must maintain at constant level
a huge number of quantities) the integrable systems not thermalize properly,
consequently have ergodicity problems, hence their behavior is far from what
we would expect from the behavior of a real system from nature. Given by these
antecedents, concentrating on the ground state and the low lying part of the
excitation spectrum, we started to develop techniques which provide exact
results in this region of the energy spectrum. The procedure starts by the
transformation of the Hamiltonian in positive semidefinite form. After this step
the ground state is deduced using positive semidefinite operator properties, the
uniqueness of the solution is proven by concentrating on the kernel of the
positive semidefinite operators, the physical characteristics of the ground
state is analysed by deducing adequate ground state expectation values, and
finally the low lying part of the excitation spectrum is studied based on the
particle number dependent chemical potential [1-3]. Several applications to
different physical systems is also presented [4-6].

[1] Z. Gulacsi, Int. J. Math. Mod. & Meth. in Appl. Sci. 9, 691, (2015).
[2] Z. Gulacsi, Int. J. Mod. Phys. B27, 1330009, (2013).
[3] Z. Gulacsi, J. Phys. Conf. Ser. 410, 012011, (2013).
[4] Z. Gulacsi, A. Kampf, D. Vollhardt, Phys. Rev. Lett. 105, 266403 (2010).
[5] M. Gulacsi, Gy. Kovacs, Z. Gulacsi, Europhys. Lett. 107, 57005, (2014).
[6] Z. Gulacsi, Eur. Phys. J. B87, 143, (2014).

C18: Momentum space reflection symmetry breaking in quasifree fermion systems

Zoltan Kadar

University of Leeds, UK

zokadar@gmail.com

Reflection symmetry breaking in the ground state and the vanishing of the spectral gap are connected in quasifree fermionic models. For translation invariant spinless fermions, the breaking signals criticality, whereas for models with spin, the spin average covariance matrix implies a similar conclusion. Our results identifies a set of models, where the generalized Hartree-Fock approximation must break down.

C19: The Description of Carrier Transport for Quantum Systems

M. Nedjalkov[1], J. Weinbub[2], S. Selberherr[1]

[1]*Institute for Microelectronics, TU Wien, Vienna, Austria*

Email: Selberherr@TUWien.ac.at, web site: http://www.iue.tuwien.ac.at/

[2]*Christian Doppler Laboratory for High Performance TCAD, Institute for Microelectronics, TU Wien, Vienna, Austria*

Basic quantum mechanics describes systems determined by Hamiltonian state vectors $|\psi\rangle$, which provide the spatial and time dependences of the physical observables. A pure state density operator $|\psi\rangle\langle\psi|$ - as obtained by a single state vector - contains the most complete information about the spatial correlations in the system. Mixed states are introduced as linear combinations of pure states with assigned probability distributions, reflecting the fact that the knowledge of the system is incomplete as a result of interactions with other systems. This is the case for carrier transport through open systems, such as nanodevices exchanging carriers through their

contacts. The carrier system is maintained in a mixed state by a competition of quantum-coherent processes of interference and correlations with processes of decoherence caused by the environment (e.g. photon/phonon interaction) [1]. The description of carrier transport falls into this setting and relies on the methods developed for quantum statistical mechanics. We critically compare the peculiarities of two such methods, those being the non-equilibrium Green's function formalism (NEGF) [2] and the Wigner function formalism [3].

The well-established and comprehensive NEGF formalism considers processes of correlations both in space (x, x') and time (t, t'). Under stationary conditions this formalism accounts for the energy dependence via a Fourier transform of the relative time $t - t'$. For purely coherent problems it provides a tomography of the generic physical quantities in terms of energy. This ability to account for the energy spectrum of the device states coupled to the states in the contacts has inspired the development of novel simulation setups. In general, NEGF is efficient for stationary problems - determined by the boundary conditions - near the coherence limit. However, the method's computational effort increases tremendously when processes of dissipation are taken into account.

The Wigner function is a single time object where one of the positions is replaced by the momentum. Being defined in the phase space x, k, the Wigner function retains many classical concepts and notions. In particular, physical averages are evaluated by classical expressions and boundary conditions are the same as for classical particles. The approach is gaining recognition as it incorporates processes of dissipation and time evolution in a computationally tractable way. Fig.1 shows one of the first two dimensional applications, where an initial Wigner function is split by a specifically engineered potential into four well-formed peaks with four mean momenta, causing them to propagate into four disparate directions. The four peaks represent a single carrier state since the Wigner evolution maintains the initial coherence. This demonstrates that the proper choice of a correct quantum initial condition is crucial to ensure physical relevance and correctness. However, the Wigner evolution cannot filter out the *unphysical* part of an improperly chosen initial state, which is an input for the formalism. Choosing a proper initial condition is thus a key challenge for using a Wigner function approach.

We see a clear advantage in combining both formalisms to describe carrier transport for quantum systems. The NEGF approach is suitable for incorporating all correlations and coherence effects in the initial condition. In turn, the Wigner evolution allows to conduct transient simulations covering time-dependence and decoherence processes. Such a coupled approach accounts for the initial coherence and the correct handling of time-dependent quantum processes.

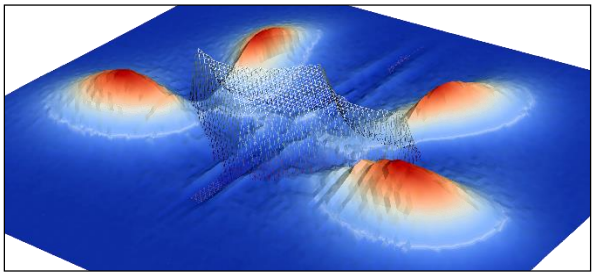

Fig 1.: An initial Wigner function corresponding to a minimum uncertainty wave packet encounters a potential with a specifically engineered shape, splitting the initial packet to four well established density peaks propagating in disparate directions. The evolution maintains the initial coherence: If time is reversed, the backward evolution recovers the initial state.

[1] C. Jacoboni, Solid-State Sciences, 2010.
[2] M. Pourfath, Computational Microelectronics Series, 2014.
[3] M. Nedjalkov et al., Nano-Electronic Devices, 2011.