MP 5: Vielteilchentheorie

Zeit: Dienstag 17:00–18:00 Raum: KGI-HS 1023

MP 5.1 Di 17:00 KGI-HS 1023

Die Grundzustandsenergie großer Atome: Die Scottkorrektur — Rupert Frank[1], •Heinz Siedentop[2] und Simone Warzel[1] — [1]Department of Mathematics, Princeton University, Princeton, NJ 08544-1000, USA — [2]Mathematisches Institut, Ludwig-Maximilians-Universität München, Theresienstr. 39, 80333 München

Die Grundzustandsenergie $E(Z)$ großer neutraler Atome (große Ordnungszahl Z) wird asymptotisch durch die Thomas-Fermi-Energie $E_{\mathrm{TF}}(Z) = E_{\mathrm{TF}}(1)Z^{7/3}$ gegeben (Lieb und Simon 1977). Die führende Korrektur, die sogenannte Scottkorrektur ist $Z^2/2$ (Siedentop und Weikard 1987). Dieses Bild der Grundzustandsenergie ist im Rahmen der nichtrelativistischen Quantenmechanik korrekt. Nun erzwingt allerdings die zunehmende Kernladung eine so schnelle Bewegung der inneren Elektronen, daß die zu Grunde liegende nichtrelativistische Schrödingergleichung unter physikalischem Aspekt fragwürdig und eine relativistische Beschreibung notwendig wird. Wir zeigen, daß die Grundzustandsenergie des von Brown und Ravenhall (1951) aus der Quantenelektrodynamik hergeleiteten Hamiltonoperators eines Atoms sich wie

$$E_{\mathrm{BR}}(Z) = E_{\mathrm{TF}}(1)Z^{7/3} + f(Z/c)Z^2 + o(Z^2)$$

verhält, wobei $f(Z/c) < 1/2$ gilt. Während der führende Energiebeitrag also unverändert bleibt, wird die Scottkorrektur erniedrigt, was eine Vermutung von Schwinger (1980) bestätigt.

MP 5.2 Di 17:20 KGI-HS 1023

The zero-entropy-density conjecture — •Zoltán Zimborás[1] and Szilárd Farkas[2] — [1]Theoretische Physik, Universität des Saarlandes, Saarbrücken 66041 Campus 1, Germany — [2]Department of Physics, University of Chicago, Chicago, Illinois 60637

A natural and long-standing conjecture in mathematical quantum statistical physic is that the entropy density vanishes for all translation-invariant pure states on a quantum spin-chain. Or equivalently, S(N), the von Neumann entropy of such a state restricted to N consecutive spins, is sublinear. We report on a new result about this conjecture. We have shown that this conjecture cannot be sharpened, i.e., translation-invariant states give rise to arbitrary fast sublinear entropy growth. The proof is constructive, and is based on a class of states derived from quasifree states on a CAR algebra. We will also discuss the d-dimensional case, and a general lower-bound on the entropy asymptotics of pure shift-invariant quasifree states will be given.

References:
1) S. Farkas and Z. Zimborás, J. Math. Phys. 48, 102110 (2007).
2) S. Farkas and Z. Zimborás, J. Math. Phys. 46, 123301 (2005).

MP 5.3 Di 17:40 KGI-HS 1023

A statistical mechanical analogue of the second law: The increase of entropy upon release of a constraint in classical systems. — •Jürgen Schlitter — Lehrstuhl für Biophysik, Ruhr-Universität Bochum, Deutschland

Computer simulations have drawn new attention to holonomic constraints being used for simplified calculations, and also for maintaining and parameterizing equilibrium states. Second-law like phenomena of relaxation and equilibration are familiar to computational physicists. Their analysis has been facilitated by methods for calculating thermodynamic potentials which now enable a new approach to the formal foundation of the observed behavior. Here, we first consider classical mechanical systems which are fixed in a conditional equilibrium by means of constraints. If there are mean forces under this condition, they are shown to be purely entropic. Next, spontaneous transitions at constant energy are considered which occur upon release of a constraint. For any such transition it is shown that it leads on average to a region of higher entropy in phase space. This is a formally derived analogue of the second law of thermodynamics. Examples of constrained systems are given which show the range of application of this approach. The result is discussed with respect to a seeming contradiction to time symmetry. The latter manifests itself by the occurrence of residual fluctuations. It is not violated during the formal derivation, but by the underlying experimental setup. Entropy is only measured at equilibrium. The two-step mode of release and constraint is essential for the formal result. Reference: J. Schlitter, Mol. Phys. 104: 2829-2834, 2006