

## DY 42 Statistical Physics (General) II

Zeit: Dienstag 14:00–15:45

Raum: TU H3010

**Hauptvortrag**

DY 42.1 Di 14:00 TU H3010

**Thermodynamics - Past, Present and Future** — ●WERNER EBELING — Institute of Physics, Humboldt-University Berlin, 12489 Berlin

We begin with historical remarks on the basic contributions to thermodynamics and statistics with some bias to scientists working in Berlin as Helmholtz, Clausius, Nernst and Einstein [1]. We underline the key role of thermodynamic ideas in the scientific revolutions in the 20th century. Further we discuss several recent applications to natural, evolutionary and informational systems [3] as well as perspectives [3].

[1] W. Ebeling, D. Hoffmann: The Berlin School of Thermodynamics. Eur.J.Phys. **12**(1991)1-9.

[2] W. Ebeling, A. Engel, R. Feistel: Physik der Evolutionsprozesse. Akademie-Verlag Berlin (1990).

[3] W. Ebeling, I. Sokolov: Statistical Thermodynamics and Stochastic Theory of Nonequilibrium Systems, World Scientific (2005), to appear.

DY 42.2 Di 14:30 TU H3010

**Coulomb Interactions via Local Dynamics: A Molecular Dynamics Algorithm Rejuvenating the Ether** — ●BURKHARD DÜNWEIG<sup>1</sup> and IGOR PASICHNYK<sup>2</sup> — <sup>1</sup>Max-Planck-Institut für Polymerforschung, Mainz — <sup>2</sup>Max-Planck-Institut für Physik komplexer Systeme, Dresden

We derive and describe a recently proposed method for obtaining Coulomb interactions as the potential of mean force between charges which are dynamically coupled to a local electromagnetic field. We focus on the Molecular Dynamics version of the method and show that it is intimately related to the Car-Parrinello approach, while being equivalent to solving Maxwell's equations with freely adjustable speed of light. Unphysical self-energies arise as a result of the lattice interpolation of charges, and are corrected by a subtraction scheme based on the exact lattice Green's function. The method can be straightforwardly parallelized using standard domain decomposition. Some preliminary benchmark results are presented.

DY 42.3 Di 14:45 TU H3010

**Casimir forces and Geometry** — ●RAUNO BUESCHER and THORSTEN EMIG — Institut fuer Theoretische Physik, Universitaet zu Koeln, Zuelpicher Str. 77, 50937 Koeln, Germany

Casimir interactions between metallic surfaces can now be measured very precisely. However, on the theoretical side there is only little knowledge about Casimir forces in geometries going beyond the simplest cases as two parallel plates or a sphere and a plate. The only available approximations start from an expansion of the force at short distances, leading to the so-called proximity force approximation (PFA). Here we present a novel approach which is based on a numerical implementation of a path integral quantization of the electromagnetic field. It can be applied to surfaces with arbitrarily strong deformations at any distance. More specifically, we consider the normal and lateral force between periodically deformed surfaces. In contrast to the in general complicated behavior at short distances, as described by the PFA, we observe a universal behavior of the force at large distances in the sense that the interaction depends only on the mode with the largest wave length of the surface deformation spectrum and the modulations at smaller scales are irrelevant. Our findings thus complement the PFA approach, and yield even the crossover between the two regimes. We find that the in recent experiments detected lateral force changes with the lateral surface displacement in a way which can be distinct from the change of the surface profile itself. Our results can be extended to finite temperatures.

DY 42.4 Di 15:00 TU H3010

**Morphological thermodynamics: shape dependence of free energies and density profiles** — ●PETER KÖNIG<sup>1</sup>, ROLAND ROTH<sup>1</sup>, and KLAUS MECKE<sup>1,2</sup> — <sup>1</sup>MPI für Metallforschung, Stuttgart — <sup>2</sup>Institut für theoretische Physik, Universität Erlangen-Nürnberg

We show that a thermodynamic potential of a fluid bounded by an arbitrarily shaped convex container can be calculated fully from the knowledge of only four morphometric measures. This result is based on the assumption that a thermodynamic potential is an 'additive' functional which can be understood as a more precise definition for the conventional term 'extensive'. As a consequence, the surface tension and other

thermodynamic quantities contain, beside a constant term, only contributions linear in the mean and Gaussian curvature of the container and not an infinite number of curvatures. Our findings are tested numerically in the entropic system of hard spheres bounded by a curved wall within the framework of density functional theory and by a systematic expansion of density profiles in powers of wall curvatures. The dependence of the fluid density on the wall shape for large distances from the wall can be derived analytically from Ornstein-Zernicke equation. The contact value of the fluid density and the asymptotic behaviour depend again only on the mean and Gaussian curvatures, i.e., on additive morphometric measures of the wall. Our approach can be generalised to systems with short-ranged fluid-fluid and wall-fluid interaction potentials, as long as intrinsic length scales remain small.

DY 42.5 Di 15:15 TU H3010

**Finding hard problems** — ●WOLFGANG BARTHEL and ALEXANDER K. HARTMANN — Institut für Theoretische Physik, Universität Göttingen, <http://www.theorie.physik.uni-goettingen.de/~barthel>

Why is it often so difficult to find the optimal solution? To answer this question computer scientists classify problems according to their complexity, i. e. how fast a worst-case realization of the problem can be solved depending on its size.

The specific problem we consider is the vertex-cover problem: Take a random graph consisting of undirected edges that meet at vertices. A vertex cover is a subset of the vertices that contains at least one of the two end vertices of every edge. Finding the vertex cover of minimal size is a NP-complete problem, i.e. the challenge of developing a fast algorithm or proving its non-existence is still open.

Typically the solution time heavily depends on the specific realization. To gain insight in the hardness of the problem one would like to compare typical realizations with the ones harder to solve. We present the results of a Monte Carlo simulation in the space of instances. Here the logarithm of the solution time plays the role of the energy, so harder instances are more favorable at low "temperature" for the dynamics.

DY 42.6 Di 15:30 TU H3010

**An EINSTEIN Memorial for Charge Transfer Reactions at the Phase Boundary of Molecular Crystals: Is it possible to Decide between FRENKEL and WANNIER Excitons by Applying his Mass-Energy Relation?** — ●HERMANN M. M. KILLESREITER — Privatgelehrter c/o TU Clausthal, priv. P. O. Box 1113, D-38669 Clausthal-Zellerfeld

One hundred years ago, EINSTEIN published amongst his current scientific considerations also his paper "Depends the Inertia of a Body from his Content on Energy?" [1905/2]. With reference to his paper on Relativity [1905/1], he assumed in a system a body which emitted two particles in opposite direction.

By comparison with earlier investigations by and with the author since his PhD Thesis [Munich 1970; 1972], dissociation of an exciton [1982] as well as sensitization from an adsorbed dye [1980] across a phase boundary is quite similar to the situation described by EINSTEIN: it corresponds to the emission of two particles from a virtual entity, remaining one part at rest. The calculated mass values are far below the mass of atoms and exclude, therefore, the assumption of WANNIER Excitons.

[1905/1] Ann. Physik 17; [1905/2] Ann Physik 18; Surveys by [1972] H. Gerischer; [1980] P. S. Vincett and G. G. Roberts and [1982] in Electronic Processes in Organic Crystals by M. Pope and Ch. E. Swenberg.