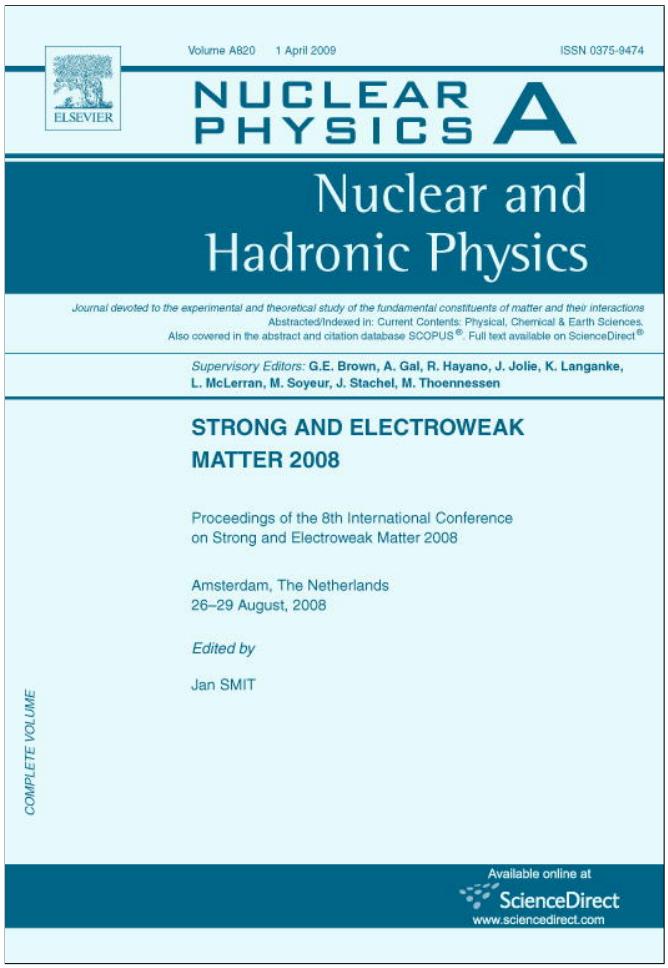

Available online at www.sciencedirect.com
ScienceDirect
ELSEVIER
Nuclear Physics A 820 (2009) 57c–64c
NUCLEAR PHYSICS A
www.elsevier.com/locate/nuclphysa

Two complex problems on the lattice: transport coefficients and finite chemical potential

Gert Aarts
Department of Physics, Swansea University, Swansea, United Kingdom

Abstract

After a few remarks about the problem of extracting transport coefficients from lattice QCD calculations, I report on recent developments in applying stochastic quantization and complex Langevin dynamics to field theories with a complex action due to a nonzero chemical potential. First results demonstrate that the sign problem poses no obstacle for this approach, even in the thermodynamic limit. I conclude with a comparison of two simple one-link models, describing a euclidean system at finite chemical potential and a Minkowski system in real time.

Key words: Lattice gauge theory, quark-gluon plasma, finite-temperature field theory
PACS: 11.15.Ha, 12.38.Mh, 11.10.Wx

1. Introduction

The euclidean lattice formulation of QCD provides a nonperturbative formulation of the theory of strong interactions, suitable for numerical simulations. This allows a detailed study of thermodynamic quantities, such as pressure, entropy and susceptibilities, and of the finite-temperature crossover between the confined and the deconfined phase (see e.g. Ref. [1]). However, for some problems standard methods are not adequate. In this contribution I discuss two of these problems. In the first case, the questions asked are not easily answered from knowledge of euclidean-time correlation functions alone, but instead require access to particular real-time correlators such as spectral functions. This is relevant for transport properties of the quark-gluon plasma and for in-medium modifications of hadrons. In the second case the weight in the euclidean path integral is not real, leading to the infamous sign problem. This prohibits the use of importance

Email address: g.aarts@swan.ac.uk (Gert Aarts).

0375-9474/$ – see front matter
doi:10.1016/j.nuclphysa.2009.01.019

sampling, the framework underlying essentially all methods used to generate ensembles in lattice QCD simulations. This is relevant for QCD at nonzero baryon density.

2. Transport and spectral functions

Conserved currents, such as the energy-momentum tensor $T^{\mu\nu}$ and the electromagnetic current j^μ, result in hydrodynamic behaviour on long length and timescales. Hydrodynamic structure is best visible in current-current correlation functions in real time, such as spectral functions. A nonperturbative determination of spectral functions ρ using euclidean correlators G_E obtained with lattice simulations, via the relation

$$G_E(\tau,\mathbf{p}) = \int_0^\infty \frac{d\omega}{2\pi}\, K(\omega,\tau)\rho(\omega,\mathbf{p}), \qquad K(\omega,\tau) = \frac{\cosh[\omega(\tau-1/2T)]}{\sinh(\omega/2T)}, \tag{1}$$

is quite involved. One widely used approach is the Maximal Entropy Method (MEM) [2]. However, in the hydrodynamical regime ($\omega, |\mathbf{p}| \ll T$) the problem is particularly difficult due the insensitivity of the euclidean correlator to details of the spectral function at small ω [3]. Moreover, the most commonly used MEM algorithm is inherently unstable at small energies and needs to be modified in order to be applicable [4]. There exist recent lattice calculations of the electrical conductivity [4], the shear viscosity [5] and the bulk viscosity [6]. Transport and hydrodynamics from the lattice have been discussed in detail in two plenary talks at the *Lattice* conferences in the past two years [7,8]. Therefore I restrict myself to some remarks and refer to those contributions for more details.

What euclidean correlators should be considered? Kubo relations relate transport coefficients to the slope of spectral functions as the energy ω is taken to zero. For example, the shear viscosity η, bulk viscosity ζ, and conductivity σ are determined by

$$\eta = \lim_{\omega\to 0}\frac{\rho^{12,12}(\omega)}{2\omega}, \qquad \zeta = \frac{1}{9}\lim_{\omega\to 0}\frac{\rho^{ii,jj}(\omega)}{2\omega}, \qquad \sigma = \lim_{\omega\to 0}\frac{\rho^{11}(\omega)}{2\omega}, \tag{2}$$

in terms of the spectral functions

$$\rho^{\mu\nu,\kappa\sigma}(\omega) = \int d^4x\, e^{i\omega t}\langle[T^{\mu\nu}(t,\mathbf{x}),T^{\kappa\sigma}(0)]\rangle, \quad \rho^{\mu\nu}(\omega) = \int d^4x\, e^{i\omega t}\langle[j^\mu(t,\mathbf{x}),j^\nu(0)]\rangle. \tag{3}$$

In analytical calculations it is sometimes useful to add an exactly conserved charge, such as $\mathcal{E} = \int d^3x\, T^{00}$ or $Q = \int d^3x\, j^0$, to the operators in Eq. (3). For instance, for the bulk viscosity one may consider correlators of T^μ_μ instead of T^{ii} [6,9]. While this is harmless in analytical calculations, it makes a difference when reconstructing spectral functions from the lattice. The reason is that lattice correlators and spectral functions are affected in a particular manner: if a conserved charge is added, lattice correlators will receive a τ-independent contribution of the form $T\Xi$, where Ξ is the corresponding charge susceptibility, while spectral functions will receive a contribution $\Xi 2\pi\omega\delta(\omega)$. This singular contribution at the origin violates the smoothness condition assumed by most methods used to obtain spectral functions from euclidean correlators and should therefore be avoided. This issue was discussed already some time ago in the context of meson spectral functions and the current $j^\mu = \bar\psi\gamma^\mu\psi$ [10,11]. For massless noninteracting fermions the delta function contribution at the origin is equal for $\rho^{00}(\omega)$ and $\rho^{ii}(\omega)$ and cancels in

the combination $\rho^\mu_\mu(\omega)$. However, interactions will smear out this delta function in the case of ρ^{ii} (resulting in a finite conductivity), whereas ρ^{00} is unchanged due to charge conservation (only the value of the susceptibility is affected). The cancelation therefore no longer holds and $\rho^\mu_\mu(\omega)$ is not smooth as $\omega \to 0$.

As a second remark, let me note again that euclidean correlators are insensitive to details of spectral functions when the transport contribution is narrow and most of the weight is concentrated at $\omega \ll T$. It is not so difficult to find cases where access to transport coefficients from euclidean correlators is virtually impossible. This has been discussed for weakly coupled theories [3], heavy quark diffusion [12] and, more recently, bulk viscosity in a weakly coupled theory or near a second order phase transition [9]. (For a lattice study of energy-momentum tensor correlators near the second order transition in SU(2) gauge theory, see Ref. [13].) From the viewpoint of the lattice, it would be more interesting to find instead examples where the transport peak is not narrow such that transport coefficients might potentially be accessible. So far this has been addressed mostly in theories with a gravity dual in the strong coupling limit [14–16]. Since these results provide an important motivation, more examples would be welcome.

3. Finite chemical potential and the sign problem

I now turn to euclidean field theories with a complex action due to the presence of a chemical potential. In this case the weight in the path integral is not real and importance sampling cannot be used. This is commonly referred to as the sign problem. If the weight is written as $e^{-S} = |e^{-S}|e^{i\varphi}$, we may consider the partition functions of the full and the phase-quenched (pq) theories, defined as

$$Z_{\rm full} = \int D\phi\, e^{-S}, \qquad Z_{\rm pq} = \int D\phi\, |e^{-S}|. \tag{4}$$

The phase-quenched theory has a real positive weight and is accessible with standard techniques. The sign problem is best demonstrated by the expression for the expectation value of the phase factor in the phase-quenched theory,

$$\langle e^{i\varphi}\rangle_{\rm pq} = \frac{Z_{\rm full}}{Z_{\rm pq}} = e^{-\Omega\Delta f}, \tag{5}$$

where Ω is the (four)volume and Δf is the difference between the free energy densities in the full and the phase-quenched theories. Eq. (5) shows that the average phase factor goes to zero in the thermodynamic limit, resulting in an overlap problem between the full and the phase-quenched theories. In other words, the important configurations in the full theory differ in an essential way from those in the phase-quenched case. The question is how to find those relevant configurations in a numerical simulation.

Recently, this problem was reconsidered [17,18] using stochastic quantization and complex Langevin dynamics [19–21]. This approach has a long history and was studied intensely in the 80's [22]. It was revived in the context of nonequilibrium quantum field dynamics in Minkowski spacetime in Refs. [23–25] and subsequently applied to euclidean theories at nonzero chemical potential. We have considered SU(3) gauge theory with heavy quarks [17] and the scalar O(2) model [18], both at nonzero chemical potential.

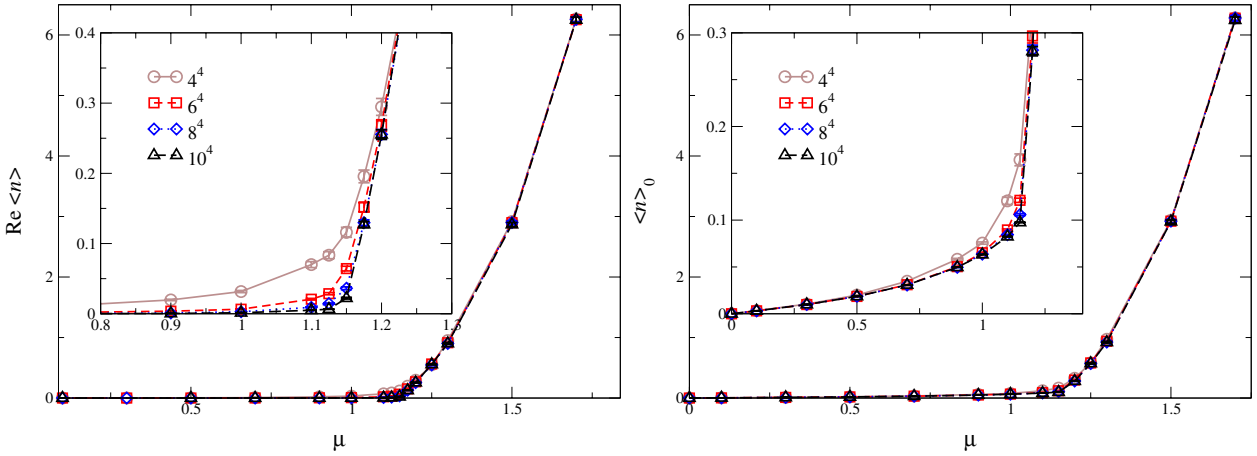

Fig. 1. Real part of the density in the full (left) and the phase-quenched (right) relativistic Bose gas as a function of chemical potential on lattices with size N^4, with $N = 4, 6, 8, 10$ ($m = \lambda = 1$).

The essence of this approach is that the weight is obtained as the equilibrium distribution of a stochastic process, described by a Langevin equation. For a scalar field the Langevin equation reads

$$\phi(x, \theta + \epsilon) = \phi(x, \theta) - \epsilon \frac{\delta S[\phi]}{\delta \phi(x, \theta)} + \sqrt{\epsilon}\eta(x, \theta), \tag{6}$$

while in SU(N) gauge theories, the links are updated according to

$$U(\theta + \epsilon) = R(\theta)U(\theta), \qquad R = \exp\left[i\lambda_a \left(\epsilon K_a + \sqrt{\epsilon}\eta_a\right)\right], \qquad K_a = -D_a S[U]. \tag{7}$$

Here $\theta = n\epsilon$ is the Langevin time, ϵ is the Langevin timestep, the noise is Gaussian

$$\langle \eta(\theta) \rangle = 0, \qquad \langle \eta(\theta)\eta(\theta') \rangle = 2\delta_{nn'}, \tag{8}$$

λ_a are the Gell-mann matrices and all other indices are suppressed. When the action is complex, the dynamics and field variables are complexified. Explicitly, a real scalar field is written as $\phi \to \phi^{\mathrm{R}} + i\phi^{\mathrm{I}}$, while an SU($N$) matrix is now an element of SL(N, $\mathbb{C}$). More details can be found in the references listed above.

I now discuss the results obtained so far. I start with the most recent results in the relativistic Bose gas, i.e. a complex scalar field with O(2) symmetry, at nonzero chemical potential [18]. The action satisfies $S^*(\mu) = S(-\mu)$. Just as QCD, this theory has what is known as a Silver Blaze problem [26]. At zero temperature the theory is in vacuum as long as the chemical potential μ is below the critical value μ_c (when interactions are ignored, $\mu_c = m$, the minimal energy of excitations). When $\mu > \mu_c$, the theory enters a Bose condensed phase and the density is nonzero. The strict μ-independence of bulk physical quantities as long as $\mu < \mu_c$, even though μ is present microscopically, is the Silver Blaze problem. We have analysed the full and the phase-quenched theory using stochastic quantization. The results for the density are shown in Fig. 1. On the left, we show the density in the full theory, as a function of the chemical potential, for lattices of size N^4, with $N = 4, 6, 8, 10$. The parameters in the scalar potential are $m = \lambda = 1$, in lattice units. The inset shows a blowup of the transition region. We observe the transition between the groundstate with zero density and the Bose condensed phase at $\mu = \mu_c \sim 1.15$. A real phase transition can only occur in the thermodynamic limit and we find that the transition becomes sharper as the volume is increased, as expected. On

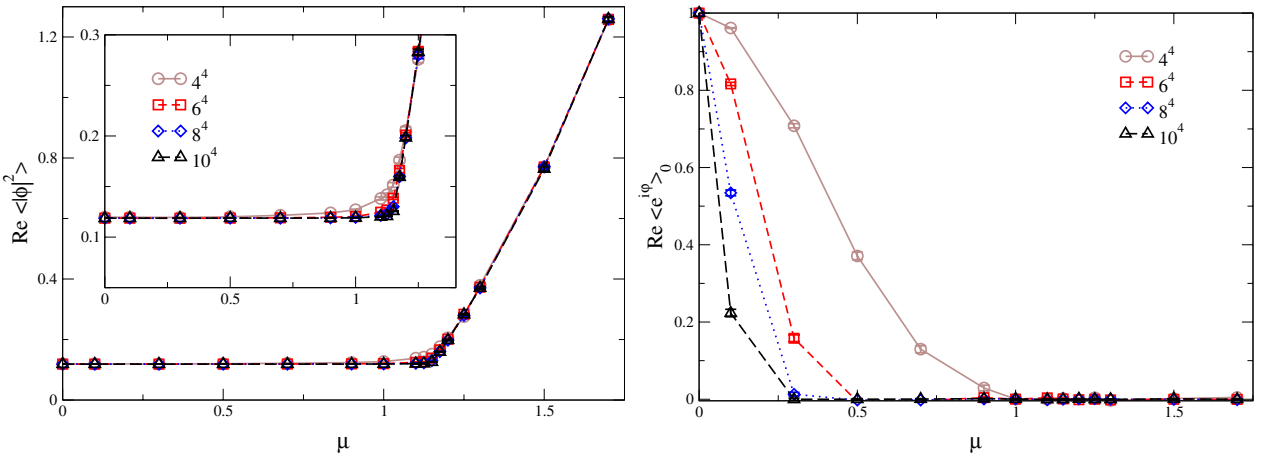

Fig. 2. Real part of the square of the field modulus in the full theory (left) and the average phase factor in the phase-quenched theory (right).

the right, the density is shown in the phase-quenched theory. Here we observe a nonzero density for all values of the chemical potential. This is similar to what is expected in phase-quenched QCD (when $m_\pi/2 < \mu < m_N/3$). The cancelation of the μ-dependence of the density in the full theory is due to the phase factor $e^{i\varphi}$ and therefore the result of the sign problem. We conclude that the complexity of the action and the Langevin dynamics deliver precisely what is expected.

The μ-independence also hold for other observables. In Fig. 2 (left) we show the square of the field modulus $|\phi|^2$ as obtained from complex Langevin dynamics. The value at zero chemical potential is nonzero due to quantum fluctuations. As μ is increased, the observable remains constant until the critical value is reached. This demonstrates the Silver Blaze feature in an impressive manner. On the right the average phase factor in the phase-quenched theory is shown. As indicated above, this observable gives an indication of the severeness of the sign problem: the phase factor goes to zero at larger chemical potential on all lattices and vanishes in the thermodynamic limit for all nonzero values of the chemical potential. This is precisely how the average phase factor is expected to behave [27]. Nevertheless, this approach can handle the sign problem without difficulties and there is no problem in taking the thermodynamic limit.

Concerning QCD we have considered SU(3) gauge theory coupled to three flavours of quarks in the heavy quark limit, starting from Wilson fermions in the hopping expansion [17]. In this limit, the complex fermion determinant is approximated as

$$\det M \approx \prod_{\mathbf{x}} \det\left(1 + he^{\mu/T}\mathcal{P}_{\mathbf{x}}\right)^2 \det\left(1 + he^{-\mu/T}\mathcal{P}_{\mathbf{x}}^{-1}\right)^2, \tag{9}$$

where $h = (2\kappa)^{N_\tau}$ and $\mathcal{P}_{\mathbf{x}}^{(-1)}$ are the (conjugate) Polyakov loops. We emphasize that the gauge action is preserved completely and that the determinant satisfies the basic property $[\det M(\mu)]^* = \det M(-\mu)$.

First results in this theory are obtained on a lattice of size 4^4, with fixed $\beta = 5.6$ and $\kappa = 0.12$. In Fig. 3 we show the (conjugate) Polyakov loops (left) and the density (right) as a function of chemical potential. The results indicate a transition from a confined low-density phase to a deconfined high-density phase. Again we address the severeness of the sign problem by studying the phase of the determinant. In this case we present the phase factor $e^{2i\phi} = \det M(\mu)/\det M(-\mu)$ in the full theory, and not in the phase-

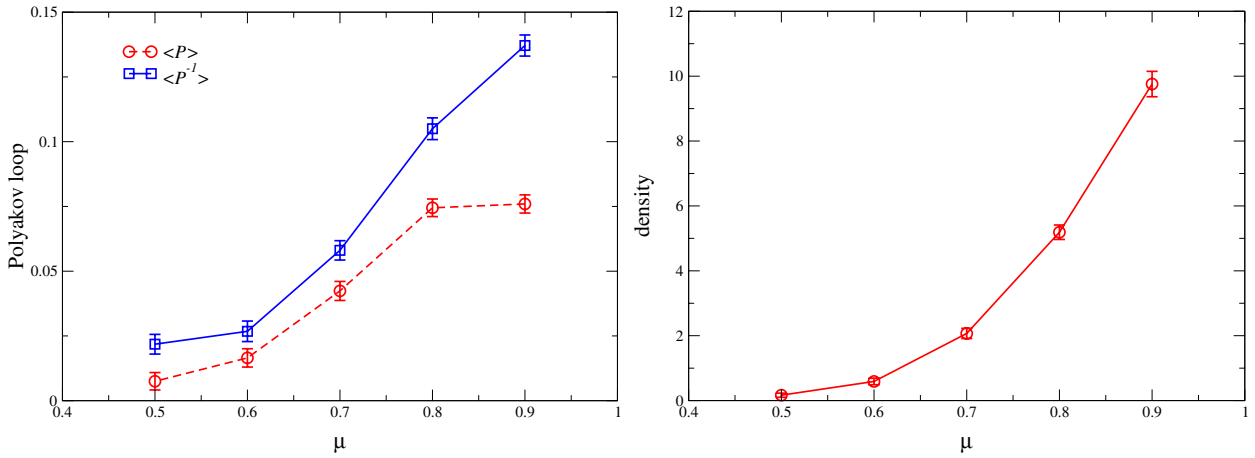

Fig. 3. Real part of the (conjugate) Polyakov loops $\langle P\rangle$ and $\langle P^{-1}\rangle$ (left) and the density $\langle n\rangle$ (right) as a function of μ for QCD in the heavy quark limit, with $\beta = 5.6$, $\kappa = 0.12$, and $N_f = 3$ on a 4^4 lattice.

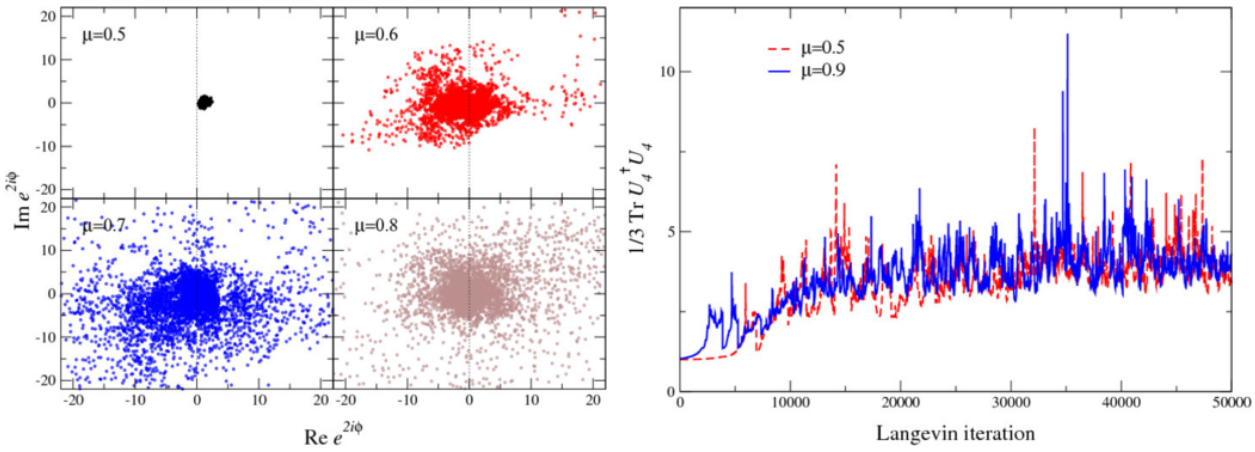

Fig. 4. Left: Scatter plot of $e^{2i\phi} = \det M(\mu)/\det M(-\mu)$ during the Langevin evolution for various values of μ. Right: Deviation from SU(3), $\mathrm{Tr}\, U_4^\dagger U_4/3$ during the Langevin evolution, for $\mu = 0.5$ and 0.9.

quenched theory. A scatter plot of the real and imaginary parts of this observable is shown in Fig. 4 (left). When the chemical potential is zero, the phase factor is equal to 1. At larger chemical potential, we find that phase fluctuations increase dramatically. Yet, observables such as the Polyakov loop and the density are under control, with reasonable errors. During the complex Langevin evolution, link variables are no longer in SU(3), instead they take values in SL(3, $\mathbb{C}$). This can analysed by computing $\mathrm{Tr}\, U_4^\dagger U_4/3$, which equals 1 in SU(3) and is ≥ 1 in SL(3, $\mathbb{C}$). We show this quantity as a function of Langevin time in Fig. 4 (right). We observe that after the initial thermalization stage it is clearly distinct from 1, but remains bounded. This indicates that the sequence of configurations generated with complex Langevin dynamics differs in an essential way from configurations constrained to be in SU(3). For more discussion, see Refs. [17,28].

4. Chemical potential versus Minkowski dynamics

At zero chemical potential the euclidean action is real. In this case one can use real Langevin evolution and apply standard proofs to demonstrate that the method will

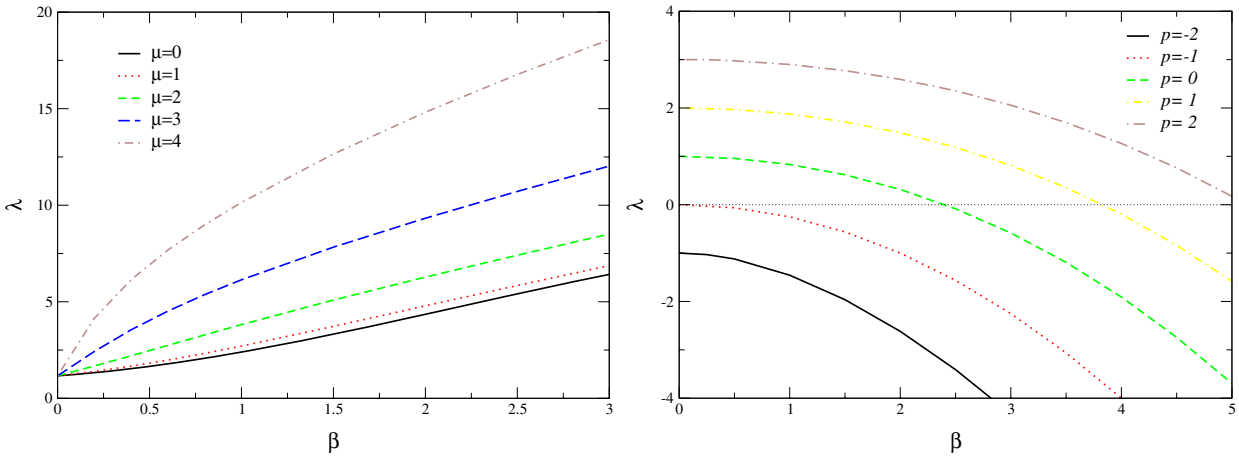

Fig. 5. Smallest nonzero eigenvalue of the complex Fokker-Planck operator in the one-link U(1) model as a function of β for various values of μ at $\kappa = 1/2$ in the euclidean case (left) and for various values of the reweighting parameter p in the Minkowski case (right).

converge to the correct distribution e^{-S}. Zero chemical potential provides therefore a useful reference point, see e.g. Fig. 2 (left). In the case of Minkowski (real-time) dynamics, where the weight in the path integral is e^{iS}, such a reference point is absent. Heuristically, one may therefore expect real time to be more difficult than nonzero chemical potential. To quantify this, we compared two simple one-link U(1) models [17], building on the work in Ref. [25]. The partition functions are

$$Z = \int_{-\pi}^{\pi} \frac{dx}{2\pi}\, e^{\beta \cos x} \left[1 + \kappa \cos(x - i\mu)\right], \tag{10}$$

at nonzero μ and

$$Z = \int_{-\pi}^{\pi} \frac{dx}{2\pi}\, e^{i\beta \cos x + ipx}, \tag{11}$$

in real time. The term px, with p integer, is a reweighting term, used to stabilize the Langevin dynamics [25]. In the euclidean case the Fokker-Planck equation for the complex distribution $P(x,\theta)$ reads

$$\frac{\partial}{\partial\theta} P(x,\theta) = \frac{\partial}{\partial x}\left(\frac{\partial}{\partial x} + \frac{\partial S}{\partial x}\right) P(x,\theta). \tag{12}$$

The zero eigenvalue, corresponding to the stationary distribution e^{-S}, always exists. The solution of the Fokker-Planck equation can therefore be written as

$$P(x,\theta) = \frac{e^{-S}}{Z} + \sum_{\lambda\neq 0} e^{-\lambda\theta} P_\lambda(x). \tag{13}$$

For the Minkowski case, $-S$ is replaced with iS in the equations above. Convergence of the complex Fokker-Planck equation is determined by the eigenvalues λ, which we studied numerically [17]. The smallest nonzero eigenvalue is shown in Fig. 5 as a function of β in the euclidean case for various values of μ (left) and the Minkowski case for various

values of p (right). In the first case, one sees that the eigenvalues are strictly positive, for all values of β and μ, indicating convergence of the complex Fokker-Planck equation. In the second case, eigenvalues turn negative for larger values of β; the value of β where this occurs depends on the parameter p. While these results do not prove or disprove convergence for the complexified Langevin dynamics (for this the real Fokker-Planck equation for the real distribution $\rho(x, y, \theta)$ has to be studied), they are an indication of the difference between the two theories when applying complex Langevin dynamics, with the euclidean one at nonzero chemical potential being better behaved.

5. Acknowledgments

It is a pleasure to thank the organizers for the stimulating Conference. In particular I am grateful to Jan Smit, not only for this event, but also for the continuous support since 1995. I thank Nucu Stamatescu for collaboration and encouragement and Simon Hands, Harvey Meyer and Erhard Seiler for discussion. This work is supported by STFC.

References

[1] C. Schmidt, these proceedings, arXiv:0810.4024 [hep-lat].
[2] M. Asakawa, T. Hatsuda and Y. Nakahara, Prog. Part. Nucl. Phys. **46**, 459 (2001) [hep-lat/0011040].
[3] G. Aarts and J. M. Martínez Resco, JHEP **0204** (2002) 053 [hep-ph/0203177].
[4] G. Aarts, C. Allton, J. Foley, S. Hands and S. Kim, Phys. Rev. Lett. **99** (2007) 022002 [hep-lat/0703008].
[5] H. B. Meyer, Phys. Rev. D **76** (2007) 101701 [0704.1801 [hep-lat]].
[6] H. B. Meyer, Phys. Rev. Lett. **100** (2008) 162001 [0710.3717 [hep-lat]].
[7] G. Aarts, PoS **LAT2007** (2007) 001 [0710.0739 [hep-lat]].
[8] H. B. Meyer, PoS **LAT2008** (2008) 017 [0809.5202 [hep-lat]].
[9] G. D. Moore and O. Saremi, JHEP **0809**, 015 (2008) [0805.4201 [hep-ph]].
[10] F. Karsch, E. Laermann, P. Petreczky and S. Stickan, Phys. Rev. D **68** (2003) 014504 [hep-lat/0303017].
[11] G. Aarts and J. M. Martínez Resco, Nucl. Phys. B **726** (2005) 93 [hep-lat/0507004].
[12] P. Petreczky and D. Teaney, Phys. Rev. D **73** (2006) 014508 [hep-ph/0507318].
[13] K. Huebner, F. Karsch and C. Pica, arXiv:0808.1127 [hep-lat].
[14] D. Teaney, Phys. Rev. D **74**, 045025 (2006) [hep-ph/0602044].
[15] P. Kovtun and A. Starinets, Phys. Rev. Lett. **96**, 131601 (2006) [hep-th/0602059].
[16] R. C. Myers, A. O. Starinets and R. M. Thomson, JHEP **0711**, 091 (2007) [0706.0162 [hep-th]].
[17] G. Aarts and I. O. Stamatescu, JHEP **0809** (2008) 018 [0807.1597 [hep-lat]].
[18] G. Aarts, arXiv:0810.2089 [hep-lat].
[19] G. Parisi and Y. s. Wu, Sci. Sin. **24** (1981) 483.
[20] G. Parisi, Phys. Lett. B **131** (1983) 393.
[21] J. R. Klauder and W. P. Petersen, SIAM J. Numer. Anal. 22 (1985) 1153; J. Stat. Phys. 39 (1985) 53.
[22] P. H. Damgaard and H. Huffel, Phys. Rept. **152** (1987) 227.
[23] J. Berges and I. O. Stamatescu, Phys. Rev. Lett. **95** (2005) 202003 [hep-lat/0508030].
[24] J. Berges, S. Borsanyi, D. Sexty and I. O. Stamatescu, Phys. Rev. D **75** (2007) 045007 [hep-lat/0609058].
[25] J. Berges and D. Sexty, Nucl. Phys. B **799** (2008) 306 [0708.0779 [hep-lat]].
[26] T. D. Cohen, Phys. Rev. Lett. **91** (2003) 222001 [hep-ph/0307089].
[27] K. Splittorff and J. J. M. Verbaarschot, Phys. Rev. Lett. **98** (2007) 031601 [hep-lat/0609076].
[28] G. Aarts and I. O. Stamatescu, PoS **LAT2008** (2008) 176 [0809.5227 [hep-lat]].