# Research statement 11/11/2011

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The present research statement briefly describes my research activity in mathematics, mathematical physics, and theoretical physics in recent years and develops prospects for future research. The research fields include the following areas ordered by decreasing number of publications.

1 Nonequilibrium quantum statistical mechanics

2 Nonlinear Schrödinger/Hartree equations

3 Weak nuclear force

4 Gravitating gauge fields

5 Dirac-Fock theory

The mathematics involved in these fields are **functional analysis**, **operator algebras**, **partial differential equations**, **calculus of variations**, **numerical** and **harmonic analysis**, and **differential geometry**.

The results will be labelled by ■ and the work in progress by □ .

## 1 Nonequilibrium quantum statistical mechanics

The main field of my present research activity in mathematical physics lies in nonequilibrium quantum statistical mechanics.[1] I'm studying the mathematically rigorous description of specific open systems within the formalism of $C^*$ algebras. A typical open system consists of a small sample coupled to several thermal reservoirs at different temperatures. Since the rigorous study of such systems is rather recent, it is of central importance for the development of the theory to have models at one's disposal which are, in some sense, exactly solvable. In sharp contrast to the case where the system is in thermal equilibrium, the nonequilibrium situation is much more complicated due to the fact the dynamics plays a crucial role. Very few nontrivial models only are integrable in the sense that their dynamics can be described in a sufficiently explicit way. One of

[1] For a more technical overview, see the habilitation thesis at *http://aschbacher.univ-tln.fr*.

the simplest examples possessing this property is the so-called XY chain. Namely, with the help of the so-called Jordan-Wigner transformation, this spin system can be interpreted, to some extent, as a gas of independent fermions. Besides the XY chain, we study different aspects of general quasifree fermionic systems. By definition, such systems consist of independent fermions, and, hence, their dynamics are implemented in the one-particle Hilbert space over which the observable algebra is built.

In order to get a concrete idea of this algebraic approach to open quantum systems, we will briefly describe in the following the ingredients of the XY chain and some of its nonequilibrium properties. The results for the more general quasifree fermionic systems will be presented subsequently.

The XY chain is a special instance of a spin system of Heisenberg type (see Lieb *et al.* [41]). Of great interest, and, hence, intensively studied, are the transport properties of such systems, as, for example, the heat conduction. Among other things, this is due to the fact that, not only theoretical and numerical investigations suggest the violation of the Fourier law,[2] but also since such an ideal conductivity can be observed in experiments (see for example Sologubenko *et al.* [44]).
The kinematical structure of the XY chain is encoded through a uniformly hyperfinite quasilocal algebra over the finite subsets of the discrete line $\mathbb{Z}$. Its formal hamiltonian is given by

$$H = -\frac{1}{4}\sum_{x\in\mathbb{Z}}\Big[(1+\gamma)\sigma_1^{(x)}\sigma_1^{(x+1)} + (1-\gamma)\sigma_2^{(x)}\sigma_2^{(x+1)} + 2\lambda\sigma_3^{(x)}\Big], \tag{1}$$

where the parameter $\lambda$ describes the strength of the external magnetic field, and $\gamma$ is the anisotropy of the spins in the transversal directions. Moreover, $\sigma_i$ denote the usual Pauli matrices. Since the interaction is short range and since it involves two spins only, the local dynamics generated by the local version of (1) has a thermodynamic limit $\tau^t$ which defines a strongly continuous group of automorphisms on the $C^*$ algebra $\mathfrak{S}$ generated by the Pauli matrices. This means that the XY chain is a so-called $C^*$-dynamical system $(\mathfrak{S},\tau)$ (see also Aschbacher *et al.* [22] for an introduction to algebraic quantum statistical mechanics).

In order to set up a nonequilibrium configuration consisting of a finite sample coupled to two thermal reservoirs, we break the bonds at two sites in (1) partitioning the discrete line into the subsets $\mathbb{Z}_L$, $\mathbb{Z}_\mathcal{S}$, and $\mathbb{Z}_R$. Doing so, we get a new hamiltonian $H_0$ whose dynamics leaves the systems over these sets decoupled. Moreover, we define a so-called initial state $\omega_0$ to be the product of three thermal equilibrium (KMS) states carrying the inverse temperatures $\beta_L$, $\beta_\mathcal{S}$, and $\beta_R$, the half-infinite systems over $\mathbb{Z}_L$ and $\mathbb{Z}_R$ playing the role of thermal reservoirs which interact with the finite system over $\mathbb{Z}_\mathcal{S}$ by the coupling $H - H_0$.

Following Ruelle [43], a nonequilibrium steady state (NESS) $\omega$ associated with the $C^*$-dynamical system $(\mathfrak{S},\tau)$ and the initial state $\omega_0$ is a weak-$*$ limit point for $t > 0$ of the net of ergodic means of $\omega_0 \circ \tau^t$.

[2] In the case of integrable systems.

In order to construct a NESS for our nonequilibrium configuration, we make use of the above mentioned Jordan-Wigner transformation which allows us to switch to a description of the system by means of independent fermions with one-particle Hilbert space $\ell^2(\mathbb{Z})$ (see Jordan and Wigner [39] and Araki [3]). The coupled and the uncoupled time evolutions then act as Bogoliubov automorphisms generated by the explicitly known one-particle hamiltonians $h$ and $h_0$. The fermions being independent, the construction of the NESS boils down to a time dependent scattering problem of the unitary groups generated by $h$ and $h_0$ on the (double) of the one-particle Hilbert space.[3]

■ **NESS existence and uniqueness – [25]** Since the spectrum of the coupled one-particle hamiltonian $h$ is purely absolutely continuous, the Møller morphism $\mu$ implementing the usual Hilbert space wave operator on the observable algebra exists and is complete.[4] This implies that the NESS is unique and that it has the form

$$\omega = \omega_0 \circ \mu. \tag{2}$$

This result constitutes the first rigorous construction of a NESS in Ruelle's framework of time dependent scattering theory. It is at the origin of the study of the more general quasifree systems (see Aschbacher *et al.* [22] and references therein).

■ **NESS properties – [25]** Due to (2), the NESS is again quasifree. Using partial wave operators and asymptotic projections, we show that the density $T$ characterizing the quasifree NESS has the form of a Fermi-Dirac distribution at mean inverse temperature $\beta$ whose exponent is augmented by a contribution proportional to the difference $\delta$ of the inverse temperatures and to the sign of the asymptotic velocity $v$ having the form

$$T = \left(1 + \mathrm{e}^{-(\beta - \delta\,\mathrm{sign}(v))\,h}\right)^{-1}. \tag{3}$$

Besides, we prove that the NESS is attractive, independent of the sample size, translation invariant, and that it is a KMS state if and only if the temperatures are equal. Moreover, it turns out that it has the following structural properties: It is primary, modular, and singular w.r.t. the initial state if and only if the temperatures are different.

The central property of such a NESS is the nontriviality of its entropy production rate $\mathrm{Ep}(\omega)$. Due to energy conservation, this quantity is proportional to $\delta$ and to the heat current through the system (see for example Aschbacher *et al.* [22]).

■ **Strictly positive entropy production – [25]** Using (3) and computing the asymptotic velocity $v$ explicitly, we derive its strict positivity,

$$\mathrm{Ep}(\omega) > 0. \tag{4}$$

This is the first rigorous result of the existence of a nontrivial thermodynamics for a NESS constructed in Ruelle's time dependent scattering approach.

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[3] The doubling of the one-particle Hilbert space is a special case of the concept of a so-called selfdual CAR algebra introduced and developed by Araki [1, 2].

[4] To my knowledge, there exist two rigorous approaches to the construction of NESS only. The approach which we describe here is the traditional one using time dependent scattering theory. A second approach has been developed more recently in Jakšić and Pillet [38] reducing the NESS construction to the spectral analysis of the so-called liouvillian.

Due to its important role, it is of great interest to have a simple criterion at one's disposal allowing to decide whether the entropy production is strictly positive.

■ **Strictly positive van Hove entropy production – [26]** We derive an algebraic criterion which ensures the strict positivity of the van Hove weak coupling entropy production $\sigma$.[5] In turn, $\sigma > 0$ leads to the desired nontrivial entropy production as soon as

$$\mathrm{Ep}(\omega) = \sigma g^2 + \mathcal{O}(g^3), \tag{5}$$

where $g$ stands for the constant which describes the strength of the sufficiently small coupling between the sample and the reservoirs. The relation (5) between the microscopic and the macroscopic regimes has been established in Jakšić and Pillet [38] for a finite sample coupled to two fermionic reservoirs and for the so-called simple electronic black box model in Aschbacher *et al.* [22].

■ **Relation between the microscopic and the van Hove regime – [13]** We rigorously study the relation (5) and the issue of strict positivity of the entropy production in the isotropic XY chain out of equilibrium. First, we construct the NESS in the same nonequilibrium setting as above, but we allow for general bond coupling perturbations and an arbitrary sample size. We then prove strict positivity of the microscopic entropy production and extract its leading second order contribution for small coupling. Furthermore, we construct the NESS in the van Hove regime and derive its entropy production. Finally, we prove that, on the level of the entropy production, the van Hove regime reproduces the leading order contribution to the microscopic regime.

Systems which are nontrivial generalizations of the XY chain exhibit even richer thermodynamical properties. We study different aspects of such systems and some of their generalizations, one of the central issues being the nonequilibrium phase transitions.

□ **Generalized XY chains – [14]** We construct NESS in such systems and study their transport properties as well as classes of important spatial and temporal correlation functions.

Motivated by the nonequilibrium situation of the XY chain, we treat the more general quasifree systems where, again, a sample is coupled to several reservoirs.

■ **Landauer-Büttiker formalism – [23]** As in the case of the XY chain, we construct the unique NESS $\omega$ by using time dependent scattering theory on the one-particle Hilbert space. Subsequently, with the help of stationary scattering theory, we derive the Landauer-Büttiker formalism for the mean heat and matter currents,[6]

$$\omega(\Phi) = \int_{\mathrm{spec}_{\mathrm{ac}}(h_0)} \mathrm{d}e \;\; \mathrm{tr}(T_0(e)[q(e) - S^*(e)q(e)S(e)]). \tag{6}$$

Here, $\Phi$ denotes the current observable generated by the charge $q$,[7] $h_0$ and $h$ again

[5] The results in Aschbacher and Spohn [26] are not restricted to the XY chain or to the more general quasifree systems but they also hold for NESS constructed with the help of the spectral approach mentioned in footnote 4.

[6] This rigorous derivation holds for couplings of trace class type.

[7] As for example the energy or the particle number in one of the reservoirs.

the uncoupled and the coupled hamiltonians, $T_0$ the density of the quasifree initial state $\omega_0$, and $S$ the scattering matrix. Specializing (6) by assuming the sample hamiltonian to have purely discrete spectrum, we arrive at the so-called Landauer-Büttiker formula. This result constitutes the first rigorous derivation of the Landauer- Büttiker formalism from Ruelle's scattering approach to NESS using simple and at the same time rather general assumptions.

■ **Strictly positive entropy production – [23]** Moreover, with the help of (6), we prove the strict positivity of the entropy production.

If the generalized forces generating such currents are sufficiently small, then the so-called kinetic transport coefficients describe the leading linear dependence of the currents on the generalized forces.

■ **Linear response – [23]** Starting again from (6), we prove the Onsager reciprocity relations. Furthermore, we derive Green-Kubo formulas for this class of models.

□ **Fluctuation theorems – [24]** We study fluctuation theorems for a wide class of correlations, as for example Gallavotti-Cohen type symmetries.

In order to get a clearer picture of the foregoing NESS, we next want to study spatial correlation functions of typical observables in these NESS.

■ **Longitudinal long range – [25]** In the above XY chain, the explicit form of the density (3) allows us to determine the spatial decay for $n \to \infty$ of the (truncated) correlation between the longitudinal spins $\sigma_3^{(0)}$ and $\sigma_3^{(n)}$. Since the Jordan-Wigner transformation is local in the longitudinal spins, the study of the correlation function reduces, for all $n$, to the computation of a fermionic four-point correlator. We show that, out of equilibrium, the decay is quadratic and, hence, it is in sharp qualitative contrast to the exponential decay behavior in equilibrium.

The correlation $C(n)$ between the transversal spins $\sigma_1^{(0)}$ and $\sigma_1^{(n)}$ (or $\sigma_2^{(0)}$ and $\sigma_2^{(n)}$) also exhibits exponential decay in thermal equilibrium (see for example [33]). How is this behavior modified in a true nonequilibrium situation?

■ **Transversal short range – [16]** Due to the nonlocal nature of the Jordan-Wigner transformation in the transversal direction, the transversal correlation function contains a with $n$ growing number of fermionic events. Moreover, as in equilibrium, it can be written as the determinant of the finite truncation of a Toeplitz operator but the Toeplitz symbol undergoes the following two main changes when leaving equilibrium: it becomes matrix-valued and loses regularity. Nevertheless, with the help of the ramifications of Toeplitz theory, we prove that the transversal correlation function still decays exponentially,

$$\limsup_{n\to\infty} \frac{\log C(n)}{n} \leq \frac{1}{2} \sum_{j=R,L} \int_{-\pi}^{\pi} \frac{\mathrm{d}k}{2\pi} \log(\tau_{\beta_j}(k)), \tag{7}$$

where $\tau_{\beta_j} = \mathrm{th}\,(\beta_j \epsilon/2)$, and $\epsilon$ is the dispersion relation. Furthermore, (7) confirms the left mover-right mover picture established in Aschbacher and Pillet [25]. This picture interprets the NESS density as being composed of two noninteracting species carrying

the inverse temperatures $\beta_R$ and $\beta_L$, respectively, stemming from the infinitely remote reservoir sources.

We want to develop the foregoing approach in order to be able to bound the decay rate of more general translation invariant quasifree fermionic systems.

■ **Exponential decay criterion – [17]** We formulate a simple sufficient condition on the spectrum of the density of the quasifree fermionic state ensuring the exponential decay for a class of typical correlation functions. We apply this criterion to the anisotropic magnetic XY chain out of equilibrium, in thermal equilibrium at positive temperature, in the ground state, and in the chaotic state.

■ **EFP decay – [9]** Furthermore, we use this method in order to derive a criterion ensuring the exponential decay of the so-called emptiness formation probability (EFP). When again applying this criterion to the XY chain in the foregoing four states, we find from the existing literature on the asymptotics of the EFP that our bound is sharp in all equilibrium cases.

Given the exponential decay in the leading order asymptotics of the foregoing correlation functions paralleling qualitatively the behavior in thermal equilibrium at positive temperature, one may wonder whether there is some characteristic signature of the nonequilibrium left at some subleading order.

■ **Qualitative nonequilibrium signature – [11]** For this purpose, we study the effect of the true nonequilibrium on the terms of subleading order in the asymptotics of the NESS EFP by using Fisher-Hartwig theory in the analysis of the occurring Toeplitz operators. We prove that the exponent of the power law contribution to the asymptotic decay behavior is strictly positive if and only if the system is truly out of equilibrium. In addition, it turns out that this behavior is indeed due to the singularities of the density of the NESS.

The foregoing methods apply to correlation observables in translation invariant states. One may wonder how some breaking of translation invariance affects the underlying Toeplitz analysis.

■ **Broken translation invariance – [12]** To this end, we construct the unique NESS in the isotropic XY chain whose translation invariance is broken by means of a local magnetization. After that, we analyze the asymptotic behavior of the expectation value of a class of spatial correlation observables in this NESS as, in particular, the EFP. We show that the magnetization has the following effects on the decay of the correlation function. On one hand, the local perturbation regularizes the scalar symbol of the corresponding Toeplitz operator and, on the other hand, it leads to an additional term of Hankel type in the correlation determinant. Furthermore, the decay is proven to be exponential and its rate again exhibits the left mover-right mover structure mentioned above which, in the present situation, is affected by the scattering at the impurity.

Finally, we study an important correlation function for spin systems, namely the von Neumann entropy which quantifies the correlation of a block of neighboring spins to the rest of the chain. At zero temperature, it is considered to be the generic measure of entanglement for bipartite systems. What happens to this object out of equilibrium?

■ **Nonvanishing entropy density – [8]** In order to tackle this question, we again use Toeplitz theory. We prove that the von Neumann entropy density has a nonvanishing thermodynamic limit. Moreover, we derive an explicit expression for it which again displays the left mover-right mover structure encountered in the foregoing correlation functions.

# 2 Nonlinear Schrödinger/Hartree equations

In this section, we are concerned with stationary and dynamical aspects of nonlinear and nonlocal partial differential equations of Schrödinger/Hartree type. We start off by studying the uniqueness of minimizers of the Hartree functional

$$\mathrm{H}[\psi] = \frac{1}{2}\|\nabla\psi\|^2 + (\psi, v\psi) + g\,(\psi, V * |\psi|^2\psi), \tag{8}$$

where $v$ is the external potential, $g$ the coupling constant, and $V$ the interaction potential (two-body potential).[8] Moreover, the function spaces involved are sufficiently regular subspaces of $L^2$ over the whole Euclidean space or subsets of it.

The functional (8) and variants of it have many physical applications. As a prominent application, it is used for the description of the condensate wave function in Bose-Einstein condensation (BEC) of dilute gases. In the standard scenario of BEC, the interatomic forces are repulsive and the nonlinearity is local. In (8), this corresponds to the choice $g > 0$ and to the formal replacement of the interaction potential by a delta function.[9]

In the case of attractive interatomic forces, *i.e.* for $g < 0$, the bosons may accumulate in clusters of high density. A simple scaling argument then shows that the GP functional does not have global minimizers (see Aschbacher *et al.* [20]). In sharp contrast, the Hartree functional has global minimizers as soon as the coupling strength exceeds a certain critical threshold value. The existence of such a threshold follows from standard arguments in the calculus of variations whereas its magnitude can be estimated with the help of Birman-Schwinger theory of binding in quantum mechanics. If there is no external potential, the latter theory implies that the threshold equals zero in dimensions one and two as well as in dimension greater or equal to three if the interaction potential has long range. If the interaction potential has short range, the threshold is strictly positive in dimension greater or equal to three.[10] On the other hand, if the external potential is nonvanishing and confining, there exist minimizers at all coupling strengths. In the following, we continue with the issue of uniqueness of attractive minimizers of (8).

■ **Spontaneous symmetry breaking – [20]** We show that, for sufficiently large attractive coupling strength, any minimizer $\Phi$ of (8) with Coulomb interaction potential

[8] The latter being of positive type, as, for example, the Coulomb potential.

[9] We will call (8) with local nonlinearity and any sign of $g$ the Gross-Pitaevskii (GP) functional.

[10] See for example the Cwikel-Lieb-Rosenbljum bound.

breaks general symmetries, possibly induced by the external potential, *i.e.* for any element $G$ of the Euclidean group, we have

$$|\Phi \circ G|^2 \neq |\Phi|^2. \tag{9}$$

The proof of this result assumes a gap between the minimizing sequences of the external potential and their image under $G$, and it is carried out in three steps. First, we show that any approximate free minimizer of (8), *i.e.* with vanishing external potential, is arbitrarily strongly concentrated, and that any minimizer of (8) with nonvanishing external potential is an approximate free minimizer localized around the minima of the external potential. Finally, assuming the minimizer to be invariant under $G$ implies the violation of mass conservation, and hence, leads to (9) by contradiction.

What happens for small attractive coupling?

■ **Uniqueness for small coupling – [20]** Using the contraction mapping principle for the ground state projection, we can show that the minimizer is unique as soon as the coupling strength drops below some critical value.

■ **Critical coupling – [20]** Moreover, we determine the magnitude of this critical coupling with the help of a numerical approach based on a finite element discretization of the configuration space (see below).

Motivated by the intense activity going on in the field of many component condensates in BEC, we want to study the minimizers of the functional associated to the system of coupled Hartree eigenvalue equations of the form

$$\begin{cases} -\Delta\Phi_1 + v_1\Phi_1 + \vartheta_1 V * |\Phi_1|^2\Phi_1 + \kappa V * |\Phi_2|^2\Phi_1 = E_1\Phi_1, \\ -\Delta\Phi_2 + v_2\Phi_2 + \vartheta_2 V * |\Phi_2|^2\Phi_2 + \kappa V * |\Phi_1|^2\Phi_2 = E_2\Phi_2, \end{cases} \tag{10}$$

where the external potentials $v_1$ and $v_2$ are nonnegative and confining. Besides, the the system is purely repulsive, *i.e.* the self-coupling constants $\vartheta_1$ and $\vartheta_2$, and the interaction strength $\kappa$ are nonnegative.

■ **Existence of a system minimizer – [27]** We prove that, for any $\kappa > 0$, there exists a system minimizer of (10). This is done by using the direct method in the calculus of variations and by exploiting the fact that the Hilbert space of the functional setting is suitably compactly embedded due to the confining external potentials.

Having this system minimizer at our disposal, we want to study the direct energy term $\mathrm{D}$ of the Coulomb interaction of its two components. In particular, we want to analyze the behavior of the latter in the limit of large interaction strength $\kappa$. To this end, we call a sequence of minimizers phase segregating if the Coulomb energy vanishes in this limit.

■ **Phase segregation – [27]** We prove that any sequence of system minimizers $\Phi_\kappa$ of fixed mass is phase segregating, and that, for large $\kappa$,

$$\mathrm{D}[\Phi_\kappa] = o(\kappa^{-1}). \tag{11}$$

■ **Separation regime – [27]** Moreover, we develop a strategy of selfconsistent iterations in order to numerically compute the decay behavior of the direct energy of the system minimizers and their transition into the phase segregated regime.

We next turn to the study of the dynamical Hartree equation,

$$\mathrm{i}\partial_t\psi = \left(-\Delta + v + gV * |\psi|^2\right)\psi, \tag{12}$$

provided with an initial condition and a Dirichlet boundary condition. In view of the numerical computation which we eventually want to carry out, we mainly stick to a domain $\Omega \subset \mathbb{R}^2$ with sufficiently smooth boundary though most of the results generalize naturally to all dimensions. In the following, we first describe the rigorous results concerning the continuum, the semidiscrete, and the fully discrete setting of (12). Subsequently, we will briefly discuss some of the numerical simulations which have been performed.

■ **Existence, uniqueness, and regularity in the continuum – [5, 10]** Under assumptions on the external potential, the interaction potential, and the initial condition motivated by the subsequent numerical computation, we prove global existence, uniqueness, and suitable space-time regularity results for the continuum initial-boundary value problem (12) by using techniques from the theory of unbounded self-adjoint operators on Hilbert space.

We next proceed to the semidiscrete and the fully discrete approximation of (12). The former one is set up in the Galerkin space of the bilinear Lagrange elements over the configuration space. Subsequently, we discretize the semidiscrete problem in time focusing on two time discretization schemes of Crank-Nicholson type. The first is the so-called one-step one-stage Gauss-Legendre Runge-Kutta method which conserves the mass of the discretized wave function under the discrete time evolution. The second one is the so-called Delfour-Fortin-Payre scheme which, besides the mass, also conserves the energy of the system.

■ **Existence and uniqueness – [5, 10]** We show that there exists a unique solution of the semidiscrete and the fully discrete schemes by using contraction methods.

■ **Quadratic space-time approximation – [5, 10]** Moreover, we derive a space and time quadratic accuracy estimate on the $L^2$-error of these approximation schemes which, in the fully discrete case, has the form

$$\max_n \|\psi_n - \psi(n\tau)\| \leq c(\psi)\,(\tau^2 + h^2). \tag{13}$$

Here, $\psi_n$ is the fully discretized wave function, and $h$ and $\tau$ denote the space and time discretization scales, respectively. Due to the above Hilbert space approach to the continuum problem, we have an explicit estimate of $c(\psi)$ at our disposal. In contrast to the usual treatment in the literature, this allows us to have a quantitative idea how to achieve a sufficiently accurate numerical control of the fully discrete approximations.

■ **Approximation convergence – [5]** Furthermore, we show that the solution of the fully discretized scheme, linearized with the help of the Picard algorithm, converges to the solution of the nonlinear problem for sufficiently small time discretization scales.

We now turn to the implementation issue and briefly discuss some of the numerical simulations performed with the following program.

■ **Software package – [5]** Using the C++ programming language, we write a software package allowing for a high performance computation both of the nonlinear and nonlocal Hartree eigenvalue problem of the type (10) and of the Hartree dynamics (12) based on their fully discrete approximation schemes discussed above.

■ **Simulation: minimizer construction – [5]** We construct the Hartree minimizer for the case of a Yukawa interaction potential. We find that it is exponentially localized. Moreover, its energy spectrum is analyzed as a function of the coupling strength.

□ **Simulation: return to equilibrium – [5, 15]** Moreover, we track the time evolution of an initial condition being close to a minimizer of the Hartree functional (8) and sitting in a external harmonic potential. We observe that the minimizer oscillates around the potential minimum while radiating off mass and energy. In order to observe return to equilibrium, the radiation has to be able to escape to spatial infinity. To this end, we develop so-called transparent boundary conditions preventing those parts of the wave function arriving at the boundary of the finite numerical configuration space from being reflected back towards the potential minimum.

■ **Simulation: coalescence, scattering, localisation, and ... – [5]** We simulate various scattering processes in order to study the effect of the nonlinear and nonlocal character of the Hartree theory: the coalescence of a binary gravitational system,[11] the scattering of Hartree solitons, the position measurement process of an electron on a screen, and some more.

Finally, we work on the following rigorous derivation of dynamical Hartree theory.

□ **Macroscopic regime – [21]** A system of two coupled time dependent Hartree equations similar to (the dynamical version of) the system (10) arises in the description of so-called monster waves in the context of gravity surface water waves (see for example Onorato *et al.* [42] and Shukla *et al.* [45]). We aim at deriving this system from the Euler equation by using methods from multiscale analysis.

# 3 Weak nuclear interaction

The rigorous study of mathematical models in quantum field theory is a growing area of intense research and fascinating progress. Most of the models whose spectral theory has been rigorously analyzed have been set up within the framework of only one of the three quantized fundamental interactions in nature known today, namely for quantum electrodynamics (QED). Thus, the natural question arises to what extent one can carry out the spectral analysis of mathematical models which stem from one or more of the other fundamental sectors of the Standard Model. As an example of such a process, we study the spectral theory of the decay of the negatively charged intermediate

[11] The Hartree equation has a Newtonian point particle limit, see Fröhlich *et al.* [36].

vector boson $W^-$ of the weak nuclear interaction into an electron $e^-$ and an electron antineutrino $\bar{\nu}_e$,

$$W^- \longrightarrow e^- + \bar{\nu}_e. \tag{14}$$

The weak nuclear interaction is the weakest quantized force of nature with the shortest range.[12] Moreover, it acts between all material particles making them eventually decay into stable leptons and hadrons. A special case of the full (electro-) weak theory is the so-called intermediate vector boson (IVB) theory whose interaction couples the charged leptonic vector current to the intermediate vector boson field.

Whereas one of the main problems in the mathematically rigorous treatment of the semi-relativistic QED models studied in the literature[13] is concerned with the control of the behavior of embedded eigenvalues under the action of a (sufficiently small) perturbation, the mathematical (pen)ultimate goal for our models from IVB theory consists in a derivation of the purely absolutely continuous nature of the spectrum above the ground state of the interacting system. This expectation is motivated by the physical fact that the weak interaction is the only one of the four fundamental forces which produces no bound states. Due to the nature of the form factor in IVB theory, such a proof can be obtained under physically suitable assumptions relaxing the sufficient conditions on the interaction found in the literature to make the available machinery for the spectral analysis work (see below).

For the sake of a simple exposition, we will stick to the decay process (14). Moreover, we assume the particles involved to be scalar. Such a simplification is irrelevant for the description of the problems occurring in the spectral analysis of the model. Nevertheless, we want to stress that the analysis in Aschbacher *et al.* [18] fully covers the real physical situation. The mathematical framework for this process involves one bosonic Fock space for the vector boson and two fermionic Fock spaces for the electron and the electron antineutrino, all of them built on the one-particle Hilbert space $L^2$ functions over the momentum coordinates of the corresponding particles. Whereas the free hamiltonian consists of the usual second quantization of the dispersion relations, being massive for the boson and the electron and massless for the antineutrino, the interaction hamiltonian is characterized by a form factor $F \in L^2$.

■ **Selfadjointness – [18]** We show that, under this assumption on the form factor, the interaction hamiltonian is relatively bounded w.r.t. the free hamiltonian, and that, for sufficiently small coupling,[14] the total hamiltonian $H$ is a self-adjoint operator on the total Fock space.

■ **Existence and uniqueness of the ground state – [18]** Under the additional assumption $F/|k| \in L^2$, where $k$ is the antineutrino momentum coordinate, we prove that there exists a unique ground state for sufficiently small coupling.

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[12] Of relative strength $10^{-15}$ w.r.t. the strong nuclear interaction and of $10^{-13}$ w.r.t. the electromagnetic interaction, and the range being $\ll 10^{-15}$ m.

[13] It is impossible to give here an exhaustive list of all the work done in this field, see for example Bach *et al.* [28, 29, 30] and references therein.

[14] Which is sensible due to the smallness of the weak coupling constant.

In Barbaroux and Guillot [32], an iterative method has been applied to derive a gap property for a certain infrared regularized total hamiltonian. The latter property together with the so-called local regularity of $H$ and the strict Mourre inequality,

$$\chi(H)[H, \mathrm{i}A]\chi(H) \geq C\chi(H), \tag{15}$$

implies that, for sufficiently small coupling, the spectrum between the ground state and the first threshold[15] is purely absolutely continuous. In (15), $\chi$ denotes the characteristic function of the desired interval, the conjugate operator $A$ is chosen to be the second quantization of the momentum dilation generator for the massless electron antineutrino, and $C > 0$. In order to prove the foregoing assertion, a cutoff in the large momenta and a quadratic infrared regularization for the antineutrinos have been used.

■ **Limiting absorption principle – [18]** Deriving a strict Mourre estimate directly for the total hamiltonian without resorting to the Feshbach-Schur procedure, we establish a limiting absorption principle near the ground state by removing the cutoff assumption on the large momenta and by relaxing the infrared regularization for the antineutrinos to

$$\|\chi_{|k|\leq\sigma}(k)F\| = \mathcal{O}(\sigma). \tag{16}$$

Since, in IVB theory, the spinors are locally bounded at the origin of the electron antineutrino momentum space, our condition (16) indeed covers the physical case.

After having analyzed the spectrum close to the ground state, we next study the spectrum between any two consecutive thresholds.

□ **Spectrum between thresholds – [19]** In contradistinction to the case near the ground state energy, we choose a conjugate operator which acts as a dilation on all the particle factors of the Fock space. We again derive a limiting absorption principle by proving the local regularity property and a strict Mourre estimate in the desired interval.

The Mourre constant tends to zero in the limit where the size of the interthreshold interval approaches the energy difference of these thresholds.

□ **Spectrum around thresholds – [19]** Hence, we cannot derive a strict Mourre estimate in the neighborhood of a threshold by perturbing naively around the free commutator. Therefore, we want to study the impact of the following two methods. First, we want to study the renormalization group scheme from Bach *et al.* [28, 29] to the process (14) or to some simplified version of it. To this end, we proceed as in our first attempt to derive (16), namely by adapting and extending the Feshbach-Schur method introduced in Chen *et al.* [35]. A second approach consists in departing from the classical Mourre theory by replacing the selfadjoint conjugate operator by the generator of a strongly continuous semigroup of isometries. This idea has been introduced in Hübner and Spohn [37] in order to treat the spin-boson model with a massive dispersion relation. As the conjugate operator they choose the second quantization of

$$a = \frac{\mathrm{i}}{2}\left(\frac{\nabla_k\omega}{|\nabla_k\omega|^2}\cdot\nabla_k + \nabla_k\cdot\frac{\nabla_k\omega}{|\nabla_k\omega|^2}\right)$$

[15] Being the electron mass since $m_e \simeq 0.5\mathrm{MeV}$ and $m_W \simeq 80\mathrm{GeV}$.

whose commutator with the bosonic field Hamiltonian equals the number operator. Using that, on the orthogonal complement of the vacuum sector, the number operator is bounded from below by the identity operator, they derive a strict Mourre estimate and prove that the spectrum is purely absolutely continuous above the unique ground state. This idea, nowadays called singular Mourre theory, triggered a still ongoing activity. In particular, it has been further developed also for Pauli-Fierz type models with massless fields. We want to apply and to extend these different approaches in order to treat the process (14), or, even simpler, to start with a process where massive particles only are involved.[16]

# 4 Gravitating gauge fields

In 1988, a countably infinite family of globally regular solutions of the Einstein-Yang-Mills (EYM) system has been found by Bartnik and McKinnon [34]. In this system, nonabelian SU(2) Yang-Mills (YM) fields are coupled to the gravitational field of general relativity. The discovery of these solutions came as a surprise since neither gravitational solitons in static curved spacetime nor YM solitons in flat spacetime exist. In contrast, in the EYM system, the attractive gravitational field manages to compensate the repulsion of the YM fields allowing for the existence of solitons.

One of the most widely studied stringy corrections stems from the superstring effective action at low energies which supplements the EYM theory, among other scalar fields, by the massless neutral dilaton with exponential coupling to matter (Kaluza-Klein theories and cosmological models also suggest such a supplementation). This stringy generalization, the so-called Einstein-Yang-Mills-Dilaton (EYMD) theory, is specified by the action

$$\mathcal{S} = \frac{1}{4\pi} \int \left( -\frac{1}{4G}\, R + \frac{1}{2}\, (\partial\varphi)^2 - \frac{\mathrm{e}^{2\kappa\varphi}}{4\gamma^2}\, F^2 \right) \sqrt{-g}\ \mathrm{d}^4x, \tag{17}$$

where $G$ is Newton's constant of gravitation, $\gamma$ the coupling of the YM field $F$, and $\kappa$ the coupling of the dilation field $\varphi$. Moreover, $R$ denotes the scalar curvature of the gravitational field $g$. As in the EYM system, there exists a countably infinite family of globally regular solutions in the EYMD system, see Lavrelashvili and Maison [40].

■ **Dynamical paths – [4]** We study the existence of dynamical paths in the space of static configurations of the EYMD system, *i.e.* those paths which pass through saddle points of the action, relate homotopically different vacua, and have finite kinetic energy. We show that any solution of the field equations possesses an underlying dynamical path if and only if the dilaton field has nonvanishing mass.

■ **Number of instabilities – [4, 7]** Moreover, the linear stability of the solutions of the EYMD system is analyzed. Applying a supersymmetry transformation, we argue that the number of odd parity instabilities is uniquely determined by the number of roots of the background gauge field.

[16] As for example in the decomposition $Z^0 \longrightarrow e^+ + e^-$.

Finally, we study further geometric aspects of gauge field theory, as, for example, the lifting problem for principal fiber bundle automorphism.

# 5 Dirac-Fock theory

Dirac-Fock theory yields a mean field approximation of the energy of a quantum mechanical many body system consisting of massive relativistic spin $1/2$ particles being exposed to an external potential and interacting via Coulomb forces. Although this theory has not yet been rigorously derived from QED, it is nevertheless used in practice, and it is in good agreement with experimental data. Progress in the direction of a rigorous justification has been achieved with the help of the electron-positron Hartree-Fock (EPHF) functional on quasifree states,

$$\mathcal{E}(\gamma) = \mathrm{tr}(H_c\gamma) + \mathcal{Q}(\gamma,\gamma). \tag{18}$$

Here, $\gamma$ denotes the density of the quasifree state, $H_c$ is the Dirac-Coulomb operator, and $\mathcal{Q}$ is the difference of the direct term and the exchange term well-known from Hartree-Fock theory. It is known from Barbaroux *et al.* [31] that the EPHF functional has a (not necessarily unique) minimizer in the set of diagonal densities of fixed mass.

■ **Lowering the energy – [6]** We prove that there exists a density matrix with non-vanishing electron-positron correlation whose EPHF energy is strictly lower than the EPHF energy for the diagonal minimizers from Barbaroux *et al.* [31].

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