Preface

This volume presents an overview of the research conducted in 2003/2004 on the high performance computing systems of the High Performance Computing Center Stuttgart (HLRS). It also reflects the changes in organization and focus of the center which are briefly described here. In 2003 HLRS has teamed up with the University of Karlsruhe in the Competence Center for High Performance Computers of the State of Baden-Württemberg (hkz-bw). This cooperation was gradually deployed during 2004 and has helped to improve the basic services. With an extension of the cooperation to other universities HLRS aims at further strengthening its ties with researchers in the State of Baden-Württemberg. Users should benefit from such a larger pool of expertise and the transformation of basic research into simulation results should be improved.

The key to high performance computing is the availability of a competitive computer system. HLRS was able to sign a contract with NEC in early 2004 for a next generation high performance computing system that will serve
as a national HPC resource for Germany. That system will be the fastest European system in sustained level of performance when being installed in early 2005. The high level of sustained performance is achieved by using vector processors. To meet the requirements of a wide variety of users the system is complemented by an HP cluster system installed at Karlsruhe. This system will serve as a state-wide simulation resource. A high level of performance can thus be achieved for at least two types of architectures, and discussions are under way how to close the PC-cluster gap.

The variety of architectures is again reflected in the contributions of this volume. They were presented at the 7th HLRS Results and Review Workshop on October 4-5 at the HLRS and show a wide spectrum of applications. Altogether 32 contributions were presented in oral and poster communications, selected from all projects processed at the HLRS and at the SSC Karlsruhe since October 2003. The investigations reported were initiated at the universities in Aachen, Berlin, Bielefeld, Bochum, Bremen, Dresden, Erlangen-Nürnberg, Freiburg, Hamburg-Harburg, Heidelberg, Jena, Karlsruhe, Konstanz, Mainz, Siegen, Stuttgart, Würzburg, and at the German Center for Aero- and Astronautics in Braunschweig, the Kiepenheuer-Institut für Sonnenphysik, Freiburg, the Landessternwarte Königstuhl, Heidelberg, the Materials Research Center, and the Fraunhofer Institute for Mechanics of Materials in Freiburg. Several foreign universities and research centers participated in the investigations: The University of Jyväskylä, Finland, the Brookhaven and the Los Alamos National Laboratories, USA, and the Institute of Theoretical and Applied Mechanics of the Russian Academy of Sciences in Akademgorodok.

The contributions are loosely arranged according to their disciplines in the six chapters physics, solid state physics, computational fluid dynamics, chemistry, computer science, and earth sciences. Seven of the 32 contributions are concerned with the numerical solution of problems in physics, six in solid state physics, eleven in computational fluid dynamics, four in chemistry, and two each in computer science, and earth sciences.

The contributions in physics cover a wide range of topics. The first two in astrophysics from the Landessternwarte Königstuhl near Heidelberg are continuations of previous work: Large scale hydrodynamic simulations of a cooled, pulsed jet in symbiotic stars, and magnetohydrodynamic simulations of the interaction of jets with a galactic wind. The third contribution is also concerned with a problem in astrophysics: Thermal convection and generation of magnetic fields inside a fully convective star is studied at the Kiepenheuer-Institut für Sonnenphysik in Freiburg. The fourth contribution describes the continuation of studies of the structural and spectroscopic properties of porphyrin-derived polymers, previously carried out at the University of Münster, and now continued at the International University Bremen. The next contribution is from the University of Mainz. It employs large scale semi-grandcanonical Monte Carlo simulations and finite size scaling to study the molecular extension and intermolecular pair-correlation function in thin films with hard, non-preferentially adsorbing surfaces. Finally the fifth and sixth
contributions deal again with problems of different nature: Simulations of suspensions are described, carried out with two different methods of solutions at Stuttgart University, and a numerical investigation of the free energies of static quark antiquark pairs in quenched QCD as well as in full QCD, being under way at the University of Bielefeld in a cooperation with Brookhaven National Laboratory.

In the chapter on solid state physics, the first contribution, carried out at the University of Konstanz, reports on new insights into electron transport in nanowires, elastic constants in model colloids and related subjects. The second paper is a continuation of the previous ab initio simulations of clusters at Freiburg University, the Fraunhofer Institute for Mechanics of Materials in Freiburg, the Freiburg Materials Center of Research, and at the University of Jyväskylä in Finland: Density-functional calculations are compared with high-resolution photoelectron spectroscopy. At the University of Mainz large scale molecular dynamics simulations are used to study amorphous alkali silicates, and at the University of Jena the adsorption on methylicloride on the Si(001) surface is studied by first-principles calculations. Quantum Monte Carlo simulations are used to study the dynamics and critical properties of strongly correlated systems relevant to cold quantum gases and high-Tc superconductivity at Stuttgart University. The last contribution comes from the University of Würzburg. It describes a numerical study of the doping dependence of the spectral function of the n-type cuprates.

In the third chapter on computational fluid dynamics the laminar-turbulent transition in a hypersonic boundary layer and - in a second project - the interaction between a shock wave and a turbulent boundary layer are studied at the University of Dresden in cooperation with the Institute of Theoretical and Applied Mechanics of the Russian Academy of Sciences in Akademgorodok. At Stuttgart University the effect of suction in a three-dimensional incompressible boundary layer is investigated. In another project the effect of enhanced mixing on supersonic combustion is studied with numerical simulations and experiments. At the Technical University of Hamburg-Harburg the incompressible flow around a sphere with a tripping wire is studied with the LES method, and at the University of Karlsruhe the passive heat transfer in a turbine cascade is investigated also with the LES method, with oncoming wakes taken into account. Extensive studies of aeroelastic problems occurring at cruise and offdesign conditions of high subsonic aircraft are studied at Aachen University of Technology. At the DLR Braunschweig high-lift conditions of aircrafts are studied solving Reynolds-averaged Navier-Stokes equations. While the previously mentioned investigations are all related to aerodynamic problems the following is of completely different nature: The electrostatic spray-painting process is studied with numerical methods at Stuttgart University. The last two contributions, carried out at the Universities of Erlangen-Nürnberg and Stuttgart, respectively, describe the application of the Lattice Boltzmann method for detailed flow simulation in complex three-dimensional geometries, and algorithmic improvements
of a numerical solution for the simulation of hypersonic non-equilibrium flows.

The chapter dealing with problems in chemistry contains four contributions. At Berlin University of Technology quantum chemical computations are carried out with the aim to assess the reactivity of various quite different Michael acceptors, while at Stuttgart University quantum chemical calculations at the MP2/[aug]-cc-pVDZ level were employed to generate a two-dimensional potential energy surface for an unusual double proton transfer reaction, in which the region around the transition state is characterized by a plateau of almost constant energy. The third investigation is from the University of Siegen, where the quantum reactive scattering for ion-neutral collisions is studied by solving the time-dependent Schrödinger equation. In the last contribution ab-initio molecular dynamics simulations of the simplest amino acid, glycine, at the water/pyrite interface under extreme pressure/temperature conditions are reported.

The last four contributions report on problems in computer science and earth sciences. At the High Performance Computing Center of the Dresden University of Technology a performance analysis of NEC computers was carried out with the PARbench benchmark system. In another investigation of this field at the University of Karlsruhe, the benchmark for MPI implementations SKaMPI is extended to the evaluation of virtual topologies and related topics, while in the first investigation in earth sciences, carried out at the Free University of Berlin, the propagation of elastic waves in two- and three-dimensional media containing cracks, pores or free surfaces is studied. The last contribution reports on a joint project of the University of Jena and the Los Alamos National Laboratory, USA. The investigation combines a two-dimensional convection-fractionation model that simulates the growth of the continents and of the geo-chemically complementary depleted mantle reservoir, with another model that simulates the three-dimensional generation of oceanic lithospheric plates sheet-like downdwellings in a spherical-shell mantle.

The continued support of the Land Baden-Württemberg in promoting and supporting high-performance computing is gratefully acknowledged. Many projects processed on the machines of the HLRS and the SSC could not have been carried out without the support of the Deutsche Forschungsgemeinschaft (DFG). As in the previous years grateful acknowledgement is also due to the Springer Verlag for publishing this volume and thus helping to position the activities of the HLRS and the SSC Karlsruhe into an international frame, by which it is hoped that this series of publications is contributing to the global promotion of high performance scientific computing.

Stuttgart, August 2004

W. Jäger
M. Resch
E. Krause
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Scientific computing on super-computers has become one of the standard methods of research in physics. This is clearly demonstrated by the articles in this section, which present a selection of projects related to physical research currently running at the HLRS. The presented work does not only cover a wide range of physics, it is also dominated by long-term projects which continuously have progressed over several years applying well established numerical methods.

A. Cavallo, M. Müller and K. Binder use large scale semi-grandcanonical Monte-Carlo simulations to analyze the chain conformations and phase separation in binary polymer blends. Testing for a large variation of chain length they were able to distinguish three regimes of film thickness with different behaviour for the critical temperature of demixing. On a much smaller length scale operate O. Kaczmarek, F. Karsch, P. Petreczky and F. Zantow, who have performed Lattice Monte-Carlo simulations of quantum chromodynamics to investigate the free energy of a static quark anti-quark pair placed in a hot strongly interacting medium. They considered not only quenched QCD but also compare with some preliminary results in full QCD.

A particular highlight is the project on simulations of particle suspensions by A. Komnik, M. Strauß, S. McNamara and H. Herrmann. They discuss the two basic approaches of how to model the combined system of fluids and grains in a suspension, either by solving for the fluid equations in high resolution and taking the grains as complex and moving boundaries, or by a coarse-grain fluid motion on scales larger than the particle sizes. For the first approach they apply the lattice-Boltzmann equation simulation technique with modifications for the interactions with the solid particles, while for the latter approach they present a new model based on mass conservation of the gas and the granular medium. This new approach is used to simulate plug conveying through pipes, and also comparisons with experiments are discussed.

With flows on much larger length-scales deal the projects by W. Dobler, and by M. Stute and M. Camenzind. W. Dobler models the thermal convec-
tion and dynamo processes in fully convective stars. To solve the compressible magneto-hydrodynamic equations he is applying an explicit high-order finite-difference code parallelized with MPI. He finds that weak initial seed magnetic fields grow exponentially and that the dynamo efficiency increases with increasing rotation rate of the star. M. Stute and M. Camenzind perform large scale simulations of cooled pulsed jets in symbiotic stars. They also use a finite-differences code (NIRVANA) to solve the equation of ideal hydrodynamics with additional non-equilibrium cooling and a network of atomic rate equations to consider radiative losses due to line emission. With their calculations they were able to continue former simulations of jets to length scales larger than 50 AU, and they found as a new and unexpected effect an inflating cocoon around the jet.

A computational study in surface physics has been presented by Dr. M. Rohlfing from the International University Bremen. Dr. Rohlfing discussed so-called image potential states on an insulator surface. Very much like in a text book example of a metal, if one considers a charge, here an electron in front of the surface, also image-effects appear in an insulator, in the studied case here of LiF surfaces. The electron then induces an “image hole”, which, in the ideal case, is located within the insulating system. This positively charged hole then creates an attractive force binding the electron very much like the electron is bound in an hydrogen atom to the positively charged nucleus. This gives rise to a kind of Rydberg series and corresponding bound image potential states which can be compared with experiments.

All these examples confirm the fact that in general the use of supercomputers has become a matter of routine. Nevertheless, there are also still reports on technical difficulties regarding the porting of codes and scripts onto these machines and regarding the configuration of the operating systems. In particular, it was noted that occasionally queueing times for moderately sized jobs are prohibitively long. Hopefully, these obstacles may be overcome with the more general availability of higher computing capacities.
Chain Conformations and Phase Behavior in Confined Polymer Blends

A. Cavallo, M. Müller and K. Binder

Institut für Physik, WA331, Johannes Gutenberg Universität, D55099 Mainz, Germany, Marcus.Mueller@uni-mainz.de

Summary. We investigate the chain conformations and phase separation in binary polymer blends. Using large scale semi-grandcanonical Monte Carlo simulations and finite size scaling, we investigate the molecular extension and the intermolecular paircorrelation function in thin films with hard, non-preferentially adsorbing surfaces. The interplay between chain conformations, demixing and the validity of mean field theory is investigated for a large variation of chain lengths $16 \leq N \leq 512$. Three regimes of film thickness $D$ can be distinguished: (i) For film thicknesses much larger than the unperturbed chain extension $R_e$, bulk behavior is observed, i.e., the critical temperature of demixing $T_c$ increases linearly with chain length, and the mean field theory becomes asymptotically correct for large $N$. (ii) For $D \sim R_e$, the critical temperature scales linearly, $T_c \sim N$, but the mean field theory overestimates the prefactor even in the limit $N \to \infty$. (iii) For ultrathin films, the chain conformations are quasi-two-dimensional, $T_c \sim \sqrt{N}$ and mean field theory completely fails.

1 Introduction

Melt blending of polymers is a promising route for tailoring materials to specific application properties: Polymeric materials in daily life are generally multicomponent systems. Chemically different polymers are “alloyed” as to design a material which combines the favorable characteristics of the individual components [1]. Clearly the miscibility behavior of the blend is crucial for understanding and tailoring properties relevant for practical applications. Miscibility on a microscopic length scale is desirable for a high tensile strength of the material. Unlike metallic alloys, however, chemically different polymers often do not mix on microscopic length scales. Rather a complicated morphology of droplets of one component dispersed into the other component forms on a mesoscopic length scale, and the blend can be conceived as an assembly of interfaces. While the detailed structure on this mesoscopic length scale depends strongly on the way the material is processed, the local properties of interfaces are certainly crucial for understanding the material properties. For instance, the interfacial width sets the length scale on which entanglement
between polymers of the different components form. Experiments [2] suggest that the mechanical strength increases if the interfacial width exceeds the entanglement length. Alternatively, the interfacial tension is important for the breaking-up of droplets under shear [3, 4]: The lower the interfacial tension is the finer are dispersed the two components.

In this report on our work at the T3E at the computing center in Stuttgart, we focus on the influence of geometrical confinement on the chain conformations and phase behavior of polymer blends. Confinement gives rise to a pronounced shift in the binodals and spinodals of polymer blends. On the one hand, the chain conformations and the intermolecular chain packing is affected by the geometrical restriction. On the other hand, surfaces often preferentially adsorb one species of the polymer mixtures, which gives rise to an interplay between wetting and phase separation. One advantage of computer simulation is that we can strictly suppress the latter effect by using neutral, i.e., non-selective surfaces and thereby highlight the effect of geometrical confinement.

In the following we consider coarse-grained models that do not capture the structure on the atomistic scale but lump a small number of chemical repeat units into a monomer of the coarse-grained model. These monomers interact via coarse-grained, simplified interactions. The reduced number of degrees of freedom and the softer interactions on a coarse scale lead to a significant computational speed-up. Hence, large system sizes and long time scales, that are inaccessible in atomistic simulations, can be studied [5]. Yet super-computers like the CRAY T3E, sophisticated simulation and analysis techniques are required to elucidate the behavior of long macromolecules.

Our report is arranged as follows: In the next section we introduce our model and briefly summarize the salient features of the simulation technique. Then, we focus on the chain conformations in thin films, and demonstrate that a significant increase in the lateral chain extension due to confinement can only be expected for ultrathin films. Thereafter, we regard the shift of the critical point of demixing due to confinement of a symmetric polymer blend by impenetrable, neutral surfaces.

2 Models and techniques

We present Monte Carlo (MC) simulations of the bond fluctuation model [6], which incorporates the relevant universal characteristics of polymer blends: connectivity of the monomers along a chain, excluded volume of the segments, and a thermal interaction between monomers. In the framework of this coarse-grained lattice model, a monomer occupies 8 corners of a unit cell from further occupancy. Monomers along a polymer are connected by one of 108 bond vectors of length 2, \(\sqrt{5}\), \(\sqrt{6}\), 3, and \(\sqrt{10}\). The bond vectors are chosen such that the excluded volume interactions prevent a crossing of bond vectors during local hopping motion. The large number of bond vectors
allows for 87 different bond angles. This is an indication for the rather good approximation of continuous space properties by this complex lattice model. \( R_e \) and \( R_g \) denote the end-to-end distance and the radius of gyration of the chains respectively.

Here and in the following all length scales are measured in units of the lattice spacing. When atomistically detailed simulations are mapped onto the bond fluctuation model a lattice unit corresponds to roughly 2\( \text{Å} \) and a monomer represents a small number – say 3 to 5 – of chemical repeat units [7]. We work at a monomer number density of \( \rho = 1/16 \), i.e., due to the extended structure of the monomers half of the lattice sites are occupied. These parameters correspond to a concentrated solution or a melt.

The conformation of polymers on the lattice evolve via local random monomer hopping [6] – a randomly chosen monomer attempts to move one lattice constant in a random direction – or slithering snake-like moves [8, 9] – a segment of the chain is removed at one end of the chain and added at the opposite one. While the former allows for a dynamical interpretation of the MC simulation in terms of a purely diffusional dynamics, the latter relaxes the chain conformations a factor \( N \) faster [9].

Blends comprise two components – denoted \( A \) and \( B \). Monomeric units of the same type attract each other whereas different monomers repel each other via a square well potential

\[
\epsilon \equiv -\epsilon_{AA} = -\epsilon_{BB} = \epsilon_{AB}. \tag{1}
\]

The potential is extended over the first peak of the pair correlation function, i.e., it incorporates the first 54 neighbors up to a distance \( \sqrt{6} \). The form of the potential is chosen by computational convenience; we expect our results to be qualitatively independent from the specific potentials used.

Being a lattice model, the bond fluctuation model is highly computationally efficient. It allows for the investigation of rather large chain lengths and large system sizes. The latter is necessary to accurately locate the critical temperature via finite size scaling analysis. As we shall illustrate, the large chain length is crucial for reaching the high molecular weight scaling limit and extrapolating some quantities to experimentally relevant chain lengths. For the present investigation chains up to 512 monomeric units have been employed.

### 3 Results

#### 3.1 Background: identification of the Flory-Huggins parameter and bulk phase behavior

By virtue of its simplicity, the Flory-Huggins theory provides a popular framework to parameterize miscibility in dense, multicomponent polymer systems. A large body of experimental data has been analyzed in terms of the mean
Fig. 1. (a) Intermolecular paircorrelation function for chain length $N = 80$ for the athermal system (triangles) and at criticality (circles and diamonds). The inset presents the scaling of the non-random mixing with increasing chain length, $\chi_A^\text{part} = \langle \phi \rangle \int d^3 r g_A^{\text{inter}}(r)$. From Müller [10]. (b) For a symmetric blend, $N = N_A = N_B = 64$, the inverse collective structure factor $1/S(q = 0)$ is plotted vs. the Flory-Huggins parameter. Symbols denote simulation results for $N = 64$ and system size $L = 96$. The dashed line shows the finite size estimate using the Ising critical behavior. Arrows mark the location of the critical temperature (MC) and the mean field estimate (FH). The straight solid line corresponds to the mean field prediction, Eq. (6), using the effective coordination number $z_c = 2.44$.

Fig. 2. Ratio of the critical temperature (as determined in MC simulations) and the Flory-Huggins estimate for binary blends. Using the scaling variable $\sqrt{N}$ the MC results for blends of linear chains and ring polymers collapse onto a common curve. From Müller [10].

field predictions in the bulk or self-consistent field theory (or approximations thereof) for spatially inhomogeneous systems.

The free energy of mixing per molecule takes a particularly simple form:

$$\frac{F_{\text{FH}}(\phi)}{T \Phi V} = \phi \ln \phi + (1 - \phi) \ln(1 - \phi) + \chi N \phi (1 - \phi),$$

(2)

where $\Phi \equiv \rho/N$ denotes the number density of polymers and $\phi$ the composition of the incompressible mixture. $T$ is the temperature and we set Boltzmann’s constant $k_B = 1$. The first two terms describe the entropy of mixing; they stem entirely from the translational entropy. The last term describes
the energy of mixing per molecule. Note that this Flory-Huggins free energy [11] does not include any contribution from the conformational entropy of the extended macromolecules. Implicitly, one assumes that the conformations of a single chain in a homogeneous system are independent from the environment (i.e., local composition and temperature).

The Flory-Huggins parameter $\chi$ encodes the local fluid structure of the polymer liquid. In a symmetric polymer blend, we can identify $\chi$ via the energy of mixing. The latter is given by the dependence of the intermolecular interactions upon changing the composition, and this leads to:

$$\chi N = \Phi N^2 \int d^3 r \left[ g_{inter}^{AB}(r) v_{AB}(r) - \frac{g_{inter}^{AA}(r) v_{AA}(r) + g_{inter}^{BB}(r) v_{BB}(r)}{2} \right]$$

$$= \frac{2N z_\epsilon \epsilon}{T} \tag{3}$$

with

$$z_\epsilon = \Phi N \int_{r \leq \sqrt{6}} d^3 r \ g_{inter}(r). \tag{5}$$

In Fig. 1(a) we present the intermolecular pair correlation function of strictly symmetric polymer blends in the athermal limit and at the critical point of the mixture in the 3d bulk. In the athermal case, $\epsilon = 0$, the distinction between the two species becomes irrelevant. The intermolecular pair correlation function mirrors two effects [8]: (i) Due to the extended monomer structure the pair correlation function vanishes for distances $r < 2$. The presence of vacancies introduces local packing effects, which give rise to a highly structured function at short distances. One can identify several neighbor shells, which are characteristic of the monomeric fluid. These packing effects are, of course, absent in simple lattice models where a monomeric unit occupies a single lattice site and are less pronounced in the bond fluctuation model than in continuum models. The length scale of these packing effects is set by the monomeric extension or the statistical segment length; the detailed shape depends strongly on the model and the degree of structure on local length scales. (ii) Furthermore, the extended structure of the macromolecules manifests itself in a reduction of contacts with other chains on intermediate length scales [14]. The length of this polymeric correlation hole is set by the size of the molecules, $R_e$, and its shape is characteristic for the large scale conformations of the molecule.

In panel (b) of Fig. 1, we plot the inverse strength of fluctuations $1/S(q \to 0)$ as a function of the $\chi N$. The second derivative of Eq. (2) yields

$$\frac{N}{S(q \to 0)} = \frac{1}{\phi g(q)} + \frac{1}{(1 - \phi) g(q)} - 2\chi N \tag{6}$$

where $g(q \to 0) = 1$ is the Debye function which characterizes the scattering from a single Gaussian chain. The identification of the $\chi$ parameter via the local fluid structure yields an accurate description of composition fluctuations.
Fig. 3. (a) Chain extension parallel to the surface normalized by the chain extension in the bulk for chain length $N = 256$ as a function of the inverse film thickness $R_g/D$. Circles denote the radius of gyration, while squares correspond to the mean squared end-to-end distance. The inset presents the dependence on the chain length at $D/R_g \approx 1$: $N = 32$ $D/R_g = 1.00$, $N = 64$ $D/R_g = 0.98$, $N = 128$ $D/R_g = 0.96$, $N = 256$ $D/R_g = 0.97$, and $N = 512$ $D/R_g = 0.97$. (b) Attempted scaling plot for all chain lengths and film thickness investigated. The data are compatible with a scaling variable $x = (R_g/\sqrt{ND})^{1/2}$. The dashed lines show the expected behavior for small and large values of the scaling variable.

away from the critical point of unmixing. In the ultimate vicinity of the critical point, there are deviations from the mean field behavior and Ising criticality is observed.

The mean field prediction of the critical incompatibility, $\chi_c N = 2$ is compared to the simulation results in Fig. 2. Upon increasing the invariant degree of polymerization $\bar{N} \equiv R_c^3 N$, the overestimation of the critical temperature by the Flory-Huggins theory decreases like $1/\sqrt{N}$ in accord with the Ginzburg criterion [12].

These considerations show that in the bulk the intermolecular chain packing determines $\chi$, and that the Flory-Huggins theory is able to describe the miscibility behavior up to corrections of order $1/\sqrt{N}$. Confining polymers into thin films will alter the chain conformations and their packing, and the confinement imparts changes onto the miscibility behavior.

3.2 Chain conformations in thin films

In many analytical approaches, e.g., self-consistent field theory (SCFT) [13] or random phase approximation (RPA) [14], polymer conformations are described by mutually non-interacting Gaussian chains in an external field. In the vicinity of a flat surface, this external field depends only on the distance perpendicular to the surface. Since the extensions of a Gaussian chain parallel and perpendicular to the surface are completely independent, the perpendicular extension remains unperturbed. This fact is at the heart of all SCF calculations of polymers in confined geometry. According to Silverberg’s
argument[15] the chain conformations can be conceived simply as random walks reflected at the surface. If a finite stiffness (or bending rigidity) along the chain is considered, parallel and perpendicular chain dimensions are no longer independent, but this short ranged correlation along the chain is not expected to affect the properties on long length scales.

At some film thickness $D$, however, the description of the polymer conformations as mutually non–interacting Gaussian chains will fail. When the film thickness becomes very small, the chain folds back many times into its own volume and the density inside of the Gaussian coil increases. The fractal structure of the segments of a single chain gradually becomes compact (i.e., space-filling). When the density inside of the coil finally becomes comparable to the average density of the melt, the parallel chain extension begins to grow such that the density of the film remains laterally homogeneous. In this limit the chains adopt disk–like compact conformations of polymers in two dimensions. The stretching parallel to the surface is only negligible when $\rho DR_{g}^{2} \ll N$ or

$$\frac{D}{R_{g}} \gg \frac{1}{\sqrt{N}} \quad \text{with} \quad \bar{N} = \left( \frac{\rho R_{g}^{3}}{N} \right)^{2}$$

where $R_{g}$ denotes the unperturbed chain extension and $\rho$ the monomer number density. $\bar{N}$ is proportional to the chain length $N$ and measures the degree of interdigitation of different polymers. This reasoning suggests the following behavior of the average chain conformation in a thin film: (i) For $D \gg R_{g}$ the chain extensions parallel and perpendicular to the surface are unperturbed. (ii) For $R_{g} \gg D \gg R_{g}/\sqrt{N}$ the parallel chain extensions are unperturbed, but the chain folds back into the volume of its own coil. Other chains are gradually squeezed out of this volume, i.e., the correlation hole in the intermolecular paircorrelation function deepens and the interdigitation of the chains decreases. (iii) For $R_{g}/\sqrt{N} \gg D$ the chains do not overlap strongly and stretch parallel to the surface as to maintain a laterally uniform density. The lateral extension scales like: $R_{\parallel}^{2} \sim R_{g}^{3}/(D \sqrt{N})$. Note that this effect occurs, when the film thickness is of the order of the excluded volume screening length $\xi \sim R_{g}/\sqrt{N}$[16]. If one of the surfaces is not a “hard wall” but rather an interface between the polymer melt and its vapor (vacuum), the surface might become rough and the ultrathin film might dewet. We start our discussion of the conformational statistics of polymers in thin films by looking at the average chain extension parallel and perpendicular to the film surfaces. For all the parameters investigated $D/R_{g} > 0.58$ the ratio of the parallel squared end-to-end distance and the squared radius of gyration $6 \leq R_{\parallel}^{2}/R_{g}^{2} \leq 6.09$ is close to the value 6 of a Gaussian chain, i.e., the chains are not two–dimensional but rather mildly perturbed from the Gaussian chain structure in the bulk. In Fig.3 (a) we plot the chain extension parallel to the film surface for chain length $N = 256$ and various film thicknesses $D$ ranging from $D = 0.58R_{g}$ to $2.03R_{g}$ in units of the radius of gyration $R_{g}$ in the bulk. As
Fig. 4. (a) Snapshot of a typical configuration for chain length \(N = 128\) at density \(\rho = 0.5\). Different chains are drawn in different grey shades. Only a fraction of size \(70 \times 70\) out of the total simulation cell \((L = 256)\) is shown. \(\epsilon/k_B T = 0.0665\). (b) Single chain structure factor for different densities. \(N = 128\). The lines mark the asymptotic power laws corresponding to Gaussian chains (RW) and self-avoiding chains (SAW) in 2d. The Debye function, which describes the structure factor of a random walk, is shown for comparison. \((\epsilon/k_B T = 0.0665, \rho = 0.5), \ (\epsilon/k_B T = 0.13, \rho = 0.4), \ (\epsilon/k_B T = 0.17, \rho = 0.36)\). The inset shows the Kratky plot. The straight line indicates the power law of a SAW.

we decrease the film thickness the lateral chain extension grows slightly, but even for the thinnest film the increase is less than 10%. In order to explore the chain length dependence, we plot in the inset of Fig.3(a) the lateral extension as a function of the chain length for \(0.96 \leq D/R_g \leq 1\). For the smallest chain length \(N = 32\) the lateral extension is increased by about 10%, but as we increase the chain length at fixed ratio \(D/R_g\) the lateral stretching decreases. Therefore, our result for chain length \(N = 256\) is rather an upper bound to the increase in chain extension observed in the experiments. In Fig.3(b) we attempt to combine the data for different film thicknesses \(7 \leq D \leq 42\) and chain length \(32 \leq N \leq 512\) to construct a scaling curve. We assume that there is a crossover from bulk-like conformations to two-dimensional configurations around \(D \sim R_g/\sqrt{N}\) and make the ansatz: \(R_{\parallel}/R_g = \mathcal{R}(x)\) with argument \(x = (R_g/\sqrt{N}D)^{1/2}\). The scaling function \(\mathcal{R}\) has the limits \(\mathcal{R}(x) \to 1\) for \(x \to 0\) and \(\mathcal{R}(x) \sim x\) for \(x \to \infty\). The latter limit assumes that the chains adopts a compact two-dimensional configuration. Within the rather large error bar of our Monte Carlo data the results are compatible with such a scaling form.

For \(R_g/\sqrt{N} \gg D\), the chains adopt quasi-two-dimensional conformations. Fig. 4 (a) presents a typical snapshot of the chain conformations in a section of the simulation box. A direct visual inspection of the chain conformation shows that the chains typically do not adopt segregated disk-like shapes. They are much more elongated and irregular. Nevertheless, each chain screens a large
part of its interior from contacts with other chains. To quantify the chain conformations we display the single chain structure factor in panel (b) on a log-log scale. One does not observe Porod scattering from an interface[17] would be characteristic of a disk with a sharp boundary, but the structure factor is compatible with Gaussian chain statistics $S(q) \sim 1/q^2$ for $2\pi/R \ll q$. This observation is in accord with previous simulations of 2d melts[17, 18] which confirmed that the excluded volume interactions are screened in the melt. At small length scales there are deviations: They stem from the local packing structure at high densities and the crossover to swollen chain conformations. From the crossover between the limiting power laws in the structure factor, we can roughly estimate the screening length $\xi \approx 15$ at $\rho = 0.5$, and $\xi$ increases with decreasing density. As $R_g/\xi \approx 1.25$ for $N = 128$ we expect deviations from the Gaussian behavior even for rather long chains. Those deviations become more apparent in the Kratky plot, i.e., the plateau in the Kratky plot exhibits additional structure. Qualitatively similar deviations are already present in the bulk[19], they become more pronounced upon confinement[21], and they are even stronger for ultrathin films.

3.3 Miscibility behavior in thin films

In the quasi-two dimensional limit, $R_g/\sqrt{N} \gg D$, the correlation hole is describable by [21]:

$$g_{\text{inter}}(r) = 1 - c \exp\left(-\frac{\text{const} \cdot r}{R_e}\right) \quad \text{for} \quad r > \xi \quad (8)$$

Fig. 5. (a) Scaling plot of the intermolecular pair correlation function $g(r)$ versus $r/N^{1/2} \sim r/R$ in quasi-two dimensional polymer films. Data are always taken close to criticality, but refer to all chains independent of their species. Chain lengths $N = 16, 32, 64, 128$, and 256 are included, as indicated in the key. For short chain lengths oscillations on the length scale of a few lattice units are visible and arise from packing effects. The inset shows $1 - g(r)$ on a logarithmic scale (cf. Eq. (8)) (b) Scaling of $T_c/N$ and $T_c/N_{zc}$ (inset) vs. $N^{-1/2}$. For comparison the results for the three-dimensional model are included. Adapted from Cavallo et al. [21].
where $c \leq 1$ is a constant. The exponential term corresponds to the correlation function of a Gaussian walk in two dimensions and the functional form suggests that the correlation hole in the intermolecular paircorrelation function in a dense melt is exactly canceled by the density of the monomers of the reference chain, as it is the case in three dimensions. The MC data for the intermolecular paircorrelation function are presented in Fig. 5 (a). The data are compatible with the value $c = 1$. Therefore, the intermolecular paircorrelation function behaves at small distances like $1 - \exp(-\text{const} \cdot r/R_c) \approx \text{const} \cdot r/R_c$ and the number of intermolecular contacts per monomer is proportional to $\rho g_{\text{inter}}(b) \sim 1/\sqrt{N}$. This implies a scaling of the critical temperature like $T_c \sim N z_c \sim \sqrt{N}$. Indeed, the simulation results [21] in Fig. 5 (b) for $T_c/N$ decreases like $N^{-1/2}$ as suggested by the scaling arguments. The incompatibility in quasi-two dimensional polymer films is therefore strongly reduced. Unlike the situation in three spatial dimensions the mean field theory does not become quantitatively correct in the limit of long chain lengths.

A crossover from two-dimensional to three-dimensional behavior in the scaling of the critical temperature $T_c$ with $N$ is observed when one increases the thickness of the film. We find that this crossover occurs for $D$ close to the screening length of the polymer melt, $\xi \sim 7$, i.e., a film thickness that is independent of the chain length. Summarizing, we can distinguish three regimes of film thickness $D$: (i) For film thicknesses much larger than the unperturbed chain extension $R_c$, bulk behavior is observed, i.e., the critical temperature of demixing $T_c$ increases linearly with $N$, (ii) For $D \sim R_c$, the critical temperature scales linearly, $T_c \sim N$, but the mean field theory overestimates the prefactor. (iii) Finally, for ultrathin films, $D \ll \xi$, the chain conformations are quasi-two-dimensional, $T_c \sim \sqrt{N}$ and mean field theory qualitatively fails. Assuming the power law $T_c \sim N^{\alpha(D)}$, for $D \ll \xi$, our results are compatible with $\alpha(D) \sim 1/2$. For $2 < D < \xi$, the exponent $\alpha(D)$ grows from 0.68 to 0.83 (15%), instead, for $\xi < D < 19$, it increases only from 0.83 to 0.9 (7%). This allows us to identify $\xi$ as a crossover length between the two regimes. This crossover can be explained in terms of geometrical arguments.

Fig 6 (a) shows the ratio $T_c/z_c N$ as a function of $1/\sqrt{N}$ for different values of the film thickness $D$. Here $z_c$ denotes the number of intermolecular contact between monomers. In the bulk, Monte Carlo simulations [20] predict $z_c = 2.1 + 2.8/\sqrt{N}$, whereas for the 2d system the data of the simulations [21] are compatible with $z_c \sim 1/\sqrt{N}$. In the limit of very long chains, $z_c$ tends to a finite number and $T_c/z_c N \to 1$, in the bulk, and $T_c/z_c N \to \text{const.}$ for a 2d system. A crossover from the 2d to the 3d behavior is observed around $D \sim \xi \approx 7$. In general, for a film with finite thickness $D$, we assume a behavior of the form: $z_c(D, N) = z_c(D, \infty) + c(D)/\sqrt{N}$. The inset of Fig. 6 (a) shows the behavior of $z_c(D, \infty)$ vs. $D$. This curve also exhibits a crossover around the film thickness $D \sim 7$. 
Confined Polymer Blends

Fig. 6. (a) Scaling of $T_c/Z_cN$ as a function of $1/\sqrt{N}$ for different film thicknesses. In the bulk $z_c = 2.1 + 2.8/\sqrt{N}$. For $N \to \infty$ the effective coordination number $z_c$ tends to a finite number and $T_c/z_cN \to 1$. For the 2d system the data of the simulations for $z_c$ are compatible with $z_c \sim 1/\sqrt{N}$ and $T_c/z_cN \to \text{const}$. A crossover from the 2d to the 3d behavior is observed around the film thickness $D \sim \xi \approx 7$. Assuming the following expression for the effective coordination number, $z_c(D,N) = z_c(D,\infty) + c(D)/\sqrt{N}$, the inset shows the behavior of $z_c(D,\infty)$ vs. the film thickness $D$. (b) Expected scaling of the number of contacts between polymers $z_{\text{pol}}$ with $1/N^{1/2}$. The inset shows the scaling plot of the number of contacts between polymers, $z_{\text{pol}}$, divided by the film thickness $D$ as a function of $D/\sqrt{N}$.

In a 3d melt, the number of polymers $z_{\text{pol}}$ in a coil of volume $R_g^3$ is proportional to $\sqrt{N}$, i.e. each chain interacts with $\sqrt{N}$ other neighbors. In the limit $N \to \infty$, the number of contacts between polymers, $z_{\text{pol}}$, tends to infinity and the mean field theory become quantitatively correct. In Fig. 6 (b) we plot the behavior of $z_{\text{pol}}$ as a function of $1/\sqrt{N}$ for different film thicknesses. The plot shows that for a system confined between to parallel walls the asymptotic value of $z_{\text{pol}}$ in the limit $N \to \infty$ is a finite number and the mean field theory will quantitatively fail. We can distinguish two different regimes: For $D \leq 7$ the number of contacts $z_{\text{pol}}$ is small (on the order of $6$) and it slightly increases with chain length. When we increase the film thickness, however, the growth of $z_{\text{pol}}$ with $N$ becomes much more pronounced. For every finite $D$, however, the number of chains a reference molecule interacts with remains finite, implying a quantitative failure of mean field theory. In the limit $D \to \infty$, $z_{\text{pol}}$ diverges and mean field theory becomes quantitatively accurate for $N \to \infty$. The inset of Fig 6 (b) shows a scaling plot for $z_{\text{pol}}$ divided by the film thickness $D$ as a function of the ratio $D/\sqrt{N}$.

4 Conclusion and outlook

Using large scale simulations of strictly polymer blends between neutral walls we have studied the interplay between confinement, chain conformations, in-
termolecular packing and miscibility behavior. For film thickness on the order of the chain dimensions in the bulk, the lateral chain dimensions are hardly extended and the Flory-Huggins theory fails to quantitatively predict the unmixing transition for large molecular weight, but linear scaling of the critical temperature with chain length is obeyed. Only for very thin films, where the thickness is on the order of the mesh size of the melt, the lateral chain dimensions drastically increase, the chains adopt quasi-two-dimensional conformations and the linear scaling $T_c \sim N$ is replaced by a much weaker dependence, $T_c \sim \sqrt{N}$, i.e., the miscibility is largely increased. A crossover from the two-dimensional to the three-dimensional behavior of the critical temperature with the chain length is observed in correspondence of a $N$–independent characteristic length of the system: the screening length.

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References


16. Since we focus on semi-dilute solutions (and melts), we express all quantities for $r > \xi_{ev}$ in terms of $R_e$ and $N$. Conceiving a chain as a random walk of blobs of size $\xi_{ev}$, we can write:

$$R^2 = b^2 N \sim \xi_{ev}^2 N / g$$

where $g$ is the number of monomeric units per blob. To a first approximation, blobs do not interdigitate and $g \sim \rho \xi_{ev}^3$. Then we obtain $\xi \sim 1 / \rho b^2 = R_e / (\sqrt{N})$. To make contact with the dilute limit, we use $R_0 \sim b_{ev} N^{\nu_{ev}}$ with $\nu_{ev} = 0.588$ for the chain extension in the limit $\rho \to 0$, and we define the overlap $s = \rho R_0^3 / N$. The extension in semi-dilute solutions is related to the properties in the dilute limit via:

$$R_e^2 \sim R_0^2 F(s) \xrightarrow{s \to \infty} R_0^2 s^{(1-2\nu_{ev})/(3\nu_{ev}-1)} \sim b_0 (\rho b_{ev}^3)^{(1-2\nu_{ev})/(3\nu_{ev}-1)} N.$$ 

Using this limiting scaling behavior we find for the screening length $\xi_{ev} \sim R_e / \sqrt{N} \sim b_0 (\rho b_{ev}^3)^{\nu_{ev}/(1-3\nu_{ev})}$ and for the overlap $s \sim N^{3\nu_{ev}-1}$.


 Thermal Quark Anti-quark Free Energies, Energies and Screening in Hot SU(3) Gauge Theory

O. Kaczmarek¹, F. Karsch¹, P. Petreczky¹², and F. Zantow¹

¹ Fakultät für Physik, Universität Bielefeld, Universitätsstraße 25, 33615 Bielefeld, Germany
² Nuclear Theory Group, Physics Department Brookhaven National Laboratory, Upton NY 11973

1 Introduction

Lattice Monte-Carlo simulations of quantum chromodynamics (QCD) have shown that strongly interacting matter undergoes a phase transition at some temperature $T_c$ [1]. Above the transition temperatures $T_c$ hadrons (the experimentally observed strongly interacting particles) cease to exist and a new state of matter, the so-called quark-gluon plasma (QGP) was predicted to exist [1]. One of the most prominent features of QGP is the screening of static chromoelectric fields. At large distances (i.e. distances much larger than the inverse temperature) the screening is exponential and can be parametrized by a temperature dependent chromoelectric screening mass. Chromoelectric screening masses have been extensively studied by us in the last few years [2-3] in the framework of our project (Nr. 11725). More recently chromoelectric screening has been studied in terms of the free energy of static quark anti-quark pair [4,5,6,7]. Moreover we developed a technique to separate energy and entropy contributions to the free energy [8, 9].

It has been observed that screening effects in a thermal medium also influence the intermediate and even short distance ($R < T$) regime of the force between quarks and gluons [4,5]. While the study of the screening at large distances is very important to understand the infrared properties of QCD at finite temperatures, possible screening effects at shorter distances are relevant for the understanding of thermal modifications of heavy quark bound states which are discussed as one of the key signatures for the formation of a quark gluon plasma that can be studied experimentally in heavy-ion collisions at RHIC (BNL) as well as SPS and LHC (CERN). The reason is that the screening of static chromoelectric fields at short distances ($R < 1 fm$) will narrow the heavy quark potential and thus forbids, for instance, the for-
mation of quarkonium bound states; the phenomenon is generally discussed as charmonium suppression [10].

As mentioned above in the past years we have extensively studied the chromoelectric screening masses as well as the thermal quasi-particle masses in SU(2) and SU(3) gauge theories. All these studies have been performed in terms of the gluon propagator. This gave direct access to the electric and magnetic screening masses. The connection to heavy quark potential or free energy, however, can be established in a straightforward way only at asymptotically high temperatures. Studies of the gluon propagator thus only provide information about screening at large distances. During the last year we investigated the properties of the free energy of a static quark anti-quark pair placed in a hot strongly interacting medium at some fixed separation R. This provides information on inter-quark forces and their screening both at small and large distances. We investigated in detail the temperature dependence of static quark free energies at large distances where their temperature dependence can be understood in terms of temperature dependent screening masses as well as their temperature dependence at short distance which is more complex. In particular, we analyzed different quantum number channels, i.e. the singlet and octet channels which show opposite behavior at short distances. The force in these channels is attractive and repulsive, respectively. For quite some time only the color averaged static quark anti-quark free energy was studied in greater detail [11]. In our previous studies we considered the case of quenched QCD (pure SU(3) gauge theory). Here we also present some preliminary results in full (2 flavor) QCD [12]. In the next section we describe how the free energy as well as the internal (potential) energy of a static quark-antiquark pair can be studied by lattice Monte-Carlo simulations. In section 3 we present our numerical results. Finally section 4 contains our conclusions.

2 Lattice calculation of the free energy of a static quark-antiquark pair

2.1 The static free energy on the lattice

We consider SU(3) gauge theory (quenched QCD) at finite temperature with tree level improved Symanzik action [13]. Simulations were performed in the temperature range $0.75T_c \leq T \leq 12T_c$ on $N^3 \times N_\tau$ lattice, with $N_\sigma = 32, 64$ and $N_\tau = 4, 8, 16$. The temperature scale was determined using the zero temperature string tension determined in [14]. In the case of 2 flavor QCD we use the so-called p4 staggered fermion action [15] and Symanzik gauge action.

The propagation of a static quark in Euclidean time is described by the Wilson line

$$W(x) = \prod_{\tau=0}^{N_\tau-1} U_0(x, \tau)$$  \hspace{1cm} (1)
with $U_0(x, \tau)$ being the link in time direction. One can then define the free energy in singlet and octet channel as \cite{16, 17}

\begin{align}
    e^{-F_s(R)/T+C} &= \frac{1}{N} \text{Tr} < W(R)W^+(0) > \\
    e^{-F_o(R)/T+C} &= \frac{1}{N^2 - 1} \left< \text{Tr} W(R) \text{Tr} W^+(0) \right> - \frac{1}{N(N^2 - 1)} \text{Tr} < W(R)W^+(0) > .
\end{align}

Here $N = 3$ for SU(3). One can also consider the color averaged free energy defined through the Polyakov loop $L(x) = \frac{1}{N} \text{Tr} W(x)$

\begin{equation}
    e^{-F(R)/T+C} = < L(R) L^+(0) > .
\end{equation}

This can be written as thermal average of the free energies in singlet and octet states (hence the name)

\begin{equation}
    e^{-F(R)/T} = \frac{1}{N^2} e^{-F_s(R)/T} + \frac{N^2 - 1}{N^2} e^{-F_o(R)/T} .
\end{equation}

Note that the free energies are defined up to a normalization constant $C$. In the deconfined phase it is customary to set $C = \ln | < L > |^2$. We use this choice of $C$ for $T > T_c$ unless stated differently. Alternatively one can choose the normalization constant $C$ such that the singlet free energy coincides with the singlet zero temperature potential at very short distances \cite{5}. The free energy of static quark anti-quark pair is not a potential energy as generally it contains an entropy contribution

\begin{equation}
    F_i(R, T) = U_i(R, T) - TS_i(R, T), i = 1, 8, \text{av.}
\end{equation}

The entropy and the internal energy can be calculated using the following formulas

\begin{equation}
    S_i = - \frac{\partial F_i}{\partial T}, \quad U_i = -T^2 \frac{\partial(F_i/T)}{\partial T} .
\end{equation}

Thus to extract the entropy and the internal energy from the Monte-Carlo data one needs to calculate numerically the derivatives with respect to the temperature. This is a tough problem as it requires fine temperature grid and high statistical accuracy.

The definitions (2) and (3) of singlet and octet free energies requires fixing a gauge ($W(x)$ is not gauge invariant). Very recently it has been shown that a gauge invariant definition of the singlet and octet potential can be achieved replacing the Wilson line in Eqs. (2), (3) by a dressed Wilson line

\begin{equation}
    \tilde{W}(x) = \Omega^\dagger(x) W(x) \Omega(x) ,
\end{equation}

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\begin{equation}
    \tilde{W}(x) = \Omega^\dagger(x) W(x) \Omega(x) ,
\end{equation}
where $\Omega(x)$ is an $SU(3)$ matrix constructed from eigenvectors of the covariant spatial Laplacian $D_i^2(A_i)$ at $\tau = 0$ [18]. Under gauge transformation $G(x)$ this matrix transforms as $\Omega(x) \rightarrow \Omega^G = G(x)\Omega(x)$ which ensures the gauge invariance of $\tilde{W}(x)$. On the other hand one can view $\Omega(x)$ as gauge transformation bringing the Wilson line to a specific gauge (spatial Laplacian gauge) [18]. Furthermore, using the transfer matrix formalism it was shown that $F_1$ and $F_2$ do not depend on choice of $\Omega$ provided that the definition of $\Omega$ is local in time [18]. This implies that any gauge where the gauge condition local in time provides a meaningful definition of the singlet and octet potential and the result does not depend on the gauge.

**Fig. 1.** The color singlet free energy at different temperatures (top) and the singlet, octet and average free energy at $0.98T_c$ (bottom) in quenched QCD.
In our study we use the Coulomb gauge which on lattice is defined by maximizing the quantity

$$ReTr \sum_{i=1}^{3} (U_i(x, \tau) + U_i(x + \hat{i}, \tau)). \quad (9)$$

This gauge condition is obviously local in time and thus provides a meaningful definition of the singlet and octet free energies. In fact in Ref. [18] the equivalence of the spatial Laplacian and Coulomb gauge was demonstrated also numerically.

3 Numerical results

3.1 Numerical results in quenched QCD

Let us start the discussion with the free energy of static quark anti-quark pair below the deconfinement transition $T < T_c$ ($T_c$ is the transition temperature). The free energy in singlet, octet and color average channels is shown in Fig. 1, where also the zero temperature potential is shown. The singlet free energy coincides with the zero temperature potential for $R^2/\sigma < 1$ for all temperatures (here and in what follows $\sigma$ is the $T = 0$ string tension). There is as small enhancement over the zero temperature potential for $1 < R^2/\sigma < 2.5$. At short and intermediate distances the octet free energy has a form which is quite different from the singlet case, in particular, it has a repulsive tail at short distances. While at short and intermediate distances the temperature dependence of singlet and octet free energies is relatively small, large temperature dependence is observed for large distances $R^2/\sigma > 3$. At large distances, interestingly enough, the singlet and octet free energies become equal. Note also, that for large distances the free energy is linearly rising with the distance as expected in the confining phase. As we will see later this is not the case in full QCD.

The singlet free energy above deconfinement is shown in Fig. 2 (top), it goes to constant at large distances indicating the presence of screening. At short distances it is temperature dependent and coincides with the zero temperature potential. The asymptotic value of the free energy

$$F^i_{\infty} = \lim_{R \to \infty} F_i(R, T) = F_{\infty}(T)$$

is independent of color channel and monotonically decreases with increasing temperature, i.e., $\partial F_{\infty}/\partial T > 0$. This means that there is an entropy contribution at large distances. Since there is no entropy contribution at short distances (there the free energy is $T$-independent) this also implies that the entropy of static quark antiquark pair is $R$-dependent. We have calculated this entropy contribution and subtracted it from the free energy,