DY 22 Quantum Dynamics II

Time: Tuesday 11:00–13:00 Room: HÜL 186

DY 22.1 Tue 11:00 HÜL 186

"Hermite"states in the quantum interaction of vortices — •Alexey Romanov, Chukbar Konstantin, and Zaburdaev Vasiliy — Russian Research Center 'Kurchatov Institute', pl. Kurchatova 1, 123182 Moscow

In this paper, we consider transition from classical dynamics of vortices to quantum. Problem of two identical cinematic vortices (each vortex produce 2d velocity field with current function $\psi(|\mathbf{r}|)$) reduces to the Hamiltonian system with Hamilton function $H(q,p) = \psi(\sqrt{q^2+p^2})$ (q=x, p=y). We perform transition to quantum vortices dynamic according to the standard rule: $q \to q, p \to -i\hbar\frac{\partial}{\partial q}$. Now we start to solve quantum problem with Hamilton operator $\hat{H} = \hat{\psi}\left(\sqrt{\hat{r}^2}\right), \hat{r}^2 = -\hbar^2\partial^2/\partial q^2 + q^2$. Operator $\hat{r}^2$ corresponds to quantum oscillator with Hermite eigenfunction, and eigenvalue spectrum (1,3,..,2n+1). So Hamiltonian $\hat{H}$, which describes dynamic of quantum vortex, has Hermite eigenfunctions and eigenvalue spectrum: $\psi\left(\sqrt{2n+1}\right)$. Quantum oscillator has, so called, coherent states, which is stable during quantum evolution. Vortex Hamiltonian doesn't have such states, because of dispersion of angular frequency. Also we consider transition for system with anisotropic current function $\psi = A\frac{x^2-y^2}{(x^2+y^2)^2}$.

DY 22.2 Tue 11:15 HÜL 186

The limited validity of the Kubo formula for thermal conduction. — •Jochen Gemmer[1], Robin Steinigeweg[1], and Mathias Michel[2] — [1]Physics Department, University of Osnabrück, Barbarastr. 7, 49069 Osnabrück — [2]Institute of Theoretical Physics I, University of Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart

The Kubo formula describes a current as a response to an external field. In the case of heat conduction there is no such external field. We analyze why and to what extend it is nevertheless justified to describe heat conduction in modular quantum systems by the Kubo formula. "Modular" we call systems that may be described as consisting of weakly coupled identical subsystems. We explain in what sense this description applies to a large class of systems. Furthermore, we numerically evaluate the Kubo formula for some finite modular systems. We compare the results with data obtained from the direct numerical solution of the corresponding time-dependent Schroedinger equation.

[1] Michel et al. *Phys. Rev. Lett.*, **95**, 180602 (2005)

DY 22.3 Tue 11:30 HÜL 186

Relevance of the electronic environment for the neutron scattering behavior of protons — •Tyno Abdul-Redah[1,2], Aris C. Chatzidimitriou-Dreismann[3], and Matthias Krzystyniak[3] — [1]ISIS Facility, Rutherford Appleton Laboratory, UK. — [2]School of Physical Sciences, The University of Kent at Canterbury, Canterbury, UK. — [3]Inst. f. Chemie, TU Berlin, Berlin, Germany.

A large number of neutron Compton scattering (NCS) experiments on hydrogen containing materials like liquid water, metal hydrogen systems and organic compounds has been reported on where a striking effect of a strong neutron proton scattering cross section shortfall has been found (for an overview, see [1]). This effect - which has been very recently confirmed using electron-proton Compton scattering on organic polymers [2] - was attributed to the existence of short lived protonic quantum entanglement and/or to the breakdown of the Born-Oppenheimer approximation during the scattering process. Recent NCS experiments on various metal hydrogen systems strongly indicate the relevance of the electronic environment surrounding the proton. Concretely, changing the electronic charge density around or the bonding conditions of the protons leads to different cross section anomalies in those materials. It is concluded that the electronic environment determines the decoherence process of the protons thus leading to these different anomalous shortfalls.

[1] T. Abdul-Redah et al., Neutron News 15 (2004) 14.
[2] C. A. C.-Dreismann et al., Phys. Rev. Lett. 91 (2003) 057403.
[3] T. Abdul-Redah et al., J. Alloys Compd. (2005), in press.

DY 22.4 Tue 11:45 HÜL 186

Novel sampling approaches for complex ensembles in ab-initio molecular dynamics — •Jochen Schmidt[1,2], Daniel Sebastiani[1], and Christopher J. Mundy[2] — [1]Max Plank Institute for Polymer Research, Mainz — [2]Lawrence Livermore National Laboratory, Livermore CA, USA

Computer simulations using ab-initio approaches are a very important and widely used tool to study the microscopic behaviour of gases, liquids and solids. The traditional simulation of an NVE-ensemble does not reflect the usual experimental setup, where temperature and pressure are monitored. Besides this, there is an extensive interest in studying properties as a function of these quantities. Therefore the simulation of an NPT-ensemble is crucial. We present the implementation of constant pressure calculations in the highly parallel DFT-code QUICKSTEP, which is a part of the CP2K program package, using a mixed Gaussian and Plane Waves approach (GPW) [1]. This enables the application of our method to extended systems. Further, we use a recently developed method to simulate shock wave propagation in condensed matter, which allows the investigation of shock compression with ab-intio methods [2]. Both theoretical background and first applications will be presented.

[1] VandeVondele J., Krack M., Mohamed F., et al., Computer Physics Communications 167, 103 (2005)
[2] Reed E. J., Fried L. E. and Joannopoulos J. D., Phys. Rev. Lett. 90, 235503 (2003)

DY 22.5 Tue 12:00 HÜL 186

Normal transport behaviour in one-dimensional chaotic quantum systems — •Robin Steinigeweg and Jochen Gemmer — Physics Department, University of Osnabrück, Barbarastr. 7, 49069 Osnabrück, Germany

We investigate the transport behaviour of several one-dimensional (1D) quantum systems neither modelling heat baths nor using standard methods as the Kubo formula for heat conduction. Instead we numerically solve the corresponding time-dependent Schrödinger equation for various initial states and model parameters. It turns out that within the parameter range where normal transport occurs, that is, Fourier's law applies the nearest neighbour level spacing distribution (NNLSD), $P(s)$, can be well described by a Wigner distribution. Amongst others we also investigate a spin system, namely a $s = 1/2$ Heisenberg chain in an external magnetic field B. Since this integrable system has a Poisson-like distribution $P(s)$ and does not show normal transport, we allow (small) local variations B_μ from the mean field B. As a consequence the distribution $P(s)$ becomes Wigner-like and normal transport occurs. This result reaffirms the assumption that normal transport behavior of 1D quantum systems is associated with a Wigner-like NNLSD.

DY 22.6 Tue 12:15 HÜL 186

Fourier's Law from Schrödinger Dynamics — •Mathias Michel[1], Jochen Gemmer[2], and Günter Mahler[1] — [1]Institut für Theoretische Physik I, Universität Stuttgart — [2]Fachbereich Physik, Universität Osnabrück

The relationship between microscopic and macroscopic levels of description has challenged physicists for centuries and in many branches of research. In this talk we demonstrate that a class of closed quantum systems gives rise to diffusive behavior (normal heat conduction, see [1]) on a mesoscopic level while the microscopic dynamics is governed by the respective Schrödinger equation only. The key to understanding such qualitative differences is not just the mere system size but rather the complete or reduced description as dictated by observation. For example, quantum thermodynamics [2] has been able to show that a partition of a closed quantum system into a small part of interest and a large environment will typically lead to thermal equilibrium properties with respect to the small part. In the same spirit, heat conduction and Fourier's law emerge from closed system quantum dynamics under appropriate coarse-graining in real space! Such a behavior may show up already in suprisingly small composite quantum objects.

[1] M. Michel et al., Phys. Rev. Lett. **95**, 180602 (2005)
[2] J. Gemmer et al., Quantum Thermodynamics, Springer (2004)

DY 22.7 Tue 12:30 HÜL 186

Effective quantum potentials — •C. Olbrich[1] and K. Morawetz[1,2] — [1]Institute of Physics, Chemnitz University of Technology, 09107 Chemnitz, Germany — [2]Max-Planck-Institute for the Physics of Complex Systems, Nöthnitzer Str. 38, 01187 Dresden, Germany

An exact correspondence is established between a N-body classical interacting system and a $N-1$-body quantum system with respect to the partition function [1]. The resulting hermitian quantum-potential is a $N-1$-body one. Inversely the Kelbg potential is reproduced which describes quantum systems at a quasi-classical level. Such quantum potential allows to simulate quantum effects within the classical moleculardynamics reproducing the quantum correlation energy. We present a simple procedure to construct such effective quantum potentials for any temperature and density and present simulation results for the conductivity in quasi two-dimensional systems.

[1] K. Morawetz; Phys. Rev. E 66 (2001) 022103

DY 22.8 Tue 12:45 HÜL 186

Continuous time quantum walks in phase space — •Oliver Mülken — Institut für Physik, Universität Freiburg

We formulate continuous time quantum walks (CTQW) in a discrete quantum mechanical phase space. We define and calculate the Wigner function (WF) and its marginal distributions for CTQWs on circles of arbitrary length \$N\$. The WF of the CTQW shows characteristic features in phase space. Revivals of the probability distributions found for continuous and for discrete quantum carpets do manifest themselves as characteristic patterns in phase space.

\Zitat{1}{arXiv: quant-ph/0509141}