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Mathematics of Complex Quantum Systems

Organised by
Volker Bach, Mainz
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August 30th – September 5th, 2009

ABSTRACT. A mathematical physics workshop focusing on the mathematics of complex quantum systems was held at MFO in September 2009. The physics topics covered included quantum chemistry, nonrelativistic QED, statistical mechanics, random matrices and disordered systems, effective equations.

Mathematics Subject Classification (2000): 81Txx.

Introduction by the Organisers

The MFO workshop 0936 on *mathematics of complex quantum systems*, organized by Volker Bach (U Mainz), Jean-Marie Barbaroux (U Toulon), and Lars Jonsson (KTH Stockholm) was held from August 30 through September 5, 2009. About 48 mathematicians and theoretical physicists accepted the invitation and came to Oberwolfach to report on their recent research results and to discuss current work progress. The mathematical field most relevant to this workshop is *analysis*, in particular, the subfields of *functional analysis*, *spectral theory*, *partial differential equations*, and *probability theory*. The physics topics whose mathematical description was covered in the workshop were

- *Quantum Mechanics of Atoms and Molecules* [M. Esteban (Paris-Dauphine), G. Friesecke (TU Munich), H. Siedentop (LMU Munich)];
- *Nonrelativistic Quantum Electrodynamics* [T. Chen (U Austin, TX), J. Dereziński (U Warsaw), J. Faupin (U Bordeaux), C. Gerard (U Orsay), A. Joye (U Grenoble), M. Lewin (U Cergy-Pontoise), O. Matte (LMU Munich), A. Pizzo (U Davies), I. M. Sigal (U Toronto)];

- *Quantum Statistical Mechanics* [V. Betz (U Warwick), W. De Roeck (ETH Zurich), G. M. Graf (ETH Zurich), E. Langmann (KTH Stockholm), M. Salmhofer (U Heidelberg), R. Seiringer (U Princeton), D. Ueltschi (U Warwick)];
- *Random Matrices and Random Schrödinger Operators* [L. Erdős (LMU Munich), F. Germinet (U Cergy-Pontoise), J. Schenker (Michigan S U), B. Schlein (U Cambridge)];
- *Effective Evolution Equations and NL PDE* [E. Lenzmann (MIT), F. Nier (U Rennes), J. Yngvason (U Vienna)];

The organizers consider the workshop a great success, and the scientific directors, the administrative, technical and kitchen staff contributed a considerable share to this - thanks a lot! Especially, we enjoyed the Barbeque on Wednesday, September 2, which is a 2009 innovation of MFO's workshop structure.

In retrospective, we think that our program with about 24 talks was too dense, and we should not have scheduled more than 20 talks.

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Abstracts

Ground state energy of the Müller functional

HEINZ SIEDENTOP

The ground state energy of the Müller functional of large (neutral) atoms of atomic number Z agrees with the quantum mechanical ground state energy up to order $o(Z^{5/3})$.

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Time ordering and counting statistics

GIAN MICHELE GRAF

(joint work with S.Bachmann, G.Lesovik)

We discuss the basic quantum mechanical relation between fluctuations of transported charge and current correlations. It is found that, as a rule, the correlators are to be time ordered in an unusual way. More precisely: upon expressing the current as the time derivative of the charge, the derivatives have to be taken after time ordering the charges. Instances where the difference with the conventional ordering matters are illustrated by means of a simple scattering model. We apply the results to resolve a discrepancy concerning the third cumulant of charge transport across a quantum point contact.

Universality for random Wigner matrices

LÁSZLÓ ERDŐS

(joint work with Benjamin Schlein and Horng-Tzer Yau)

Consider $N \times N$ random hermitian matrices $H = (h_{ij})$, $h_{ij} = \overline{h_{ji}}$. They form a *hermitian Wigner ensemble* if

$$(1) \quad h_{ij} = N^{-1/2}(x_{ij} + \sqrt{-1}y_{ij}), \quad (i < j), \quad \text{and} \quad h_{ii} = N^{-1/2}x_{ii},$$

where $x_{ij}, y_{ij} \in \mathbb{R}$ ($i < j$) and $x_{ii} \in \mathbb{R}$ are independent random variables with mean zero and we assume that x_{ij}, y_{ij} ($i < j$) all have a common distribution $d\nu$ with variance $1/2$. The diagonal elements, x_{ii} , also have a common distribution with mean zero and variance one. Let \mathbb{P} and \mathbb{E} denote the probability and the expectation value w.r.t the joint distribution. We assume that there are positive δ, γ such that

$$(2) \quad \mathbb{E} e^{\delta|x_{ij}|^\gamma} < \infty, \quad \mathbb{E} e^{\delta|x_{ii}|^\gamma} < \infty.$$

The *symmetric Wigner ensemble* is defined analogously. In this case, the matrix elements are real, i.e. we set $y_{ij} = 0$ and we assume that the variance of x_{ij} is

one. If the matrix elements are Gaussian random variables, then the corresponding ensembles are called *Gaussian Unitary Ensemble* (GUE) and *Gaussian Orthogonal Ensemble* (GOE).

Let $\lambda_1 \leq \lambda_2 \leq \dots \leq \lambda_N$ denote the eigenvalues of H . The normalization is chosen such that the bulk of the spectrum of H is $[-2, 2]$. In particular, the typical scaling between neighboring eigenvalues is of order $1/N$, $\lambda_j - \lambda_{j-1} \sim O(1/N)$. It is well known that the density of eigenvalues follows the Wigner semicircle law. More precisely, for any $I \subset \mathbb{R}$ let \mathcal{N}_I denote the number of eigenvalues in I . Wigner's theorem [19] states that for any fixed interval I

$$\frac{\mathcal{N}_I}{N} \rightarrow \int_I \varrho_{sc}(x) dx$$

almost surely as $N \rightarrow \infty$, where

$$\varrho_{sc}(x) := \frac{1}{2\pi} \sqrt{(4-x^2)_+}$$

is the density of the semicircle law. This result can be interpreted as a law of large numbers for the empirical eigenvalue density on macroscopic scales, i.e. for intervals that contain $O(N)$ eigenvalues.

The following result from our earlier paper shows that the semicircle law holds on intervals I of length $|I| = \eta \geq K/N$ for sufficiently large K .

Theorem 0.1. [7, Theorem 3.1] *Suppose that (2) with $\gamma = 2$ holds. Let $\kappa > 0$ and fix an energy $E \in [-2 + \kappa, 2 - \kappa]$. Consider the interval $I = [E - \frac{\eta}{2}, E + \frac{\eta}{2}]$ of length η about E . Then there exist positive constants C, c , depending only on κ , and a universal constant c_1 such that for any $\delta \leq c_1\kappa$ there is $K = K_\delta$ such that*

$$(3) \quad \mathbb{P}\left\{\left|\frac{\mathcal{N}_I}{N\eta} - \varrho_{sc}(E)\right| \geq \delta\right\} \leq Ce^{-c\delta^2\sqrt{N\eta}}$$

holds for all η satisfying $K/N \leq \eta \leq 1/K$.

In particular, this result shows that $\mathcal{N}_I/N\eta$ converges to $\varrho_{sc}(E)$ in probability as long as $\eta = \eta(N)$ is such that $\eta(N) \rightarrow 0$ and $N\eta(N) \rightarrow \infty$. The Gaussian decay condition on the matrix elements can be relaxed to (2) if $\eta \geq N^{-1+\varepsilon}$ with any $\varepsilon > 0$ at the expense of a weaker bound on the right hand side of (3), see Section 5 of [10]. The estimate also deteriorates if the energy is close to the edge, see Proposition 4.1 of [9] for a more precise statement. Based upon our proofs, similar estimates were given in [17, Theorem 56] for energies in the bulk and somewhat stronger bounds in [18, Theorem 1.7] for the edge.

In this talk we prove that not only the density, but more general local statistics of eigenvalues follow a universal pattern, namely the two-point correlation function is given by the Wigner-Dyson sine kernel, and higher order correlations are given by a determinant.

More precisely, let $f(\lambda_1, \lambda_2, \dots, \lambda_N)$ denote the symmetric joint density function of the eigenvalues of the $N \times N$ Wigner matrix H . For any $k \geq 1$ we define the

k -point correlation functions (marginals) by

$$p_N^{(k)}(\lambda_1, \dots, \lambda_k) = \int_{\mathbb{R}^{N-k}} f(\lambda_1, \lambda_2, \dots, \lambda_N) d\lambda_{k+1} \dots d\lambda_N.$$

We will use the notation $p_{N,GUE}^{(k)}$ and $p_{N,GOE}^{(k)}$ for the correlation functions of the GUE and GOE ensembles.

We consider the rescaled correlation functions about a fixed energy E under a scaling that guarantees that the local density is one. The sine-kernel universality for the GUE ensemble states that the rescaled correlation functions converge weakly to the determinant of the sine-kernel, $K(x) = \frac{\sin \pi x}{\pi x}$, i.e.

$$(4) \quad \frac{1}{[\varrho_{sc}(E)]^k} p_{N,GUE}^{(k)}\left(E + \frac{x_1}{N\varrho_{sc}(E)}, \dots, E + \frac{x_k}{N\varrho_{sc}(E)}\right) \rightarrow \det\left(K(x_\ell - x_j)\right)_{\ell,j=1}^k$$

as $N \rightarrow \infty$ for any fixed energy $|E| < 2$ in the bulk of the spectrum [14, 4]. Similar result holds for the GOE case; the sine kernel being replaced with a similar but somewhat more complicated universal function, see [13]. Our main result is that universality (4) holds for general hermitian or symmetric Wigner matrices after averaging in the energy E :

Theorem 0.2. [8] *Let H be an $N \times N$ symmetric or hermitian Wigner matrix with the given normalization. Suppose that the distribution ν of the matrix elements has subexponential decay (2). Let $k \geq 1$ and $O : \mathbb{R}^k \rightarrow \mathbb{R}$ be a continuous, compactly supported function. Then for any $|E| < 2$, we have*

$$(5) \quad \lim_{\delta \rightarrow 0} \lim_{N \rightarrow \infty} \frac{1}{2\delta} \int_{E-\delta}^{E+\delta} dv \int_{\mathbb{R}^k} d\alpha_1 \dots d\alpha_k O(\alpha_1, \dots, \alpha_k) \\ \times \frac{1}{[\varrho_{sc}(v)]^k} \left(p_N^{(k)} - p_{N,\#}^{(k)}\right)\left(v + \frac{\alpha_1}{N\varrho_{sc}(v)}, \dots, v + \frac{\alpha_k}{N\varrho_{sc}(v)}\right) = 0,$$

where $\#$ stands for GOE or GUE for the symmetric or hermitian cases, respectively.

For the *hermitian case*, the first result on universality beyond the GUE was due to Johansson [12] (based upon [2]) under the condition that ν has a Gaussian component with a positive variance independent of N . His method was extended in [1] to Wishart matrices. The variance of the necessary Gaussian component was reduced to $N^{-3/4+\varepsilon}$ in [9] under the additional technical assumptions that the measure ν is smooth and it satisfies the logarithmic Sobolev inequality. The local statistics was identified via orthogonal polynomials. The Gaussian component assumption was first removed completely in [10] under the condition that the density of the probability measure ν is positive and it possesses a certain number of derivatives. Shortly after [10] appeared on the arXiv, the same result using a different method has been posted [17] without any regularity condition on ν provided that the third moment vanishes and ν is supported on at least three points. Combining the two methods, all conditions on ν apart from the subexponential decay (2) were removed in a short joint paper [11].

The methods of [10] and [17] both rely on the explicit formula of Brézin and Hikami [2], exploited also in [12], for the correlation functions of the Wigner matrix with Gaussian convolution. This formula reduces the problem to a saddle point analysis. The saddle points are identified by solving an equation involving the Stieltjes transform $m_N(z) = \frac{1}{N} \sum_{\alpha=1}^N (\lambda_\alpha - z)^{-1}$ of the eigenvalues with $\eta = \text{Im } z$ corresponding to the variance of the Gaussian component: precise information on $m_N(z)$ for a smaller η implies that a smaller Gaussian component is sufficient.

In our work [10] we used the convergence of $m_N(z)$ to $m_{sc}(z)$ for very small $\eta = N^{-1+\varepsilon}$ established along the proof of Theorem 0.1. To remove this tiny Gaussian component, we have compared the local eigenvalue statistics of a given Wigner matrix H with that of $\widehat{H}_s + sV$ for which the saddle point analysis applies. Here $s^2 = \eta = N^{-1+\varepsilon}$ and the new Wigner matrix \widehat{H}_s was chosen such that the law of $\widehat{H}_s + sV$ be very close to H . Since Gaussian convolution corresponds to running a heat flow on the matrix elements, \widehat{H}_s could, in principle, be obtained by running the *reverse heat flow* on the elements of H . Although the reverse heat flow is undefined for most initial conditions, one can construct an approximation to the reverse heat flow that is well defined and yields \widehat{H}_s with a required precision assuming sufficient smoothness on ν . Technically, we use Ornstein-Uhlenbeck process instead of the heat flow to keep the variance constant. We also mention that the result of [10] is valid for any fixed energy E , i.e. $d\nu$ averaging in (5) is not necessary.

Tao and Vu [17] have directly compared local statistics of the Wigner matrix H and that of the matrix with order one Gaussian component for which Johansson has already proved universality. Their main technical result [17, Theorem 15] states that the local eigenvalue statistics of two Wigner matrices coincide as long as the first four moments of their single site distributions match. It is then an elementary lemma from probability theory ([17, Corollary 23] based upon [3]) to match to order four a given random variable with another random variable with a Gaussian component.

The proof of Theorem 0.2 for the *symmetric* case requires a new idea since the formula of Brézin and Hikami is not available. While the four moment theorem of [17] also applies to this case, there is no reference ensemble available. In the next sections we describe our new approach that proves universality for both hermitian and symmetric matrices without relying on any explicit formulae.

Our main idea is to use the Dyson Brownian motion which is a stochastic flow for the eigenvalues as the matrix elements evolve according to an Ornstein-Uhlenbeck process. The equilibrium measure of this stochastic dynamics is the GUE or GOE ensembles. We can localize this dynamics to construct a *local relaxation flow* that has approaches to local equilibrium faster. In this way we can show that matrices of the form $\widehat{H} + sV$ with $s = O(N^{-\delta})$ has the universal local statistics *without using the explicit formula of [2]*.

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**Resonances and lifetime of metastable states in Non-relativistic
Quantum Electrodynamics**

J ER EMY FAUPIN

(joint work with W.K. Abou Salem, J. Fr ohlich, I.M.Sigal)

We consider a finite number of non-relativistic particles interacting with the quantized electromagnetic field in the standard mathematical model of non-relativistic

QED. After recalling some results on the existence of resonances in this context, we relate the lifetime of metastable states to the imaginary part of the resonances.

Charge Renormalization in a Nonlinear Model of Quantum Electrodynamics

MATHIEU LEWIN

(joint work with Philippe Gravejat and Éric Séré)

Renormalization is an essential tool in Quantum Electrodynamics (QED). In my talk I have presented a nonlinear model derived from QED in which the charge of the electron has to be renormalized, but not its mass. The model, based on the Dirac operator, takes into account vacuum polarization effects. It is a rather simple effective theory which however reproduces several general features of the true QED.

In [7, 6, 5] we studied the following time-independent self-consistent equation:

$$(1) \quad \begin{cases} P = \chi_{(-\infty, \mu)}(D) \\ D = D^0 + \alpha(\rho_{P-1/2} - \nu) * |x|^{-1}. \end{cases}$$

Here $D^0 = \boldsymbol{\alpha} \cdot (-i\nabla) + \beta$ is the free Dirac operator (with mass $m = 1$ for simplicity) acting on $L^2(\mathbb{R}^2, \mathbb{C}^4)$ and ν is an external density of charge modeling for instance a (smeared) nucleus. The operator P should be interpreted as the one-body density matrix of a Hartree-Fock state containing infinitely many particles (both the real electrons and the virtual electrons of the Dirac sea). The associated density of charge $\rho_{P-1/2}$ is *formally* defined by

$$\rho_{P-1/2}(x) = \text{tr}_{\mathbb{C}^4}(P - 1/2)(x, x) = \frac{1}{2} \sum_{i \geq 1} |\varphi_i^-(x)|^2 - |\varphi_i^+(x)|^2$$

where $\{\varphi_i^-\}_{i \geq 1}$ is an orthonormal basis of $PL^2(\mathbb{R}^3, \mathbb{C}^4)$ and $\{\varphi_i^+\}_{i \geq 1}$ is an orthonormal basis of $(1 - P)L^2(\mathbb{R}^3, \mathbb{C}^4)$. Note the subtraction of half the identity, which is a kind of renormalization, necessary to impose charge conjugation invariance [8]. In (1), the real number μ is a chemical potential used to fix the correct total charge of the system.

Equation (1) is well-known in Physics. For instance it appears (possibly with an additional exchange-correlation term) in Relativistic Density Functional Theory [4, 3]. But Dirac already considered in [1] the first order term obtained from (1) by expanding in powers of α . Equation (1) (or more precisely its regularized version (2)) may also be deduced by a thermodynamic limit procedure from QED [8] by restricting to no-photon Hartree-Fock states and neglecting the so-called exchange term.

When $\nu \equiv 0$, Equation (1) has a trivial solution: $P = P_-^0 := \chi_{(-\infty, 0)}(D^0)$, the free Dirac sea. This comes from the fact that $\rho_{P_-^0-1/2} \equiv 0$, as is seen by writing

in the Fourier representation

$$(P_-^0 - 1/2)(p) = -\frac{\alpha \cdot p + \beta}{2\sqrt{1 + |p|^2}}$$

and using that the Dirac matrices are trace-less.

When $\nu \neq 0$, Equation (1) has *no solution* [7] and adding an ultraviolet cut-off is mandatory. The simplest method (although probably not optimal regarding regularity issues [6]) is to impose a cut-off at the level of the Hilbert space, that is to work in

$$\mathfrak{H}_\Lambda := \{f \in L^2(\mathbb{R}^3; \mathbb{C}^4), \text{supp}(\widehat{f}) \subset B(0; \Lambda)\}$$

and to solve, instead of (1), the regularized equation in \mathfrak{H}_Λ :

$$(2) \quad \begin{cases} P = \chi_{(-\infty, \mu)}(D) + \delta \\ D = \Pi_\Lambda \left(D^0 + \alpha(\rho_{P-P_-^0} - \nu) * |x|^{-1} \right) \Pi_\Lambda \end{cases}$$

where Π_Λ is the orthogonal projector onto \mathfrak{H}_Λ in $L^2(\mathbb{R}^3; \mathbb{C}^4)$. Note we have replaced $\rho_{P-1/2}$ by $\rho_{P-P_-^0}$ since $\rho_{P_-^0-1/2} \equiv 0$. Recall however that solutions of (2) do *not* depend on the reference P^0 and the subtraction P_-^0 is only a convenient algebraic manipulation (in practice P will not be “too far” from P^0 hence it makes sense to use $P - P_-^0$ as main variable). Also we have added in (2) the possibility of having a density matrix in the Fermi level $0 \leq \delta \leq \chi_{\{\mu\}}(D)$ as is usually done in reduced Hartree-Fock theory. In principle P is not a projector anymore but we still use the letter P for convenience.

Because of the Shale-Stinespring theorem, it is natural to look for a solution of (2) such that $P - P^0$ is a Hilbert-Schmidt operator on \mathfrak{H}_Λ ($\in \mathfrak{S}_2(\mathfrak{H}_\Lambda)$). If P is a projector, it will then yield a Fock representation equivalent to that of P_-^0 . Even when P is not a projector, it will be associated with a unique Bogoliubov state in the Fock space representation of P_-^0 . This is a mathematical formulation of the statement that P should not be too far from P_-^0 . When $P - P_-^0 \in \mathfrak{S}_2(\mathfrak{H}_\Lambda)$, the associated density $\rho_{P-P_-^0}$ is a well-defined function thanks to the ultraviolet cut-off. One can even check that $\rho_{P-P_-^0} \in L^2(\mathbb{R}^3)$.

For convenience we introduce the Hilbert space

$$\mathcal{C} := \left\{ f : \int_{\mathbb{R}^3} |k|^{-2} |\widehat{f}(k)|^2 dk < \infty \right\}$$

and assume that $\nu \in \mathcal{C} \cap L^2(\mathbb{R}^3)$. It was then proved in [7] (for $\mu = 0$) and in [6] (for $\mu \in (-1, 1)$) that (2) has at least a solution such that $P - P_-^0 \in \mathfrak{S}_2(\mathfrak{H}_\Lambda)$. Such solutions are in general not unique but the corresponding density $\rho_{P-P_-^0}$ is always *unique*, hence so is D (only δ is *a priori* not unique). Existence was obtained in [7, 6] by identifying solutions of (2) with minimizers of a convex Hartree-Fock-type functional. This gave as a byproduct the following information on solutions:

$$(3) \quad P - P_-^0 \in \mathfrak{S}_2(\mathfrak{H}_\Lambda), \quad P_\pm^0(P - P_-^0)P_\pm^0 \in \mathfrak{S}_1(\mathfrak{H}_\Lambda), \quad \rho_{P-P_-^0} \in \mathcal{C} \cap L^2(\mathbb{R}^3)$$

where $\mathfrak{S}_1(\mathfrak{H}_\Lambda)$ is the space of trace-class operators on \mathfrak{H}_Λ and $P_\pm^0 = 1 - P_-^0$.

In [6] it was shown that if additionally $\nu \in L^1(\mathbb{R}^3)$, then $\rho_{P-P_-^0} \in L^1(\mathbb{R}^3)$ and that the following relation holds:

$$(4) \quad \int_{\mathbb{R}^3} \nu - \int_{\mathbb{R}^3} \rho_{P-P_-^0} = \frac{\int_{\mathbb{R}^3} \nu - \text{tr}_{P_-^0}(P - P_-^0)}{1 + \alpha B_\Lambda}$$

where by definition $\text{tr}_{P_-^0}(A) = \text{tr}(P_-^0 A P_-^0) + \text{tr}(P_+^0 A P_+^0)$ which is well-defined for $P - P_-^0$ by (3). In (4), B_Λ is a universal function of Λ which diverges logarithmically

$$B_\Lambda = \frac{2}{3\pi} \log \Lambda - \frac{5}{9\pi} + \frac{2 \log 2}{3\pi} + O(1/\Lambda^2).$$

Let us emphasize that (4) in particular implies that solutions of (2) are in general *not trace-class*, although the corresponding density is always in $L^1(\mathbb{R}^3)$. This mathematical odd property is at the origin of charge renormalization. Let us also remark that (4) is fully non perturbative.

Equation (4) leads to the following charge (or rather coupling constant) renormalization formula:

$$(5) \quad \alpha_{\text{ph}} = \frac{\alpha}{1 + \alpha B_\Lambda} \iff \alpha = \frac{\alpha_{\text{ph}}}{1 - \alpha_{\text{ph}} B_\Lambda}.$$

In practice $\alpha_{\text{ph}} \simeq 1/137$ is the real physical constant since we will always observe the nucleus together with the vacuum polarization density. Therefore in our theory we must fix α_{ph} and see α as a function of α_{ph} and Λ . Renormalization could mean that if we express any physical observable in terms of α_{ph} , Λ and μ , then it must stay finite in the limit $\Lambda \rightarrow \infty$. Unfortunately it holds $\alpha_{\text{ph}} B_\Lambda < 1$ hence it makes no sense to take $\Lambda \rightarrow \infty$ while keeping α_{ph} fixed (this is the so-called Landau pole [9]) and one has to look for a weaker definition of renormalization.

In [7], Formula (5) was already proposed and used to reinterpret the self-consistent equation. The idea is to define a physical density containing both the true density ν and the vacuum polarization by

$$\alpha_{\text{ph}} \rho_{\text{ph}} = \alpha (\nu - \rho_{P-P_-^0})$$

in such a way that $D = D^0 - \alpha_{\text{ph}} \rho_{\text{ph}} * |x|^{-1}$. This procedure is similar to wave-function renormalization. By uniqueness we can see ρ_{ph} as a function of α_{ph} and Λ (it is in general also a function of μ which we take equal to 0 for simplicity). The self-consistent equation for ρ_{ph} was derived in [7].

In [5] we show that one can expand $\rho_{\text{ph}} = \rho_{\text{ph}}(\alpha_{\text{ph}}, \Lambda)$ as follows:

$$(6) \quad \rho_{\text{ph}}(\alpha_{\text{ph}}, \Lambda) = \sum_{n=0}^{\infty} \nu_{n,\Lambda}(\alpha_{\text{ph}})^n$$

where $\{\nu_{n,\Lambda}\}_k$ is a sequence depending only on the external density ν and the cut-off Λ . Assuming $\widehat{\nu}$ decays fast enough, one can prove that for any fixed n , $\nu_{n,\Lambda} \rightarrow \nu_n$ in $L^2(\mathbb{R}^3) \cap \mathcal{C}$. This is what is usually meant by renormalization in QED: each term of the perturbation series in powers of the physical α_{ph} has a limit

when the cut-off is removed. The sequence $\{\nu_n\}_n$ is the one which is calculated in practice. One has for instance $\nu_0 = \nu$ and

$$\nu_1 * |x|^{-1} = \frac{1}{3\pi} \int_1^\infty dt (t^2 - 1)^{1/2} \left[\frac{2}{t^2} + \frac{1}{t^4} \right] \int_{\mathbb{R}^3} e^{-2|x-y|t} \frac{\nu(y)}{|x-y|} dy,$$

which is usually called the Uehling potential [10]. All the others ν_n can be calculated by induction in terms of ν_0, \dots, ν_{n-1} .

The next natural question is to understand the link between the well-defined, cut-off dependent, series (6) and the *formal series* $\sum_{n=0}^\infty \nu_n (\alpha_{\text{ph}})^n$, which is expected to be divergent [2]. Recall that $\alpha_{\text{ph}} B_\Lambda < 1$ by construction so one is in principle not allowed to take the limit $\Lambda \rightarrow \infty$ while keeping α_{ph} fixed.

In [5] we give to renormalization an *asymptotic meaning* as follows:

Theorem 0.3 (Asymptotic renormalization [5]). *Let $\mu = 0$ and $\nu \in L^2(\mathbb{R}^3) \cap \mathcal{C}$ such that, for some $m \geq 1$,*

$$\int_{\mathbb{R}^3} \log(1 + |k|)^{2m+4} |\widehat{\nu}(k)|^2 dk < \infty.$$

Let $\epsilon > 0$. There exist two constants $C(\nu, m, \epsilon)$ and $a(\nu, m, \epsilon)$ depending on m, ν and ϵ such that one has

$$(7) \quad \left\| \rho_{\text{ph}}(\alpha_{\text{ph}}, \Lambda) - \sum_{n=0}^m (\alpha_{\text{ph}})^n \nu_n \right\|_{L^2(\mathbb{R}^3) \cap \mathcal{C}} \leq C(\nu, m, \epsilon) (\alpha_{\text{ph}})^{m+1}$$

for all $0 \leq \alpha_{\text{ph}} \leq a(\nu, m, \epsilon)$ with $\epsilon \leq \alpha_{\text{ph}} B_\Lambda \leq 1 - \epsilon$.

The interpretation of the theorem is that for α_{ph} small enough, then $\rho_{\text{ph}}(\alpha_{\text{ph}}, \Lambda)$ is, to any order in α_{ph} , essentially independent of the value of Λ in a very large range of values, essentially $C_1 e^{3\epsilon\pi/2\alpha_{\text{ph}}} \leq \Lambda \leq C_2 e^{3(1-\epsilon)\pi/2\alpha_{\text{ph}}}$.

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Existence of Ground States of Hydrogen-like Atoms in Semi-relativistic QED

OLIVER MATTE

(joint work with Edgardo Stockmeyer, Martin Könenberg)

We consider two different models of a hydrogenic atom interacting with the quantized electromagnetic field that treat the electron relativistically. The first one is given by a no-pair operator, the second one by the semi-relativistic Pauli-Fierz operator. We prove that both operators are semi-bounded below, that their low-lying spectral subspaces are exponentially localized (w.r.t. the electron coordinates), and that they possess an eigenvalue at the lower end of their spectra. These results hold true, for arbitrary values of the fine structure constant and the ultraviolet cut-off, and for Coulomb coupling constants less than the critical constants without quantized radiation field.

A 2D analogue of the Luttinger model

EDWIN LANGMANN

(joint work with Jonas de Woul)

We report on a project with the aim to develop reliable computation methods for two dimensional (2D) lattice fermion systems of Hubbard type. These systems are well-understood only at *half filling*, i.e. when the fermion density is half the maximal one. In this case the ground state is typically insulating, i.e. the fermions have a gap. The challenge is to understand such systems away from half filling. One indication for the difficulty of this is mean field theory: this standard method allows a simple description of the half filled insulating state, but it typically fails away from half filling.

To motivate our approach we recall a well-known strategy which has been used successfully in 1D: starting from a model for spin-less fermions on a 1D lattice one can perform a particular continuum limit and derive a quantum field theory model. Away from half-filling one thus obtains the so-called Luttinger model that can be solved exactly by a technique known as *bosonization* [1]. Thus an exactly solvable quantum field theory model provides a low-energy effective description of 1D lattice fermions.

We present a natural generalization of this to 2D [2-4]. We propose a method to overcome the above mentioned difficulty of mean field theory away from half filling as follows. There exists a natural 2D analogue of the Luttinger model obtained as a continuum limit of a model for spin-less fermions on a square lattice. This

2D Luttinger model can be partly solved exactly by bosonization: it contains two kinds of fermion degrees of freedom which we call *nodal* and *anti-nodal*, and the nodal fermions can be treated exactly by bosonization. This yields a model of the anti-nodal fermions coupled to bosons. The latter can be treated by mean field theory. We find that there is a regime away from half filling where only the anti-nodal fermions have a gap and the nodal fermions have a Fermi surface.

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The critical temperature of dilute Bose gases

ROBERT SEIRINGER

(joint work with Daniel Ueltschi)

The effect of interparticle interactions on the critical temperature for Bose-Einstein condensation has been a controversial issue in the literature. Various approximation schemes lead to different conclusions, concerning both the sign and the magnitude of the shift in the critical temperature. We shall examine this question from the point of view of rigorous bounds. While lower bounds seem to be out of reach of present methods, we show that a rigorous upper bound can be established rather easily. Our bound shows that in the presence of repulsive interactions the critical temperature can not increase by more than the square root of $a\rho^{1/3}$, with ρ the density and a the scattering length of the interaction potential.

Our method also yields valuable information in the case of a two-dimensional Bose gas. While there is no Bose-Einstein condensation in this case, a Kosterlitz-Thouless type phase transition is expected at a definite critical temperature. We prove that off-diagonal correlations decay exponentially above this temperature.

Explicit quantum states of atomic ions as $Z \rightarrow \infty$ and basic aspects of the periodic table

GERO FRIESECKE

(joint work with Benjamin Goddard)

In my talk I present joint work with Ben Goddard (Warwick) which seeks to understand how basic *chemically specific* properties of atoms emerge mathematically from the *universal* equations of quantum mechanics.

Some history. The original grouping of atoms into a “periodic table” was done

on purely empirical grounds, due to striking chemical differences between some elements and great similarities between others (Meyer and Mendelejew, 1869). The first to develop a partial theoretical picture was Bohr (1913–1922). He argued that chemical differences come from different *electronic structure*. The electrons were pictured on Bohr orbits with three quantum numbers n , ℓ , m . In 1924 Pauli introduced a fourth quantum number (spin), and postulated, on empirical grounds, a sub-shell ordering rule: each Bohr orbit can accommodate two electrons of opposite spin, and the sub-shells (= collections of Bohr orbits with same n and ℓ) are occupied in the order 1s 2s 2p 3s 3p 4s 3d ... Here the numbers are the values of n and the letters s, p, d stand for $\ell = 0, 1, 2$. Hund (1925) added empirical selection rules governing the filling order within sub-shells. The next advance was made by Slater and Hartree in the years 1928–1930. After the Schrödinger equation had been introduced (and solved for the H atom) in 1926, they argued that the Bohr orbits in the above picture should be replaced by hydrogen orbitals, respectively “self-consistent” orbitals. Explanations of the filling order via numerical solutions to Hartree or Hartree-Fock equations began with work of Hartree on rubidium in 1928; for treatments of large classes of atoms see e.g. the books by Hartree (1957) and Froese-Fischer (1977).

Mathematical perspective. Starting from a universal quantum mechanical model (such as the many-electron Schrödinger equation), we would like to answer the following questions. 1. Are there well defined and natural equivalence classes corresponding to the chemical notion of “two atoms belonging to the same group”. 2. Can one derive which atom is in which group. 3. Can one extract a rigorous picture of the electronic structure of atoms which shares the simplicity of the famous hydrogen orbital configurations.

Preliminary considerations on Question 1. We argue that a natural mathematical answer to Question 1 is as follows: *Two atoms are in the same equivalence class if their many-electron Schrödinger ground states have the same quantum numbers L , S and p* (corresponding to total angular momentum, total spin and total parity). Unlike the quantum numbers for individual orbitals which appear in the Bohr-Pauli-Hund-Slater picture, L , S and p are good quantum numbers, resulting from the invariance of the atomic Schrödinger equation (2)–(3) under the symmetry group

$$(1) \quad SO(3) \times SU(2) \times \mathbb{Z}_2$$

(corresponding to simultaneous rotation of electron positions and spins, and simultaneous inversion of electron positions). Experimentally, only five different (L, S) pairs occur for the first 20 atoms (see the Table below). This yields a classification in to 5 classes. Each class is either a ‘group’, or a union of 2 ‘groups’. Thus predicting an atom’s group is achieved, up to at most two possibilities, by predicting L and S of the Schrödinger ground state.

H							He
Li	Be	B	C	N	O	F	Ne
Na	Mg	Al	Si	P	S	Cl	Ar
L=0 S=½	L=0 S=0	L=1 S=½	L=1 S=1	L=0 S=3/2			

Results. We have shown that questions 2 and 3 can be answered for highly charged atomic ions. The details are as follows. We start from the (nonrelativistic, Born-Oppenheimer) time-independent Schrödinger equation for atoms and ions,

$$(2) \quad H\Psi = E\Psi,$$

where, for nuclear charge $Z > 0$ and N electrons and in atomic units, the Hamiltonian is

$$(3) \quad H = \sum_{i=1}^N \left(-\frac{1}{2}\Delta_{x_i} - \frac{Z}{|x_i|} \right) + \sum_{1 \leq i < j \leq N} \frac{1}{|x_i - x_j|},$$

$E \in \mathbb{R}$, and Ψ belongs to the usual Hilbert space $L^2_a((\mathbb{R}^3 \times \mathbb{Z}_2)^N)$ of square-integrable, antisymmetric functions $\Psi : (\mathbb{R}^3 \times \mathbb{Z}_2)^N \rightarrow \mathbb{C}$. By Zhislin’s theorem, for $N < Z - 1$ (neutral atoms and positive ions), there exist countably many discrete eigenvalues below the bottom of the essential spectrum. Consideration of the symmetry group and the associated conserved quantities shows that on each irreducible eigenspace, the operators \mathbf{L}^2 and \mathbf{S}^2 have only one eigenvalue, of form $L(L + 1)$ respectively $S(S + 1)$, with integer L and half-integer S .

Our results are associated with the limit of fixed electron number N and nuclear charge $Z \rightarrow \infty$. Physically, this limit corresponds to considering iso-electronic sequences like Li, Be⁺, B⁺⁺, C⁺⁺⁺, ...

Theorem 1 [FG09] (Spin and angular momentum quantum numbers) *For $N = 1, \dots, 10$, and sufficiently large Z , the angular momentum and spin quantum numbers, and the dimension, of the Schrödinger ground state are:*

Iso-electronic sequence	H	He	Li	Be	B	C	N	O	F	Ne
‡ electrons	1	2	3	4	5	6	7	8	9	10
L	0	0	0	0	1	1	0	1	1	0
S	½	0	½	0	½	1	¾	1	½	0
Chemist’s notation	² S	¹ S	² S	¹ S	² P	³ P	⁴ S	³ P	² P	¹ S
dimension	2	1	2	1	6	9	4	9	6	1

All numbers agree with experiment for all $Z \geq N$, including neutral atoms ($Z = N$). Open problem: Prove that the theoretical numbers do not change as Z is decreased down to $Z = N$.

Theorem 2 [FG09] (Ground states) *For $N = 1, \dots, 10$, and in the limit $Z \rightarrow \infty$,*

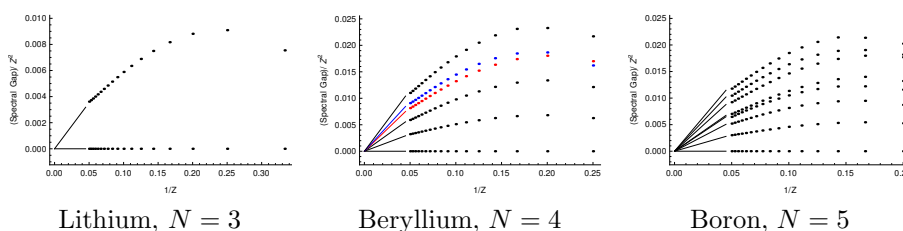
the Schrödinger ground state is asymptotic to the explicit vector space given in the table below, in the sense that the projection operators P_0, \tilde{P}_0 onto these spaces satisfy $\lim_{Z \rightarrow \infty} \|P_0 - \tilde{P}_0\| = 0$, the norm being the operator norm on L^2 .

Iso-el. Seq.	Sym.	Exact ground state in large Z limit	Dim.
H	2S	$ 1s\rangle, \bar{1}s\rangle$	2
He	1S	$ 1s^2\rangle$	1
Li	2S	$ 1s^2 2s\rangle, 1s^2 \bar{2}s\rangle$	2
Be	1S	$\frac{1}{\sqrt{1+c^2}} \left(1s^2 2s^2\rangle + c \frac{1}{\sqrt{3}} (1s^2 2p_1^2\rangle + 1s^2 2p_2^2\rangle + 1s^2 2p_3^2\rangle) \right)$ $c = -\frac{\sqrt{3}}{59049} (2\sqrt{1509308377} - 69821) = -0.2310995 \dots$	1
B	$^2P^o$	$\frac{1}{\sqrt{1+c^2}} \left(1s^2 2s^2 2p_i\rangle + c \frac{1}{\sqrt{2}} (1s^2 2p_i 2p_j^2\rangle + 1s^2 2p_i 2p_k^2\rangle) \right)$ $\frac{1}{\sqrt{1+c^2}} \left(1s^2 2s^2 \bar{2}p_i\rangle + c \frac{1}{\sqrt{2}} (1s^2 \bar{2}p_i 2p_j^2\rangle + 1s^2 \bar{2}p_i 2p_k^2\rangle) \right)$ $(i, j, k) = (3, 1, 2), (1, 2, 3), (2, 3, 1)$ $c = -\frac{\sqrt{2}}{393660} (\sqrt{733174301809} - 809747) = -0.1670823 \dots$	6
C	3P	$\frac{1}{\sqrt{1+c^2}} (1s^2 2s^2 2p_i 2p_j\rangle + c 1s^2 2p_k^2 2p_i 2p_j\rangle)$ $\frac{1}{\sqrt{1+c^2}} \left(\frac{1}{\sqrt{2}} (1s^2 2s^2 2p_i \bar{2}p_j\rangle + 1s^2 2s^2 \bar{2}p_i 2p_j\rangle) + c \frac{1}{\sqrt{2}} (1s^2 2p_k^2 2p_i 2p_j\rangle + 1s^2 2p_k^2 \bar{2}p_i 2p_j\rangle) \right)$ $\frac{1}{\sqrt{1+c^2}} (1s^2 2s^2 \bar{2}p_i 2p_j\rangle + c 1s^2 2p_k^2 \bar{2}p_i 2p_j\rangle)$ $(i, j, k) = (3, 1, 2), (1, 2, 3), (2, 3, 1)$ $c = -\frac{1}{98415} (\sqrt{221876564389} - 460642) = -0.1056317 \dots$	9
N	$^4S^o$	$ 1s^2 2s^2 2p_1 2p_2 2p_3\rangle$ $\frac{1}{\sqrt{3}} (1s^2 2s^2 \bar{2}p_3 2p_1 2p_2\rangle + 1s^2 2s^2 2p_3 \bar{2}p_1 2p_2\rangle + 1s^2 2s^2 2p_3 2p_1 \bar{2}p_2\rangle)$ $\frac{1}{\sqrt{3}} (1s^2 2s^2 \bar{2}p_3 2p_1 \bar{2}p_2\rangle + 1s^2 2s^2 \bar{2}p_3 \bar{2}p_1 2p_2\rangle + 1s^2 2s^2 3 \bar{2}p_1 2p_2\rangle)$ $ 1s^2 2s^2 \bar{2}p_1 2p_2 2p_3\rangle$	4
O	3P	$ 1s^2 2s^2 2p_i^2 2p_j 2p_k\rangle$ $\frac{1}{\sqrt{2}} (1s^2 2s^2 2p_i^2 2p_j 2p_k\rangle + 1s^2 2s^2 2p_i^2 \bar{2}p_j 2p_k\rangle)$ $ 1s^2 2s^2 2p_i^2 2p_j 2p_k\rangle$ $(i, j, k) = (3, 1, 2), (1, 2, 3), (2, 3, 1)$	9
F	$^2P^o$	$ 1s^2 2s^2 2p_i^2 2p_j^2 2p_k\rangle$ $ 1s^2 2s^2 2p_i^2 2p_j^2 \bar{2}p_k\rangle$ $(i, j, k) = (3, 1, 2), (1, 2, 3), (2, 3, 1)$	6
Ne	1S	$ 1s^2 2s^2 2p_1^2 2p_2^2 2p_3^2\rangle$	1

Note the close similarity to the semi-empirical hydrogen orbital configurations. In the table, $1s, 2s, 2p_i$ ($i=1,2,3$) are dilated hydrogen orbitals, $1s(x) = Z^{3/2} e^{-Z|x|} / \sqrt{\pi}$, $2s(x) = Z^{3/2} (1 - Z|x|/2) e^{-Z|x|/2} / \sqrt{8\pi}$, $2p_i(x) = Z^{5/2} (x \cdot e_i) e^{-Z|x|/2} / \sqrt{32\pi}$, e_1, e_2, e_3 are orthonormal basis vectors of \mathbb{R}^3 , the overbar or its absence gives the spin state (down respectively up), a square (as in $1s^2$) indicates that both spin states are occupied, and $|\varphi_1 \dots \varphi_N\rangle$ stands for the Slater determinant of the orbitals

$\varphi_1, \dots, \varphi_N$.

We have also determined the low-lying excited states, for the above N and in the limit $Z \rightarrow \infty$, as well as two-term expansions of the Schrödinger energy levels, $\frac{E_j(N, Z)}{Z^2} = a^{(0)}(N) + \frac{1}{Z}a_j^{(1)}(N) + O(\frac{1}{Z^2})$. The first two terms are the exact eigenvalues of the reduced Hamiltonian PHP in eq. (4) (lines in the plots below), and compare very well to the experimental energy levels of highly charged ions (dots, taken from the NIST atomic spectra database).



Proofsketch, Step 1 (Derivation of a reduced Hamiltonian) Use of rescaled position coordinates $\tilde{x} = Z^{-1}x$ removes the factor Z from (3) and creates a small factor, $1/Z$, in front of electron interaction. Applying degenerate first order perturbation theory and scaling back to the original variables yields that for large Z , the lowest eigenvalues and eigenstates of (2), (3) are governed by the finite-dimensional reduced problem

$$(4) \quad (a') \quad PHP\Psi = E\Psi, \quad (b') \quad \Psi \in V_0.$$

Here P is the projector onto the non-interacting ground state V_0 (lowest eigenspace of (3) with electron interaction deleted). Rule (b') is the same as the postulate that the electrons occupy hydrogen orbitals, while (a') replaces the postulates of Pauli and Hund (sub-shell ordering; Hund's rules), instead selecting the correct hydrogen orbital configurations from theory.

Proofsketch, Step 2 (Determining the eigenvalues and eigenstates of the reduced Hamiltonian) Evaluating the matrix elements of PHP is achieved by successively reducing the domain of integration from \mathbb{R}^{3N} to \mathbb{R}^6 to \mathbb{R}^3 to \mathbb{R} via Slater's rules, Fourier analysis, and spherical polar coordinates, and evaluating the remaining one-dimensional integrals by residue calculus.

Diagonalization of PHP is possible by careful use of the symmetry group (1) and its representation theory, despite the fact that the matrix is quite high dimensional ($d \times d$, where $d = \binom{8}{N-2}$ corresponds to the number of possible assignments of the $N-2$ valence electrons to the 8 valence orbitals; thus, 70×70 for the Carbon sequence).

Summary. Our results provide a theoretical alternative to the usual discussions of the periodic table in the literature, in which non-trivial empirical postulates such as sub-shell ordering or Hund's rules are replaced by careful analysis of a reduced Hamiltonian emerging from the Schrödinger equation. The price to pay is that this works only for highly charged ions, not neutral atoms.

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Level and level spacings statistics for random Schrödinger operators

FRANÇOIS GERMINET

(joint work with J.M. Combes, A. Klein, F. Klopp)

We show absence of energy levels repulsion for the eigenvalues of random Schrödinger operators in the continuum. We derive a Minami estimate for continuum Anderson Hamiltonians,

$$H_\omega = -\Delta + V_{per} + V_\omega.$$

The Minami's estimate follows from new local Wegner estimates. It is valid for bounded distribution densities and a single covering condition. We also give a simple and transparent proof of Minami's estimate for the (discrete) Anderson model. We prove then that, in the localization region at the bottom of the spectrum, the properly rescaled eigenvalues of a continuum Anderson Hamiltonian are distributed as a Poisson point process with intensity Lebesgue. We also obtain simplicity of the eigenvalues. As a byproduct of our analysis, we show that a Lifshitz tail bound on the Integrated Density of States implies the same decay for its derivative, the Density of States. Joint work with JM Combes and A. Klein.

We next study the level spacings statistics and the statistics of the centers of localization. To do so, we prove that, with probability one in the large volume limit, the eigenvalues of the random Hamiltonian restricted to the cube inside the interval are given by independent identically distributed random variables, up to an error of size an arbitrary power of the volume of the cube. This enables us to prove the convergence in probability of the spacing distribution to the exponential e^{-s} for levels and e^{-s^d} for centers of localization, as expected. Joint work with F. Klopp.

Are there mysteries in quantum mechanics?

JÜRIG FRÖHLICH

The short answer to this question is: no! The somewhat more elaborate answer I sketched in my lecture can be summarized as follows:

- (1) One tries to convince oneself that the puzzling features of quantum mechanics originate in the combination of a quantum-theoretical description of matter with its atomistic constitution. (The atomistic constitution of matter can be interpreted as arising from a process of quantization.)

- (2) As a consequence of atomism and of the nature of quantum-mechanical correlations one shows that quantum mechanics is fundamentally *indeterministic*. It can only predict the frequencies (or probabilities) of possible future events.
- (3) One then develops a *calculus of frequencies* of causal sequences of possible events (histories), following *Wigner*. One introduces a notion of "evidence for an event to have happened". This evidence approaches 1 (i.e., certainty) if and only if the history in question is "*consistent*", in the sense of *Griffiths*.
- (4) One convinces oneself that "(almost) consistent histories" emerge thanks to the phenomenon of *decoherence*, (which was first discussed by Hepp), etc.

"All" mysteries disappear!

Bulk universality for Wigner matrices

BENJAMIN SCHLEIN

We consider ensembles of $N \times N$ random matrices whose entries are, up to some symmetry constraints, independent and identically distributed random variables with zero average and variance $1/N$.

We prove that, as $N \rightarrow \infty$, the density of states on microscopic intervals (intervals containing only order one eigenvalues) converges to Wigner's semicircle law.

Using the local validity of the semicircle law, we establish the complete delocalization of the eigenvectors, and the level repulsion among the eigenvalues.

Moreover, extending an approach introduced by Jhansson, and combining it with a new time-reversal idea, we show universality of the correlation functions for a large class of hermitian ensembles (convergence to the sine-kernel).

On the well-posedness of the Cauchy problem for focusing and defocusing Gross-Pitaevskii hierarchies

THOMAS CHEN

(joint work with Natasa Pavlovic)

We present some recent results, all from joint work with Natasa Pavlovic, related to the Cauchy problem for the Gross-Pitaevskii (GP) hierarchy. first, we address the local well-posedness theory, in various dimensions, for the cubic and quintic case. We then introduce new conserved energy functionals which we use in the following contexts:

- (1) In a joint work with N.Tzirakis (UIUC), we prove, on the L^2 critical and supercritical level, that solutions for focusing GP hierarchies with a negative average energy per particle blow up in finite time.

- (2) We prove the global well-posedness of the Cauchy problem for energy subcritical, defocusing GP hierarchies, based on the conservation of higher order energy functionals.
- (3) We prove global well-posedness of focusing and defocusing GP hierarchies on the L^2 subcritical level, based on a generalization of the Gagliardo-Nirenberg (and Sobolev) inequalities, which we establish for density matrices.

Renormalization Group and Resonances in Non-relativistic QED

ISRAEL MICHAEL SIGAL

I.M. Sigal, Renormalization Group and Resonances in Non-relativistic QED

Abstract In this talk I describe a proof of existence of a ground state and resonances in the standard model of the non-relativistic quantum electro-dynamics (QED) with no extra assumptions on the infra-red behaviour of the interactions. The proof I outline is based on the spectral renormalization group approach developed in a joint work with Volker Bach and Jürg Fröhlich. It has two new elements: (a) a new canonical transformation of QED Hamiltonians and (b) a new - momentum anisotropic - Banach space on which the renormalization map acts.

The critical temperature of dilute Bose gases: A tentative exact approach using spatial permutations

VOLKER BETZ, DANIEL UELTSCHI

We attempt to calculate the change of critical temperature of the dilute Bose gas, that is due to interactions. The system of N bosons in the three-dimensional cubic box Λ is described by the Schrödinger operator

$$H = - \sum_{i=1}^N \Delta_i + \sum_{1 \leq i < j \leq N} U(x_i - x_j),$$

acting in $L^2_{\text{sym}}(\Lambda^N)$. We always suppose that the interaction potential U is repulsive and finite range; we let a denote its scattering length.

Our approach starts with the Feynman-Kac representation, where quantum particles are represented by Brownian bridges, and the restriction to the symmetric subspace is implemented by explicitly summing over permutations $\pi \in \mathcal{S}_N$. A good reference is [4]. We are led to a model of “spatial random permutations”, whose state space is $\Lambda^N \times \mathcal{S}_N$, i.e. it consists of all pairs (\mathbf{x}, π) , with $\mathbf{x} = (x_1, \dots, x_N)$ representing N positions in Λ , and π a permutation of N elements. One considers the Gibbs weight $e^{-H(\mathbf{x}, \pi)}$ with “Hamiltonian”

$$H_1(\mathbf{x}, \pi) = \frac{1}{4\beta} \sum_{i=1}^N |x_i - x_{\pi(i)}|^2 + \sum_{1 \leq i < j \leq N} V_{ij}(\mathbf{x}, \pi).$$

The first term is due to Brownian bridges and it forces the spatial permutation to have only small jumps. The second term gives the interaction between the jumps $x_i \mapsto x_{\pi(i)}$ and $x_j \mapsto x_{\pi(j)}$. Its explicit expression is a bit complicated, namely

$$V_{ij}(\mathbf{x}, \pi) = \int [1 - e^{-\frac{1}{4} \int_0^{4\beta} U(\omega(s)) ds}] d\widehat{W}_{x_i - x_j, x_{\pi(i)} - x_{\pi(j)}}^{4\beta}(\omega) = K(x_i - x_j, x_{\pi(i)} - x_{\pi(j)}).$$

Here, \widehat{W} denotes the normalized Wiener measure for Brownian bridges, and K is the integral kernel of the operator $e^{2\beta\Delta} - e^{\beta(2\Delta - U)}$. Notice that $V_{ij}(\mathbf{x}, \pi)$ depends only on $x_i, x_{\pi(i)}, x_j, x_{\pi(j)}$. Our system is not exactly equivalent to the Bose gas, but it should describe it exactly in the dilute regime $a\rho^{1/3} \ll 1$ [8].

The usual definition of the Bose-Einstein condensation involves the off-diagonal correlations $\langle a^*(x)a(y) \rangle$. But in this approach we consider an alternate criterion pioneered by Feynman [3] and Sütő [6, 7], and that should be equivalent when interactions are weak. Namely, there is Bose-Einstein condensation if and only if there are infinite permutation cycles.

At this stage we perform certain expansions and simplifications, which we hope to retain the main features of the model — the critical temperature should be identical to first order in $a\rho^{1/3}$. But these steps remain to be justified in a mathematically rigorous fashion. We then obtain the simpler Hamiltonian

$$H_2(\mathbf{x}, \pi) = \frac{4\pi\beta aN^2}{|\Lambda|} + 8\pi\beta\rho_c^{(0)}aN + \frac{1}{4\beta} \sum_{i=1}^N |x_i - x_{\pi(i)}|^2 + \sum_{\ell \geq 1} \alpha'_\ell r_\ell(\pi),$$

where $r_\ell(\pi)$ gives the number of cycles of length ℓ in the permutation π . The weights α'_ℓ are given by

$$\alpha'_\ell = \frac{2\ell a}{(4\pi\beta)^{1/2}} \left[\frac{1}{2} \sum_{j=1}^{\ell-1} \left(\frac{\ell}{j(\ell-j)} \right)^{3/2} - \zeta\left(\frac{3}{2}\right) \right].$$

One can check that the weights are negative, and that they converge to $-(6 - \gamma_{1/2})(4\pi\beta)^{-1/2}a$ as $\ell \rightarrow \infty$. The critical density of this model is conjectured to be

$$\rho_c^{(a)} = (4\pi\beta)^{-3/2} \sum_{\ell \geq 1} \frac{e^{-\alpha'_\ell}}{\ell^{3/2}}.$$

This was rigorously proved in the case where the weights α'_ℓ go to 0 faster than $1/\log \ell$ as $\ell \rightarrow \infty$ [2]. We assume here that the formula remains true with the present weights. Let $\rho_1^{(a)}$ be the critical density for the occurrence of infinite cycles in this model. To first order, the change in the critical temperature is given by

$$\frac{\rho_c^{(a)} - \rho_c^{(0)}}{\rho_c^{(0)}} \approx -\frac{1}{\zeta\left(\frac{3}{2}\right)} \sum_{\ell \geq 1} \frac{\alpha'_\ell}{\ell^{3/2}} = \frac{2\sqrt{\pi}a\beta^{-1/2}}{\zeta\left(\frac{3}{2}\right)}.$$

In the physics literature, people have rather consider the change in the critical temperature. The result above translates into

$$\frac{T_c^{(a)} - T_c^{(0)}}{T_c^{(0)}} \approx -\frac{8\pi a\rho^{1/3}}{3\zeta(\frac{3}{2})^{4/3}} \approx -2.33 a\rho^{1/3}.$$

We have found that the change in the critical temperature is linear in a and that it is negative. The latter point is totally unexpected, as it goes against the findings of the physics community. Indeed, many papers have been devoted to this question, and physicists have recently reached the consensus that $\frac{T_c^{(a)} - T_c^{(0)}}{T_c^{(0)}} \approx 1.3 a\rho^{1/3}$. See [5] for a review of the physics literature, and also for a rigorous upper bound on the critical temperature. The discrepancy between our result and the physics consensus is puzzling. We trust the physics literature, especially when over a dozen articles point towards the same conclusion. On the other hand, our approximations seem reasonable and they should lead to the correct critical temperature, to first order in the scattering length. This conundrum will hopefully be solved in the future.

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Towards Diffusion from Hamiltonian Quantum Systems

WOJCIECH DE ROECK

We report on recent work on deriving diffusive motion from Hamiltonian dynamics.

In [1], we consider a quantum particle coupled to an array of thermal baths. In this setup, the reservoir correlation function can be chosen to decay exponentially in time, uniformly in the spatial coordinates. This allows us to use cluster expansion techniques to control the long time behavior of the particle, and we prove diffusion in all dimensions.

In [2], we consider a heavy quantum particle with an internal degree of freedom moving on the d -dimensional lattice \mathbb{Z}^d (e.g., a heavy atom with finitely many excited states). The particle is coupled to a thermal bath consisting of free relativistic bosons through an interaction of strength λ linear in creation and annihilation operators. Since the local momentum conservation induces a slow decay of correlations, we cannot use the techniques of [1]. Instead, the mass of the quantum particle is assumed to be of order λ^{-2} , and we assume that the internal degree of freedom is coupled “effectively” to the thermal bath. With these simplifications in place, we prove that the motion of the quantum particle is diffusive in $d \geq 4$ and for λ small enough.

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Symmetry breaking in atomic multi-configuration calculations

MARIA J. ESTEBAN

(joint work with Mathieu Lewin, Andreas Savin)

In atomic relativistic calculations, one usually imposes the total angular momentum $J^2 = (L + S)^2$ whereas in nonrelativistic calculations both L^2 and S^2 are imposed. It has been observed by Kim et al in [3] that a certain multiconfiguration ground state of the symmetry space $J = 1$ for *Be*-like (Beryllium-like) atoms, was converging in the nonrelativistic limit to a state which was not an eigenfunction of S^2 and L^2 . This led to erroneous values of certain transition probabilities like spin-forbidden ones.

More concretely in [3] we find the following sentence “*For the last 30 years during which many researchers have used the MCDF method, it was assumed that MCDF wave functions would reduce to the correct NR limit, without verification of the limiting values of L and S in each case. We found that the calculated MCDF wave functions sometimes fail to reduce to the eigenfunctions of L and S* ”.

Other discussions about symmetry-breaking phenomena in the physical and chemical literature can be found in [1, 2, 4].

In this talk we have discussed the fact that the above issue has nothing to see with the nonrelativistic limit, because we prove that the above phenomenon of symmetry breaking takes already place when considering the (nonrelativistic) multi-configuration Hartree-Fock model. What induces symmetry breaking is the high nonlinearity of the model.

In the multiconfiguration methods, the wavefunction is taken to be a linear combination of certain configurations. Both the linear coefficients and the orbitals in the configurations are variational parameters, leading to a highly nonlinear problem (with respect to variations of the orbitals). Each configuration is itself a

sum of Slater determinants whose coefficients are fixed such that the configuration belongs to a chosen symmetry subspace ($J = 1$ in the case of the example studied in [3]).

Typically, if for instance we consider the Beryllium atom (4 electrons), and we decide that we fill the first shell with two electrons in the $1s_{1/2}$ state, and in the second shell there are two electrons, one s and one p , or one p and one d , then the general wave function for the multiconfiguration method can be written as

$$(*) \quad \Psi = a\Phi(1s_{1/2}^2 2s_{1/2} 2p_{1/2})(R_0, R_1, R_2) + b\Phi(1s_{1/2}^2 2s_{1/2} 2p_{3/2})(R_0, R_1, R_3) \\ + c\Phi(1s_{1/2}^2 2p_{1/2} 3d_{3/2})(R_0, R_2, R_4) + d\Phi(1s_{1/2}^2 2p_{3/2} 3d_{3/2})(R_0, R_3, R_4) \\ + e\Phi(1s_{1/2}^2 2p_{3/2} 3d_{5/2})(R_0, R_3, R_5),$$

where each function Φ is an eigenstate of \mathbf{J}^2 with eigenvalue $J(J+1)$, $J = 1$.

The 4-body Hamiltonian is chosen to be:

$$H := \sum_{i=1}^4 \left(\frac{-\Delta_i}{2} - \frac{4}{|x_i|} \right) + \sum_{1 \leq i < j \leq 4} \frac{1}{|x_i - x_j|}.$$

So the problem to look at when one wants to compute the ground state energy for $J = 1$ in the above class of functions is

$$E_{sp+pd}(J=1) := \inf_{\Psi \text{ of type } (*)} \langle \Psi, H\Psi \rangle,$$

where the variational parameters are the radial orbital functions R_0, \dots, R_5 and the coefficients a, b, \dots, e .

Now, if we want to consider states which are eigenstates of \mathbf{J}^2 , of \mathbf{L}^2 and of \mathbf{S}^2 , we introduce the usual notation: a state is denoted by ${}^{2S+1}L_J$ when it is an eigenfunction of \mathbf{S}^2 with eigenvalue $S(S+1)$, of \mathbf{L}^2 with eigenvalue $L(L+1)$ (with the identification P, D, F, \dots for $L = 1, 2, 3, \dots$), and of \mathbf{J}^2 with eigenvalue $J(J+1)$.

For Be -like atoms in the symmetry $J = 1$ with $sp + pd$ configurations, we will see that 3 nonrelativistic symmetries occur with well defined values of L and S : 1P_1 , 3P_1 and 3D_1 .

Of course, one has:

$$E_{sp+pd}(J=1) \leq \min \left\{ E_{sp+pd}({}^3P_1), E_{sp+pd}({}^1P_1), E_{sp+pd}({}^3D_1) \right\},$$

where

$$E_{sp+pd}({}^3P_1) := \inf_{\Psi \in {}^3P_1} \langle \Psi, H\Psi \rangle, \quad E_{sp+pd}({}^1P_1) := \inf_{\Psi \in {}^1P_1} \langle \Psi, H\Psi \rangle, \\ E_{pd}({}^3D_1) := \inf_{\Psi \in {}^3D_1} \langle \Psi, H\Psi \rangle.$$

The main question is then to see whether the above inequality is strict or not. By proving the first kind of Hund's rule in this context we verify that

$$E_{sp+pd}({}^3P_1) < E_{sp+pd}({}^1P_1).$$

Then, we use numerical computations performed with the ATSP package (see <http://atoms.vuse.vanderbilt.edu/>) to verify that

$$E_{sp+pd}(^3P_1) < E_{sp+pd}(^3D_1).$$

Remains then the question of whether or not

$$E_{sp+pd}(J=1) < E_{sp+pd}(^3P_1).$$

We then prove that both the simplet 1P_1 and the triplet 3D_1 are stationary points of the E_{sp+pd} energy, but none of them is a local minimum. Moreover, by performing again numerical computations with Mathematica, based of the data provided by calculations done with the ATSP package, we see that the triplet 3P_1 is not even a stationary point for E_{sp+pd} . So, the triplet P is not even a bound state for the multi-configuration Hartree-Fock model when one considers $sp + pd$ configuration in the symmetry class $J = 1$.

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Determinant bounds and dilute fermion systems in three dimensions

MANFRED SALMHOFER

After a brief review of the ultraviolet and infrared problems in the construction of coherent-state functional integrals for nonrelativistic quantum many-body systems, I present some recent results about many-fermion systems. The first are determinant bounds, developed in joint work with Walter Pedra [1], that allow for a simple proof that the time continuum limit of regularized functional integrals exists and that ℓ^1 clustering bounds hold [2]. The second is a construction of the correlation functions for a dilute three-dimensional gas of fermions with a weak, short-range interaction [3]. The diluteness condition places a temperature-dependent restriction on the fermion density. It has the physical interpretation that the thermal de Broglie wavelength of the particles is at most a multiple of the average interparticle distance. Besides the above-mentioned proof of convergence of the time continuum limit, the construction of the correlation functions requires dealing with the infrared problem arising from the slow falloff of the fermionic covariance. This is done by a multiscale expansion and an analysis of the corresponding sequence of effective actions. This *renormalization group (RG) flow* has

the feature that, due to the smallness of the density, the corrections to the two-particle interaction function decreases along this sequence (i.e. they are irrelevant in the RG sense). For this reason, all correlation functions are close to those of an ideal Fermi gas.

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Uniqueness of ground states for fractional non-linear Schrödinger equations

ENNO LENZMANN

(joint work with Rupert Frank)

Ground states play an eminent role in our rigorous understanding of solitary waves and blowup for dispersive equations with focusing nonlinearity. Indeed, many key results in this area depend on fundamental properties of ground states such as their uniqueness, radial symmetry as well as the so-called nondegeneracy of the linearized operator. In the well-studied case of classical NLS/NLW, all these issues have found a satisfactory answer by using classical elliptic theory and techniques from ordinary differential equations. However, the current status of affairs about ground states for fractional NLS (involving fractional powers of the Laplacian) is mainly open. In this talk, I will present a new result that enters this "terra incognita", by proving the uniqueness and radial symmetry of ground states for a certain class of fractional NLS, which arise in astrophysics. Time permitting, I will discuss some applications too.

Solution of the Infrared Catastrophe Problem in Non-relativistic QED

ALESSANDRO PIZZO

We construct infraparticle scattering states for Compton scattering in the standard model of non-relativistic QED. In our construction, an infrared cutoff initially introduced to regularize the model is removed completely. We rigorously establish the properties of infraparticle scattering theory predicted in the classic work of Bloch and Nordsieck from the 1930's, Faddeev and Kulish, and others.

Leaky Repeated Interaction Quantum Systems

ALAIN JOYE

(joint work with Laurent Bruneau, Marco Merkli)

We consider a small reference system \mathcal{S} interacting with two large quantum systems of a different nature. On the one hand the system \mathcal{S} interacts for a fixed duration with the successive elements E of an infinite chain \mathcal{C} of identical independent quantum subsystems \mathcal{E} . And, on the other hand, it interacts continuously with a heat reservoir \mathcal{R} at a some inverse temperature given by an infinitely extended Fermi gas. The reservoir and the chain are not coupled. When the reservoir is absent, the state of the repeated interaction quantum system defined by \mathcal{S} and the chain \mathcal{C} approaches a non-equilibrium asymptotic state for large times. When the chain is absent, the system \mathcal{S} and the reservoir \mathcal{R} reach an equilibrium state at large times. Our goal is to describe the large time behaviour of the fully coupled system $\mathcal{S} + \mathcal{R} + \mathcal{C}$. We describe the asymptotic state of this system and the heat fluxes between the chain \mathcal{C} and the reservoir \mathcal{R} through the small system \mathcal{S} .

Some results on the Nelson model with variable coefficients

CHRISTIAN GÉRARD

The Nelson model with variable coefficients describes a quantized scalar bosonic field linearly coupled with a non-relativistic particle.

Contrarily to the usual Nelson model, where the scalar field is obtained by quantization of the free Klein-Gordon equation, in our case the Klein-Gordon equation comes from a variable, static Lorentzian metric on \mathbf{R}^{1+3} . The mass term is also allowed to be position-dependent. Examples of this type of Klein-Gordon equation are obtained if we add a scalar curvature term (conformal wave equation).

We present proofs of the following results:

1) Removal of the UV cutoff: as in the standard Nelson model, the UV cutoff in the interaction can be removed, and a local Hamiltonian can be constructed. Instead of simple Fourier analysis, we use here some results from pseudodifferential calculus.

2) Existence of a ground state for the Hamiltonian: if the mass decays at infinity like $\langle x \rangle^{-\mu}$ for $\mu < 2$, then the Hamiltonian has a ground state. This follows by combining known results on the abstract Nelson model with some (new?) lower bounds on differential operators.

3) Non-existence of a ground state for the Hamiltonian: if the mass decays at infinity like $\langle x \rangle^{-\mu}$ for $\mu > 2$, then the Hamiltonian has no ground state. This is shown by adapting the proof of Lorinczi-Minlos-Spohn to the variable coefficients case. At the end the key ingredient is some lower bounds on heat kernels for Schroedinger operators, due to Semenov.

Mean field limits and semiclassical analysis

FRANCIS NIER

(joint work with Z. Ammari, S. Breteaux)

Very early, the bosonic Fock space has been identified as the quantization of the classical phase-space. In this spirit the mean field limit can be viewed as a semiclassical limit. The coherent state method introduced by Hepp in the 70's is an application of this point of view. In the mean time the attempts to develop an infinite dimensional pseudodifferential calculus had to face obstructions or subtle differences between an inductive approach with Hilbert-Schmidt conditions like in Shale's theorem and a projective approach more naturally related with the stochastic processes framework. With Zied Ammari and more recently with Sébastien Breteaux, we have tried to analyze more precisely this question by making use of the developments on finite dimensional semiclassical analysis in the 80-90's. Wigner measures (or semiclassical measures) can be introduced and bring some flexibility on mean field limits while infinite dimensional phenomena can still be specified. Higher order expansions can also be considered.

This lecture gives an account of recent works of the author with Z. Ammari and S. Breteaux on the subject (see [AmNi][AmNi2][AmBre] where an extended bibliography can be found).

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Diffusion of a Wave Packet in a Markov Random Potential

JEFFREY SCHENKER

It is generally expected that over long times the amplitude of a wave propagating in a weakly disordered background will be well described by a diffusion, at least in dimension $d \geq 3$. This expectation stems from a picture of wave propagation as a multiple scattering process. Scattering off the disordered background results in random phases, and the build up of these phases over multiple scattering events leads eventually to a loss of coherence in the wave. Decoherent propagation of the wave may be understood as a classical superposition of reflections from random obstacles. As long as recurrence does not dominate the evolution, the central limit theorem suggests that the amplitude is given in the long run by a diffusion.

So far it has not been possible to turn this heuristic argument into mathematical analysis, at least without restricting the time scale over which the wave evolution is followed as in [1, 2, 3]. One major obstacle is a lack of control over recurrence:

the wave packet may return often to regions visited previously, denying us the independence needed to carry out the central limit argument.

A natural way to avoid recurrence difficulties is to bring a time dependence into the disordered background — to suppose that the environment evolves as the packet propagates. With Yang Kang, we considered a stochastic environment evolving independently of the wave packet. Specifically, we studied the unitary evolution

$$(1) \quad i\partial_t\psi_t(x) = H_0\psi_t(x) + \omega_t(x)\psi_t(x)$$

on $\ell^2(\mathbb{Z}^d)$ where H_0 is a translation invariant hopping term satisfying a non-degeneracy condition spelled out in [5], and $\omega_t(x)$ is a time dependent random potential, which evolves in time as a Markov process. The key assumption is that the process has a “spectral gap,” which means roughly that

$$\left| \mathbb{E}(f(\omega_t)) - \int_{\Omega} f(\omega)d\mu(\omega) \right| \leq e^{-t/T},$$

for some $T > 0$ with $d\mu$ a non-trivial invariant measure.

For this evolution, we obtained the following result which shows that the density of the wave converges, in a scaling limit, to a solution of a heat equation:

Theorem 1 (Kang and Schenker 2009 [5]). *For solutions to (1), with the assumptions of [5], we have*

$$\lim_{\tau \rightarrow \infty} \sum_{x \in \mathbb{Z}^d} e^{-i \frac{k}{\sqrt{\tau}} \cdot x} \mathbb{E}(|\psi_{\tau t}(x)|^2) = e^{-t \sum_{i,j} D_{i,j} k_i k_j},$$

with $D_{i,j}$ a positive definite matrix. Furthermore

$$\lim_{T \rightarrow \infty} \frac{1}{T} \sum_{x \in \mathbb{Z}^d} |x|^2 \mathbb{E}(|\psi_T(x)|^2) = \sum_i D_{i,i}.$$

The proof relies on an “augmented space” representation, similar to that used in the study of random walk in a random environment [6, 4].

Recently this has been extended to the following evolutions:

$$(2) \quad i\partial_t\psi_t(x) = H_0\psi_t(x) + (w(x) + \omega_t(x))\psi_t(x),$$

where w is a static random potential with a translation invariant distribution.

Theorem 2 (Schenker 2009). *For solutions to (2) we have*

$$\lim_{\tau \rightarrow \infty} \eta \int_0^\infty e^{-\eta t} \sum_{x \in \mathbb{Z}^d} e^{-i \frac{k}{\sqrt{\tau}} \cdot x} \mathbb{E}(|\psi_{\tau t}(x)|^2) dt = \frac{1}{\eta + \sum_{i,j} D_{i,j} k_i k_j},$$

and

$$\lim_{\eta \rightarrow 0} \eta^2 \int_0^\infty e^{-\eta t} \sum_{x \in \mathbb{Z}^d} |x|^2 \mathbb{E}(|\psi_t(x)|^2) dt = \sum_i D_{i,i},$$

with $D_{i,j}$ a positive definite matrix.

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