# DY 29: Soft matter

Time: Thursday 14:00–15:45                                    Location: H3

DY 29.1    Thu 14:00    H3

**Polymers and star polymers in correlated environments** —
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We show that correlated environments have significant and quantita-
tively measurable impacts on the scaling properties of polymers and
branched polymer structures such as star polymers. These result in
experimentally accessible effects on their osmotic behavior in differ-
ently correlated environments. We calculate these quantitative effects
by appropriately extending a field theoretic renormalization group ap-
proach for spin models in long range correlated disorder [Weinrib and
Halperin, Phys Rev B (1983)]. We find new universal scaling exponents
for linear and star polymers in such environments with consequences
for their entropic behaviour as well as for the effective interactions be-
tween these polymers. Surprisingly, these effects have opposite signs
for linear and star polymers. We predict quantitatively measurable
segregation effects at the interface between correlated and uncorre-
lated environments, e.g. introduced by an aerogel-structure immersed
in a solution of a mixture of linear and star polymers.
Yu.H. was supported by FWF (Austria), Project P16574.
V Blavats'ka, C v Ferber, Yu Holovatch, Phys Rev E, 74 031801 (2006)

DY 29.2    Thu 14:15    H3

**Elasticity of randomly cross-linked particles** — •Stephan
Ulrich[1], Annette Zippelius[1], Xiaoming Mao[2], and Paul
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Starting from a microscopic model of randomly cross-linked particles
with quenched disorder, we calculate the Landau-Wilson free energy $\mathcal{S}$
for arbitrary cross-link densities. Considering pure shear deformations,
$\mathcal{S}$ takes the form of the elastic energy of an isotropic amorphous solid
state, from which the shear modulus can be identified. It is found to be
an universal quantity, not depending on any microscopic length-scales
of the model.

DY 29.3    Thu 14:30    H3

**Collective Monte Carlo updating for off-lattice systems**
— •Markus Bellion[1], Werner Krauth[2], Heiko Rieger[1], and
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The introduction of Cluster Monte Carlo algorithms led to much larger
computational efficiency compared to (conventional) local Monte Carlo
schemes. For example, by using cluster algorithms it was possible to
reduce critical slowing down or even to avoid this problem. Unfor-
tunately, up to now most such cluster algorithms have been designed
for classical and quantum mechanical models that are defined on a
lattice. In fact, currently there is only one known cluster algorithm
for off-lattice models which is based on the exchange of clusters gen-
erated by overlaying a rotated particle configuration with the orig-
inal (non-rotated) configuration [1,2]. Although this algorithm has
been successfully applied to a number of models (phase separation in
fluid mixtures, stabilisation of colloidal suspensions by nanoparticles,
polydisperse systems), it works rather inefficiently for higher densities.
Here we present an alternative approach, which iterates a translational
move in order to generate particle clusters. The main advantage of this
approach is that the distribution of cluster sizes can be tuned by vary-
ing the step width of the elementary move.
[1] C. Dress and W. Krauth, J. Phys. A 28, 597 (1995).
[2] J. Lui and E. Luijten, PRL 92, 035504 (2004).

DY 29.4    Thu 14:45    H3

**Structure of the inhomogeneous hard-spherocylinder fluid
from an improved density functional theory** — •Hendrik
Hansen-Goos[1,2] and Klaus Mecke[3] — [1]Max-Planck-Institut für

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The performance of a new density functional theory (DFT) for fluids of
nonspherical hard particles is tested in a study of structural properties
of the inhomogeneous hard-spherocylinder fluid. The new DFT results
from an extension of Rosenfeld's fundamental measure theory (FMT)
[1] which is based on a deconvolution of the Mayer-$f$-function into
weight functions encoding the geometry of the constituents. While in
the case of hard-sphere mixtures an exact deconvolution is feasible, for
nonspherical particles it holds only as an approximation. Using a result
from differential geometry it is possible to improve the approximate de-
convolution compared to the one of Rosenfeld. The performance of the
resulting DFT is shown to improve w.r.t. the original FMT by compar-
ing with results from Monte-Carlo simulations of the inhomogeneous
hard-spherocylinder fluid. The connection of the new FMT with the
version of Tarazona [2] is established. Tarazona's modification in or-
der to avoid spurious divergencies for the hard-sphere crystal can be
understood as a stabilization of the theory against deviations from
sphericity.
[1] Y. Rosenfeld, Phys. Rev. Lett. **63**, 980 (1989); [2] P. Tarazona,
Phys. Rev. Lett. **84**, 694 (2000).

DY 29.5    Thu 15:00    H3

**Influence of long-range correlated surface and near the
surface disorder on the process of adsorption of long-
flexible polymer chains** — •Zoryana Ustenko[1,2] and Jens-Uwe
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The influence of long-range correlated surface and decaying near sur-
face disorder with correlation function for the defects of the form $\frac{e^{-z/\xi}}{r^a}$
, where $a < d - 1$ and $z$ being the coordinate in the direction perpen-
dicular to the surface and $r$ denotes the distance parallel to the surface.
We investigate the process of adsorption of long-flexible polymer chains
with excluded volume interactions on a "marginal"and attractive wall
in the framework of renormalization group field theoretical approach
up to first order of perturbation theory in a double$(\epsilon,\delta)$- expansion
$(\epsilon = 4 - d, \delta = 3 - a)$ for the semi-infinite $|\phi|^4$ $O(m,n)$ model with
the above mentioned type of surface and near the surface disorder in
the limit $m, n \to 0$. We obtained series for bulk and the whole set
of surface critical exponents, characterizing the process of adsorption
of long-flexible polymer chains at the surface. The polymer linear di-
mensions parallel and perpendicular to the surface and the behavior
of monomer density profiles and the fraction of adsorbed monomers at
the surface and in the interior are studied.

DY 29.6    Thu 15:15    H3

**Quantifying Cation Transport in Polymer Electrolytes in
Terms of Microscopic Properties** — •Arijit Maitra[1,2] and An-
dreas Heuer[1] — [1]Institute of Physical Chemistry, University of
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We present an analytical approach to relate the *macroscopic* cation
dynamics in polymer electrolytes via three principal time scales which
characterize the *local* modes of cation transport. These are: poly-
mer/segmental relaxation, the motion of the cation along the chain
and cation jump events between different chains. With the knowl-
edge that cationic motion is coupled to the segmental dynamics of
polymers and applying the concept of renewal process (from dynamic
bond percolation model) we are able to express the cation diffusion
constant in terms of these three time scales. For the description of
polymer dynamics, depending on chain length, we invoke the Rouse
model and the Reptation model. Our theory is complemented by all-
atom molecular dynamics simulation of a model system comprising of
poly(ethylene oxide) and lithium tetrafluoroborate. Apart from fur-
nishing a complete picture (both quantitative and qualitative) of the
variety of cation transport mechanisms through the combination of
theory and simulation, we are able to explain the chain length (N)
dependence of lithium diffusivity (D) over a large range of N. This is
supported by experimental data. Specifically, we find that the plateau

regime of D(N) for large N does not require the presence of polymer entanglements, as has been speculated in the literature.

DY 29.7 Thu 15:30 H3

**Magnetische Eigenschaften und magnetoelastisches Verhalten eines CoFe$_2$O$_4$-basierten Ferrogels im homogenen Magnetfeld** — •Stefan Monz, Andreas Tschöpe und Rainer Birringer — Universität des Saarlandes, F.R. 7.3 Technische Physik, Geb. D 2.2, D-66123 Saarbrücken

Aus einem CoFe$_2$O$_4$-basierten Ferrofluid wurde durch chemische Vernetzung von gelöstem Polyvinylalkohol und Glutardialdehyd ein Ferrogel hergestellt. Die magnetfeldsensitiven viskoelastischen Eigenschaften der so erhaltenen Körper einerseits und der Einfluss der Matrix auf die magnetischen Eigenschaften andererseits wurden untersucht. Durch das Anlegen eines homogenen Magnetfeldes während der Vernetzung besteht die Möglichkeit, die makroskopische Gelprobe magnetisch zu texturieren. Des Weiteren wurde gezeigt, dass sich ein solches Ferrogel auf Grund dieser magnetischen Textur und seiner besonderen elastischen Eigenschaften im homogenen Feld deformiert; je nach den gewählten Randbedingungen kommt es zu einer Rotation oder zu einer Torsion des Ferrogels. Zusätzlich wird ein einfaches Modell vorgestellt, mit dessen Hilfe man mittels magnetischer Messungen Zugang zu den elastischen Eigenschaften der weichen Matrix erhält.