quad \rightarrow \quad \text{thermal fluctuation} \quad \sim \quad \frac{1}{2} + \frac{1}{e^{\frac{E}{T}} - 1}.$$

In the IR for a weakly coupled quantum theory at large temperatures $T \gg m$, we can expand

$$\frac{1}{2} + \frac{1}{e^{\frac{E}{T}} - 1} \approx \frac{T}{E} + \frac{1}{12}\frac{E}{T} + \mathcal{O}\left(\frac{E^3}{T^3}\right).,$$

Classical perturbation theory on the other hand has the same temperature dependence as the leading order term $\mathcal{O}(T/E)$.

Alternative:
⇒ The leading order correspondence in an $\hbar$ expansion, with quantum corrections turning put to be of $\mathcal{O}(\hbar^2)$ has also shown in

„Classical Real Time Correlation Functions and Quantum Corrections at Finite Temperature“

Dietrich Bödeker, *Nucl. Phys. B486 (1997) 500-514*

Lattice implementation

This discussion follows: „*Real time simulations in lattice gauge theory*“

Guy D. Moore, *Nucl. Phys. B (Proc. Suppl.) 83-84 (2000) 131-135*

Recall: The classical theory is UV (Rayleigh-Jeans) divergent.

$\Rightarrow$ Nonperturbative regulation required, that will preserve exact gauge invariance and removes the unwanted UV degrees of freedom.

$\Rightarrow$ **The lattice is the ideal candidate.**

Considering the lattice formulation of Yang-Mills theory

$$\mathcal{L}_{YM} = \frac{2}{g^2 a^4} \mathrm{Retr}\left[\frac{a^2}{a_t^2} \sum_i \left(1 - U_{i0}\right) - \sum_{i<j} \left(1 - U_{ij}\right)\right].$$

- To each link U_i a (dimensionless) canonical conjugate momentum field E_i in the Lie algebra is associated.
- Construct the lattice Hamiltonian of the theory

$$\mathcal{H}_{YM} = \frac{1}{g^2 a^4} \mathrm{Retr}\left[\sum_i E_i E_i + 2 \sum_{i<j} \left(1 - U_{ij}\right)\right].$$

Equations of motion

Usually: Fix temporal gauge $A_0 = 0 \ \rightarrow \ U_0 = 1$.

$\Rightarrow$ The equation of motion of the chromo-electric field E_i is obtained from Hamilton's equations of motion

$$\partial_t E_i^a(x) = -g^2 a^4 \frac{\partial \mathcal{H}}{\partial A_i^a(x)} = 2 \sum_{i \neq j} \mathrm{Imtr}\Big[T^a \big(U_{ji}(x) + U_{-ji}(x)\big)\Big]$$

$\Rightarrow$ The equation of motion of the gauge link is obtained via the temporal plaquette

$$U_{0i}(x) = U_i(x + \hat{t}) U_i^\dagger(x) = \exp\Big[\mathrm{i} g a_t a F_{0i}(x) + \mathcal{O}(a^3)\Big] = \exp\Big[\mathrm{i} g a_t a E_i(x) + \mathcal{O}(a^3)\Big].$$

$\Rightarrow$ **Beware!** Additional constraint has to be satisfied: Gauss law.
Can be derived before fixing gauge, using the Euler-Lagrange equations with respect to A_0

$$0 = -\frac{2}{g a^2 a_t} \sum_i \mathrm{Imtr}\Big[T^a \big(U_{i0}(x) + U_{-i0}(x)\big)\Big]\Big|_{A_t = 0}$$

Note: Equations of motion in real Minkowski time $\rightarrow$ Derivation of time dependent observables possible.

Simulation „receipt“

1. Specify the initial conditions, generating a starting configuration $\{U_{init}\}$.
   $\Rightarrow$ Physical system that satisfies the necessary conditions to be described classically.
2. Make sure, that Gauss law is satisfied.
   $\Rightarrow$ Requires some specific algorithm applied on the initial configuration.
3. Evolve the system in time with timestep a_t, making use of the classical equations of motion.
4. If necessary, fix the gauge completely, e.g. using an algorithm to apply Coulomb gauge.
5. Determine the gauge variant or gauge invariant observable, making use of the classical gauge links U_i and chromo-electric fields E_i.
6. Repeat 2.-5. until the maximum amount of timesteps is reached.

Conclusion

$\Rightarrow$ Lattice simulation of a physical system, making it possible to calculate real time observables.

$\Rightarrow$ The dynamics is governed by solving classical equations of motion.

$\Rightarrow$ Additional constraint „Gauss law“ needs to be satisfied, especially for the initial configuration.

Open problem: Classical theory is UV divergent $\rightarrow$ no continuum limit possible.

$\Rightarrow$ The theory requires some „scale setting“, connecting the lattice spacing a to the physical scale of the system, since observables are cutoff dependent.

Applications:

Sphaleron transitions

E.g. *„Lattice Simulations of electroweak sphaleron transitions in real time"*
J. Ambjorn, T. Askgaard, H. Porter, M.E. Shaposhnikov, *Phys. Letters B 244 (1990)*

- Sphaleron as classical transition between gauge vacua of different topological number.
- The barrier seperating these vacua (the sphaleron mass) can be crossed by sphaleron fluctuations if the temperature of the system is comparable with its size.
- **Especially:** Characteristic momenta of the fluctuations forming a sphaleron are much smaller than the generic momenta of quantum excitations in the hot plasma
  $\rightarrow$ Separation of IR and UV physics makes an application of the classical approximation possible.

$\Rightarrow$ Real time dependent observable: The topological charge

$$Q(t) = \frac{1}{32\pi^2} \int_0^t dt' \int d^3x F^a_{\mu\nu} \tilde{F}^{\mu\nu,a}.$$

$\Rightarrow$ Relation between lattice spacing and temperature calculating the energy of the continuum free bosonic system and relating it to the lattice result $\rightarrow (aT)^3 = 30/\pi^2$.

Applications

Nonequilibrium physics

E.g. *„Nonequilibrium Quantum Fields and the Classical Field Theory Limit"*
Jürgen Berges, *Nucl. Phys. A (2002), 351-355*

- Study of a N-component scalar quantum field theory with ϕ^4-type of interaction.
- Comparing perturbative methods (2 PI 1/N expansion of Kadanoff-Baym equations) to the classical limit.

Strongly-coupled QCD

E.g. *„Heavy Quark Thermalization in Classical Lattice Gauge Theory: Lessons for Strongly-Coupled QCD"*
Mikko Laine, Guy D. Moore, Owe Philipsen, Marcus Tassler, *JHEP 05 (2009) 014*

- QCD at temperatures far above the confinement scale, such that g is small as multiscale problem with momentum scales $\sim T, \sim gT$ and $\sim g^2 T$.
- Physics on the scales $\sim gT$ and $\sim g^2 T$ is describable by classical statistical field theory.
- Of course, no quarks in the classical theory, but Lorentz force acting on a charge carrying heavy can be calculated.
- Scale setting is performed by connecting the lattice spacing and the Debeye mass m_D

$$m^2_{D,cont} = \frac{2N_c + N_f}{6} g^2 T^2, \quad m^2_{D,latt} = \frac{2N_c \Sigma}{4\pi} \frac{g^2 T}{a}, \quad \Sigma = 3.1759115...$$

Applications

Heavy ion collisions

First classical aspects of gluon fields in a heavy ion collision discussed in:

„Computing quark and gluon distribution functions for very large nuclei"
Larry McLerran, Raju Venugopalan, *Phys. Rev. D, Vol. 49/5 (1994), 2233-2241*

- Modeling the initial state of heavy ion collisions → nuclei with densely packed gluons at very high energy densities.
- In a collision with sufficiently large momentum transfer („small x physics") the parton distribution function is dominated by the gluonic contribution.
- Separation of two degrees of freedom:
  Color charge densities ρ of the colliding nuclei, modeled by McLerran and Venugopalan (MV-model), forming a color current

$$J^{\mu,a}(x) = \delta^{\mu,+}\rho_1^a(x_\perp, x^-) + \delta^{\mu-}\rho_2^a(x_\perp, x^+)$$

  Dynamical gauge fields A^μ, which are coupled to the static current via the classical Yang-Mills equation

$$D_\mu F^{\mu\nu} = J^\nu$$

  ⇒ Starting point to generate an initial configuration and perform a classical real time evolution, calculating physical observables as energy density and pressure, looking for indications on thermalization of the system.

Demonstration

Initial state of a heavy ion collision in a static box, as first presented in

„Turbulent pattern formation and diffusion in the early-time dynamics in the relativistic heavy-ion collision"

Kenji Fukushima, *Phys. Rev. C89 (2014)*

- Generation of the initial configuration $\{U_i\}$ via the MV-model.
- Enforcement of Gauss law, as discussed earlier.
- Evolution via the classical equations of motion

$$E_i^a(x+\hat{t}) = E_i^a(x) + 2a_t \sum_{j\neq i} \mathrm{Imtr}\Big[T^a\big(U_{ji}(x) + U_{-ji}(x)\big)\Big], \qquad U_i(x+\hat{t}) = \exp\Big[iga_t a E_i(x)\Big] U_i(x)$$

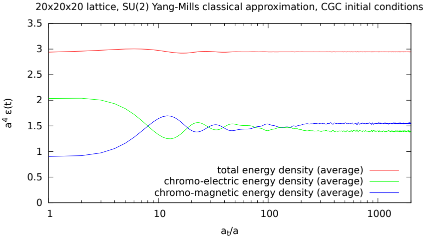
- Derivation of the real time dependent energy density and longitudinal/transversal pressure

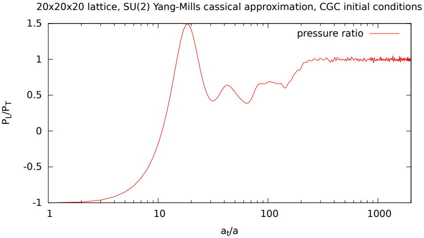
$$\langle\epsilon\rangle(t) = \frac{1}{V}\sum_{\mathbf{x}} \mathrm{Retr}\Big[\sum_i E_i^2(x) + 2\sum_{i<j}\big[1 - U_{ij}(x)\big]\Big] = \langle\epsilon_E\rangle(t) + \langle\epsilon_B\rangle(t).$$

$$\langle P_T\rangle(t) = \frac{1}{V}\sum_{\mathbf{x}} \mathrm{Retr}\Big[E_3^2(x) + 2\big(1 - U_{12}(x)\big)\Big]$$

$$\langle P_L\rangle(t) = \frac{1}{V}\sum_{\mathbf{x}} \mathrm{Retr}\Big[E_1^2(x) + E_2^2(x) - E_3^2(x) + 2\big(1 + U_{12}(x) - U_{13}(x) - U_{23}(x)\big)\Big]$$

Energy density and pressure

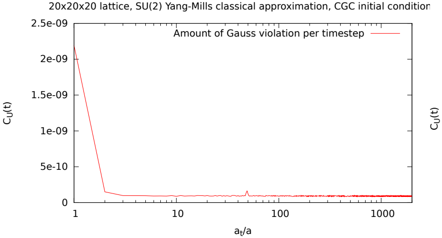


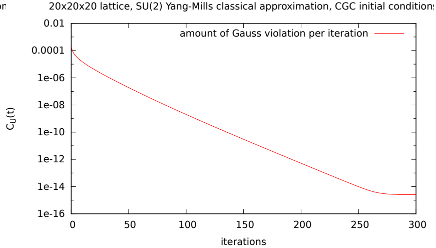


$\Rightarrow$ Computation of time dependent observables.

$\Rightarrow$ **Beware!** At this stage the results are cutoff dependent $\rightarrow$ real cutoff independence remains an open problem in real time classical simulations of heavy ion collisions (at least to my knowledge)

Gauss constraint





$\Rightarrow$ Gauss constraint has to be satisfied at every timestep, especially in the beginning

$\rightarrow$ It is violated by the initial configuration and needs to be restored.

$\rightarrow$ Although it is preserved by the EoM, it is violated numerically.

$\Rightarrow$ Details on the algorithm can be found in:

„Motion of Chern-Simmons number at High Temperatures under a chemical Potential"

Guy D. Moore, *Nucl. Phys. B 480 (1996) 657-688*

Beyond the classical approximation

Interactions between IR and UV:

$\Rightarrow$ Avoid the „scale setting“ problem and treat the UV properly.

Different approaches, e.g.:

- „N-body approach“: Adding a large number of „particle“ degrees off freedom to the lattice gauge theory. Derivation of interaction rules between these additional degrees of freedom and lattice degrees of freedom modeling the UV interaction *Moore, Hu, Müller, Phys . Rev. D58 (1998)*.
- „Boltzmann-Vlasov approach“: Consider continous particle population functions, resulting in Vlasov fields $W^a(x,\vec{v})$. The Vlasov field itself satisfies an EoM and induces a current on the classical EoM

$$D_\nu F^{\nu\mu,a} = j^{\mu,a}, \quad j^{\mu,a} = m_D^2 \int v^\mu W^a(x,\vec{v}) \frac{d\Omega_v}{4\pi}, \quad v_\mu D^\mu W^a(x,\vec{v}) = v_\mu F^{0\mu,a}(x)$$

Fermions:

$\Rightarrow$ Inclusion of fermion fields, that can not be treated classical, due to the Pauli principle.

- Induced fermion current on the classical Yang-Mills equation

$$\partial_\mu F^{\mu\nu,a} - g f^{abc} A_\mu^b F^{\mu\nu,c} = j^{\nu,a} = -g\mathrm{tr}\Big[F_A(x,x)\gamma^\nu T^a\Big],$$

with $F_A(x,x)$ the fermion statistical propagator evaluated in the background of the classical field A_μ.

Final conclusion

$\Rightarrow$ Hot bosonic theories can be approximated as classical statistical field theories within certain limits (weak coupling, MV-model,...).

$\rightarrow$ IR field modes need to be highly occupated, suppressing UV quantum effects.

$\Rightarrow$ Evolution of the physical system is governed by solving classical field equations of motion on the lattice. An additional constraint, referred to as Gauss law has to be satisfied.

$\rightarrow$ Real time is preserved, making it possible to calculate time-dependent observables.

$\Rightarrow$ No continuum limit can be achieved, since the classical theory is Rayleigh-Jeans divergent. Observables are lattice spacing/cutoff dependent.

$\rightarrow$ Some additional „scale setting“ or special treatment of the UV is required.

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