Application of Ewald's Method for Efficient Summation of Dyon Long-Range Potentials

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Motivation / Dyons in SU(2) YM Theory

- aim: understand quark-antiquark interaction for finite temperature $T < T_c$ (related talk: Müller-Preussker)
- evaluation of observable O with path integral

$$\langle O \rangle = \frac{1}{Z} \int \mathcal{D}A \; O[A] \exp\left(-S_{\mathrm{YM}}[A]\right) \qquad \text{Euclidean action } S_{\mathrm{YM}}[A]$$

$$Z = \int \mathcal{D}A \; \exp\left(-S_{\mathrm{YM}}[A]\right)$$

- approach to solve path integral: semi-classical approximation ⇒ fields with small action

⇒ modular space integration

$$\int \mathcal{D}A \rightarrow \prod_{j=1}^{n_D} \int d^3\mathbf{r}_j$$

- KvBLL calorons, (anti) selfdual classical solutions of YM equations for $T > 0$, periodic instantons with non-trivial holonomy, Kraan, van Baal ('98), Lee, Lu ('98)
- consider calorons to be dissolved in their constituents ⇒ dyon gas
- dyons: magnetic monopoles, splitting up the calorons topological charge

Procedure of Observable Evaluation

- calculate free energy between a static quark antiquark pair at separation $d = |\mathbf{r} - \mathbf{r}'|$ from

$$F_{Q\bar{Q}}(d) = -T \ \log \left\langle P(\mathbf{r}) P^{\dagger}(\mathbf{r}') \right\rangle$$

- choose dyon density ρ, temperature T
- consider dyons to be located in a volume at positions $\{\mathbf{r}_k\}$
- Polyakov-loop correlator $\langle P(\mathbf{r}) P^{\dagger}(\mathbf{r}') \rangle$ via

$$P(\mathbf{r}) = -\sin\left(\frac{1}{2T}\Phi(\mathbf{r})\right)$$

- gauge field (superposition of relevant component of the dyon gauge field in Abelian limit with magnetic charges $q = \pm 1$)

$$\Phi(\mathbf{r}) = \sum_{i=1}^{n_D} \frac{q_i}{|\mathbf{r}_i - \mathbf{r}|}$$

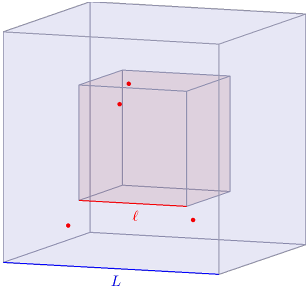
$\Rightarrow$ investigate behavior of free energy for growing quark separation

Problems with Long-range Dyon Fields

problem long-range potential $q/r \Rightarrow$ rather large volume is needed

$\Rightarrow$ two possible solutions

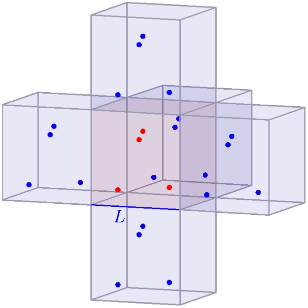
1. simulating a cubic spatial volume of length L, but evaluate observables within a spatial volume of length $\ell < L$



- slow convergence expected

$\Rightarrow$ extrapolation to infinite volume in ℓ and L

2. copy the cubic volume of length L infinitely often in all directions

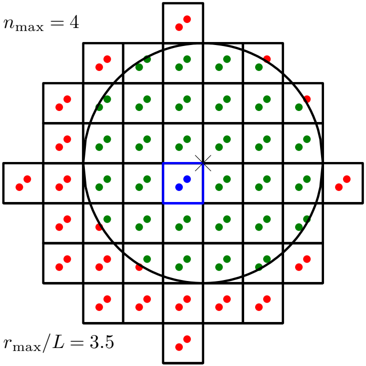


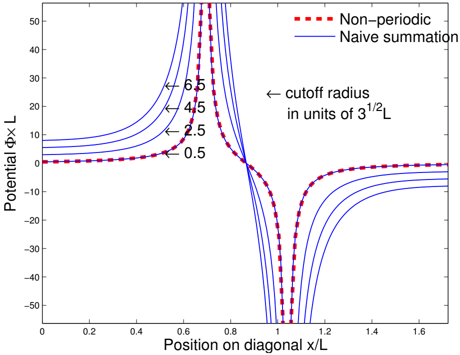
$\Rightarrow$ extrapolation in L

Naive periodic summation

1^{st} idea: sum all $1/r$ contributions in original volume and copies within radius r_{max}

$$\Phi(\mathbf{r}) = \underbrace{\sum_{\mathbf{n}\in\mathbb{Z}^3}^{|\mathbf{n}|\le n_{\text{max}}}}_{\text{sum over copies of volume}} \underbrace{\sum_{j=1}^{j<n_D,|\mathbf{r}-\mathbf{r}_j-\mathbf{n}L|<r_{\text{max}}}}_{\text{sum over dyons within sphere}} \frac{q_j}{|\mathbf{r}-\mathbf{r}_j+\mathbf{n}L|}$$





$\Rightarrow$ Better:
Ewald's method

Ewald's Method

- Ewald '21: split superposition of dyon potentials into short range part and long range part

$$\Phi(\mathbf{r}) = \sum_{\mathbf{n}\in\mathbb{Z}^3} \sum_{j=1}^{n_D} \frac{q_j}{|\mathbf{r}-\mathbf{r}_j-\mathbf{n}L|} = \Phi^{\text{Short}}(\mathbf{r}) + \Phi^{\text{Long}}(\mathbf{r})$$

- Φ^{Short} converges exponentially

$$\Phi^{\text{Short}}(\mathbf{r}) = \sum_{\mathbf{n}\in\mathbb{Z}^3} \sum_{j=1}^{n_D} \frac{q_j}{|\mathbf{r}-\mathbf{r}_j-\mathbf{n}L|} \operatorname{erfc}\left(\frac{|\mathbf{r}-\mathbf{r}_j-\mathbf{n}L|}{\sqrt{2}\lambda}\right)$$

- Φ^{Long} converges exponentially in Fourier space (with momenta $\mathbf{k} = \frac{2\pi}{L}\mathbf{n}$)

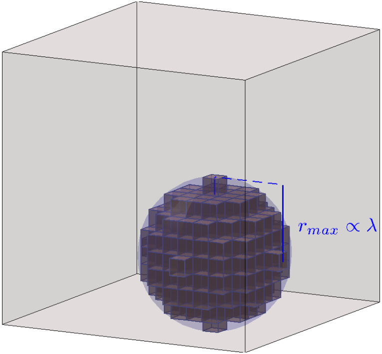
$$\Phi^{\text{Long}}(\mathbf{r}) = \frac{4\pi}{L^3} \sum_{\mathbf{k}\neq 0} \sum_{j=1}^{n_D} q_j e^{i\mathbf{k}(\mathbf{r}-\mathbf{r}_j)} \frac{e^{-\lambda^2\mathbf{k}^2/2}}{\mathbf{k}^2}$$

- divergences cancel in case of neutrally charged volume
- pedagogical introduction: "Ewald Summation for Coulombic Interactions in a Periodic Supercell", Lee, Cai ('09)

Ewald's Method more in Detail

Short-range

$$\Phi^{\text{Short}}(\mathbf{r}) = \sum_{\mathbf{n}\in\mathbb{Z}^3} \sum_j \frac{q_j}{|\mathbf{r}-\mathbf{r}_j-\mathbf{n}L|} \operatorname{erfc}\left(\frac{|\mathbf{r}-\mathbf{r}_j-\mathbf{n}L|}{\sqrt{2}\lambda}\right)$$

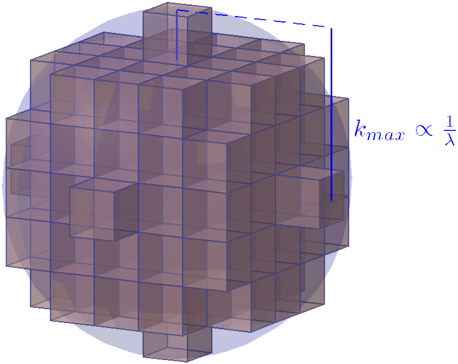


- λ: arbitrary parameter which controls the tradeoff between Φ^{Short} and Φ^{Long}
- due to exponential convergence of Φ^{Short}, evaluation can be restricted to dyons within a sphere of radius $r_{\text{max}} \propto \lambda$

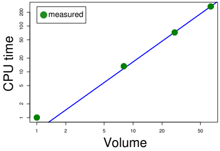
Ewald's Method more in Detail

Long-range

$$\Phi^{\text{Long}}(\mathbf{r}) = \frac{4\pi}{L^3} \sum_{\mathbf{k}\neq 0} e^{+i\mathbf{k}\mathbf{r}} \frac{e^{-\lambda^2\mathbf{k}^2/2}}{\mathbf{k}^2} \left(\sum_{j=1}^{n_D} q_j e^{-i\mathbf{k}\mathbf{r}_j} \right), \qquad \mathbf{k} = \frac{2\pi}{L}\mathbf{n}$$



- perform a sum over momenta pointing on volume copies (within a sphere of radius $k_{\text{max}} \propto \frac{1}{\lambda}$)
- calculate the structure functions once
- performance for evaluating Φ on a grid of $M \propto V$ points $\mathbf{r}$
  - Short-range: $\mathcal{O}(V\lambda^3)$
  - Long-range: $\mathcal{O}(V^2/\lambda^3)$



$\Rightarrow$ choose $\lambda^3 \propto \sqrt{V}$ for scaling of $\mathcal{O}(V^{3/2})$

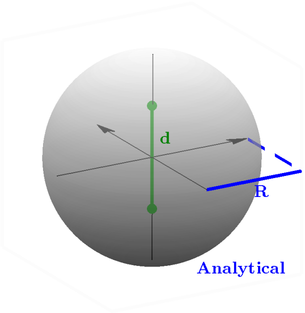
Numerical Results - Ewald's method

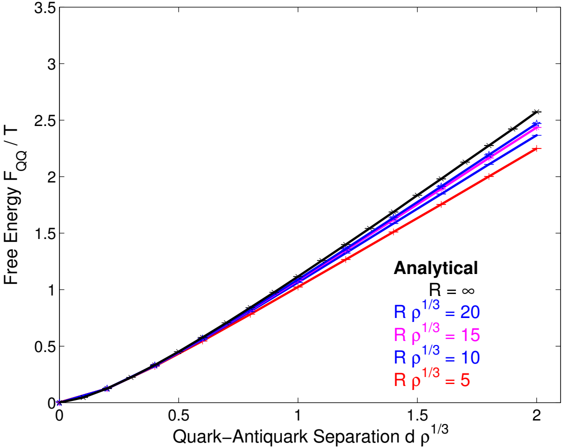
Setup and method of computation

- choose dyon density ρ and temperature T
- put dyons on random positions in a cubic spatial volume for 30 to 800 configurations
- vary dyon number (between 1 000 and 125 000) at fixed density to make extrapolation possible
- evaluate $\Phi(\mathbf{r})$ at various points $\mathbf{r}$ (analytical and Ewald's method)
- evaluate Polyakov-loop correlator and free energy from Φ

Numerical Results - Ewald's method

F. Bruckmann, S. Dinter, E.-M. Ilgenfritz, B. Maier, M. Müller-Preussker, M. Wagner, (2012), arXiv:1111.3158v2 [hep-ph]





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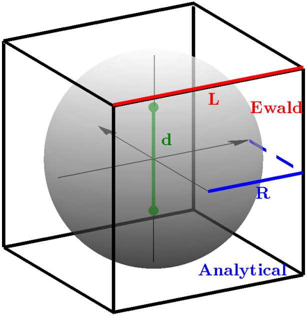

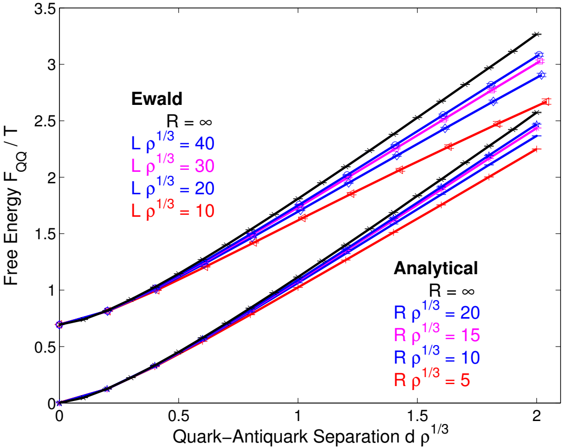

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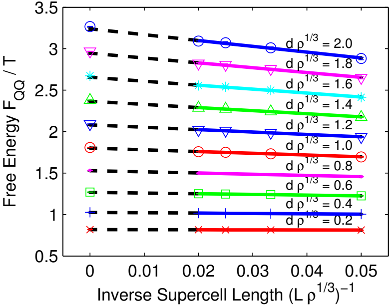

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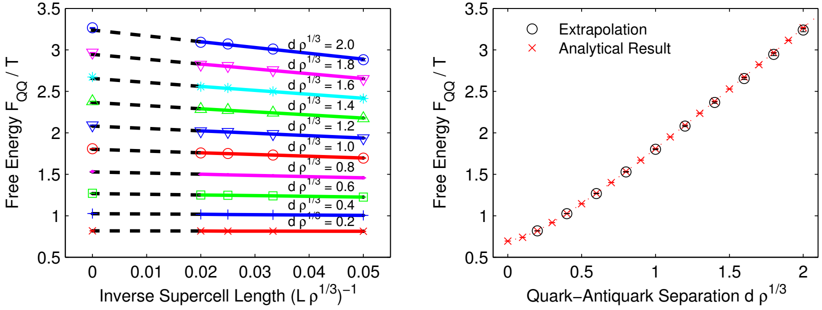

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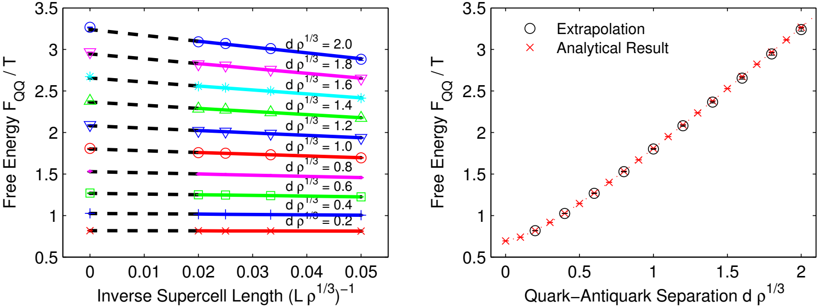

Result

- Ewald's method: controlled extrapolation to infinite volume – equal results to analytical calculations

Long-range Objects of Other Kind

- evaluate long-range potentials in powers of inverse distance

$$\Phi(\mathbf{r}) = \frac{\#}{r} + \frac{\#}{r^2} + \frac{\#}{r^3} + \ldots$$

- use **general** Ewald's method for power $p \geq 1$ – (Essmann, *et. al.* '95)

$$\Phi_p^{\text{Short}}(\mathbf{r}) = \sum_{\mathbf{n}} \sum_{j=1}^{n_D} \frac{q_j}{|\mathbf{r} - \mathbf{r}_j + \mathbf{n}L|^p} \, g_p\left(\frac{|\mathbf{r} - \mathbf{r}_j + \mathbf{n}L|}{\sqrt{2}\lambda}\right)$$

$$\Phi_p^{\text{Long}}(\mathbf{r}) = \frac{\pi^{3/2}}{V\left(\sqrt{2}\lambda\right)^{p-3}} \sum_j \sum_{\mathbf{k}} q_j \, \exp\left(i\,\mathbf{k}(\mathbf{r} - \mathbf{r}_j)\right) f_p\left(\frac{k\lambda}{\sqrt{2}}\right)$$

- with decay functions

$$g_p(x) = \frac{2}{\Gamma(p/2)} \int_x^\infty s^{p-1} \exp\left(-s^2\right) \, ds,$$

$$f_p(x) = \frac{2x^{p-3}}{\Gamma(p/2)} \int_x^\infty s^{2-p} \exp\left(-s^2\right) \, ds.$$

$\Rightarrow$ long-range potentials can be evaluated in powers of $1/r$ for an efficient algorithm

Summary & Outlook

Summary

- Ewald's method: controlled extrapolation to infinite volume for long-range objects
- nice agreement with infinite volume analytical results for dyon model
- potential power to treat any long-range objects

Possibilities for Dyon Model

- simulate an interacting dyon model by expanding an "effective action" $S_{\mathrm{eff}} = \frac{1}{2}\sum_j \sum_i \log\left(1 - \frac{2q_i q_j}{\pi|\mathbf{r}_i - \mathbf{r}_j|}\right)$ (based on the moduli space metric) in inverse powers of r using Ewald's method
- understand effects of interacting/non-interacting dyon model on the free energy

SU(2) YM Action

$$S[A] = \frac{1}{4g^2} \int d^4x \; F^a_{\mu\nu} \; F^a_{\mu\nu},$$

$$F^a_{\mu\nu} = \partial_\mu A^a_\nu - \partial_\nu A^a_\mu + \varepsilon^{abc} A^b_\mu A^c_\nu$$