MATHEMATISCHES FORSCHUNGSINSTITUT OBERWOLFACH

TAGUNGSBERICHT 31/1999

LARGE COULOMB SYSTEMS

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Large Coulomb systems is a special interdisciplinary topic in mathematical physics joining the sciences of mathematics and physics. Indeed, “Coulomb systems” refers to the mathematically rigorous description of electrons in atoms, molecules, and solids in the absence or presence of an electromagnetic field. These “Coulomb systems” can be “large”, which means that the # electron number N and the number of nuclei K is allowed—and sometimes even desired—to be large. The limit $N \to \infty$ often corresponds to the limit $\hbar \to 0$, where $\hbar$ is Planck's constant. This correspondence intimately connects large Coulomb systems, as physical models, with the mathematical disciplines of partial differential equations, pseudo-differential operators, semiclassical analysis, spectral theory and the calculus of variations. Specifically, the topics of the workshop included

- Stability of matter (nonrelativistic, relativistic, and with classical electromagnetic field),
- Semiclassical Schrödinger operators with and without magnetic field, in particular, Lieb-Thirring inequalities,
- Nonrelativistic quantum electrodynamics,
- Ground state asymptotics for large, (asymptotically) neutral Coulomb systems, e.g., energy, density, surplus negative ionization,
- Ground state asymptotics for atoms in homogeneous magnetic fields.

This meeting was organized by Volker Bach and Heinz Siedentop.

1. **G. Friesecke:** The configuration-interaction equations for atoms and molecules: Charge quantization and existence of solutions

The configuration-interaction equations of rank K for atoms and molecules are a natural hierarchy of exactifications of the Hartree-Fock equations to which they reduce in the lowest rank case where K equals the number N of electrons in the system. In the highest rank case, $K = \infty$, they turn into the full Schrödinger N-body equation. The ground state energy for large finite K approaches the 'exact' (non-relativistic, Born-Oppenheimer) quantum mechanical energy of the system delivered by the Schrödinger equation.

The CI equations are central to the understanding of electron correlation, which is neglected by the Hartree-Fock approximation. They have an enormous physics and quantum chemistry literature, but very little was known rigorously: mathematically, they are a system of K coupled nonlinear partial integrodifferential equations.

The new result is that charge in the CI equations is integer-quantized and that ground state solutions for atoms and molecules exist whenever the total nuclear charge excedds $N-1$, where N is the number of electrons. (This is new even for the Helium atom.)

2. **T. Weidl:** Classical constants in Lieb-Thirring inequalities

Let $H = -\Delta - V$ be the Schrödinger operator on $L^2(\mathbb{R}^d)$. We consider potentials V for which the negative spectrum of H is discrete, let $\{E_j\}$ be the sequence of these negative eigenvalues. Consider the Riesz means of these eigenvalues

$$S_{\gamma,d}(V) = \sum(-E_j)^\gamma, \quad \gamma \geq 0.$$

It is well-known that for $d = 1, \gamma \geq 1/2$ or $d = 2, \gamma > 0$ or $d \geq 3, \gamma \geq 0$ the bound

$$S_{\gamma,d}(V) \leq R(\gamma, d) \iint_{\{H<0\}} (-H(x,\xi))^\gamma \frac{dx d\xi}{(2\pi)^d} = R(\gamma, d) L^{cl}_{\gamma,d} \int_{\{V>0\}} V^{\gamma+d/2}\, dx,$$

holds, where

$$L^{cl}_{\gamma,d} = \frac{\Gamma(\gamma+1)}{2^d \pi^{d/2} \Gamma(\gamma+1+d/2)}.$$

¿From the quasi-classical limit it is known that $R(\gamma, d) \geq 1$. Moreover, $R(\gamma, 1) = 1$ for $\gamma \geq 3/2$.

We prove that $R(\gamma, d) = 1$ for all $\gamma \geq 3/2$ and all $d \in \mathbb{N}$.

Joint work with A. Laptev.

3. **M.J.Esteban and E. Séré:** The Dirac-Fock equations

The Dirac-Fock equations are the relativistic analogue of the well-known Hartree-Fock equations. They are used in computational chemistry, and yield results on the inner-shell elctrons of heavy atoms that are in very good agreement with experimental data. By a variational method, we prove the existence of infinitely many solutions of the Dirac-Fock equations 'without projector', for Coulomb systems of electrons in atoms, ions or molecules, with $Z \leq 124, N \leq 41, N \leq Z$. Here, Z is the sum of the nuclear charges in the molecule, N is the number of electrons.

M.J.Esteban and E. Séré (CEREMADE, Université Paris-Dauphine, France).

Solutions of the Dirac-Fock equations for atoms and molecules, Comm. Math. Phys. 203, 499-530 (1999).

4. **J. Yngvason:** The ground state of Bosons in a trap

The ground state properties of interacting Bose gases in external potentials, as considered in recent experiments, are usually described by means of the Gross-Pitaevskii energy functional

$$\mathcal{E}^{GP}[\phi] = \int_{\mathbb{R}^3} |\nabla\phi|^2 - V|\phi|^2 + 4\pi a|\phi|^4.$$

Here V is an external potential (often $\approx |x|^2$) and a is the scattering length of the interaction potential, v, between the Bosons. The corresponding ground state energy, $E^{GP}(N,a)$, is the minimum of $\mathcal{E}^{GP}$ under the condition $\int |\phi|^2 = 1$.

We have proved the asymptotic exactness of this approximation for the quantum mechanical ground state energy $E^{QM}(N,a)$ as $N \to \infty$ with Na fixed:

$$\lim_{N\to\infty} \frac{E^{QM}(N,a)}{E^{GP}(N,a)} = 1.$$

A corresponding theorem holds also for the particle density. These results are obtained under the assumption that $v \geq 0$, spherically symmetric, and of short range.

J. Yngvason (Univ. of Vienna): Joint work with E. H. Lieb (Princeton) and R. Seirinzer (Vienna).

5. **M. Salmhofer:** Positivity and convergence in fermionic quantum field theory

I discuss norm bounds that imply the convergence of perturbation theory for the effective action of fermionic quantum field theories with cutoffs. These bounds are sufficient for an application in renormalization group studies. I sketch our proof of these bounds; it clarifies how the applicability of Gram bounds with uniform constants is related to positivity properties of matrices associated to the procedure of taking connected parts of Gaussian convolutions. This positivity is preserved in decouplings that also preserve stability in the case of two-body interactions. The physical systems to which these techniques apply include the Gross-Neveu model and many-fermion models with short-range interactions, such as the Hubbard model, at weak coupling.

M. Salmhofer (ETH Zürich): Joint work with C. Wieczerkowski (Münster).

6. **J. Fröhlich:** Open systems

We present a general introduction to the quantum theory of *open systems* consisting of a 'compact system' coupled to an infinite dispersive medium. The analysis of such systems is important in attempting to understand *friction* and *dissipation* in unitary quantum dynamics, the *emergence of classical behaviour* in quantum systems and a *'quantum theory of experiments'*. As typical examples of dissipative behaviour we discuss 'relaxation to a groundstate' and 'return to equilibrium'. We then exemplify our general theory on the example of systems consisting of a finite number of *atoms* with static nuclei and non-relativistic quantum-mechanical electrons coupled to the *quantized radiation field.* The interaction between the electrons and the quantized electromagnetic vector potential is cutoff at large photon wave vectors.

At zero temperature, we develop a mathematically rigorous theory of the *Lamb shift*, of the *decay of resonances* corresponding to excited states of the atoms and of the existence of *ground states.* We also analyse the spectral type of the basic Hamiltonian of the system.

At positive temperature, we construct the *KMS* (thermal equilibrium) *states* of these systems and prove *'return to equilibrium'.*

J. Fröhlich: Joint work with V. Bach, I.M. Sigal (et.al.).

7. **I. Catto:** Thermodynamic limit problems for Hartree and Hartree-Fock type models

We consider a neutral molecular system consisting of a given number of point nuclei located on a (finite) set of points of integer coordinates in $\mathbb{R}^3$, and we let asymptotically this set of locations fill in the entire lattice $\mathbb{Z}^3$. We consider next the behaviour of the ground state energy per unit volume for various well-known models in Quantum Chemistry. By this process, we wish to set a limit problem for the ground state energy of a crystal, that is well-posed mathematically, in particular with a view to give a sound ground to numerical simulations of the condensed phase.

For the Thomas-Fermi type models, following the ground-breaking work of Lieb and Simon on Thomas-Fermi models, we have proved that the ground state energy per unit volume converges to a periodic minimization problem, and that the electronic density also becomes asymptotically periodic.

For the more complicated Hartree and Hartree-Fock models, we are only able to define periodic problems which are likely to be the thermodynamic limits, and to prove that they are mathematically well-posed. Nevertheless, we are able to prove the thermodynamic limit for a simplified version of the Hartree-Fock model, namely the reduced Hartree-Fock model.

I. Catto (CNRS and CEREMADE, Université Paris-Dauphine): Joint work with C. Le Bris (ENPC, Marne-la-Vallée, France) and P.L. Lions (CEREMADE, Paris).

8. **A. Knauf:** The n-centre problem for large energies

The motion of a fast comet in the gravitational field of n fixed celestial bodies is considered. Their positions are $s_1, \cdots, s_n \in \mathbb{R}^3$, and their masses $Z_1, \cdots, Z_n \neq 0$ (Because of applications in molecular scattering repelling forces are considered, too). The Hamiltonian $\hat{H} : T^*\hat{M} \to \mathbb{R}$ (with $\hat{M} = \mathbb{R}^3 \setminus \{s_1, \cdots, s_n\}$ is of the form $\hat{H}(p,q) = \frac{1}{2}p^2 + V(q), V(q) = -\sum_{l=1}^{n} \frac{Ze}{|q-s_l|} + W(q)$ with $W \in C^\infty(\mathbb{R}^3, \mathbb{R})$ decaying at infinity. We first uniquely complete the Hamiltonian System $(T^*\hat{M}, \sum dq, \hat{H})$, obtaining (P, ω, H), where P is a smooth $6D$ mainfold, ω a smooth symplectic form and $H : P \to \mathbb{R}$ smooth. Then we study the complete flow $\Phi^t : P \to P$. For large energies E we get a complete symbolic dynamics on $H^{-1}(E)$, assuming that no three centres s_l are on one line (NC condition), whereas

- for $n = 1$ (Kepler pr.) there is no bounded orbit,
- for $n = 2$ (Jacobi pr.) there is just one,
- for $n \geq 3$ there is a Cantor set of bounded orbits in $H^{-1}(E)$.

The Hausdorff and box counting dimension of b_E are both of the order

$$\dim(b_E) = 1 + d(E)(1 + O(\frac{1}{E \ln E})),$$

where $d(E)$ is explicit.

The topological entropy of $\Phi_E^t \equiv \Phi^t|_{H^{-1}(E)}$ is given by

$$h_{top}(\Phi_E^1) = h_{top}(\Phi_E^1|_{b_E}) = c_1\sqrt{2E}(1 + c_2\frac{\ln E}{E} + O(\frac{1}{E})),$$

with explicit constants c_1, c_2.

Although for $n \geq 3$ there is a Cantor set of scattering orbits with given incoming and outgoing directions $\hat{\theta}^-, \hat{\theta}^+ \in S^2$, the Rutherford cross section (for the Kepler problem with $\omega = 0$) is a good approximation to the differential cross section of the n-centre problem:

$$\frac{d\sigma}{d\hat{\theta}^+}(E, \hat{\theta}^-, \hat{\theta}^+) = \frac{d\sigma}{d\hat{\theta}^+}(E, \hat{\theta}^-, \hat{\theta}^+)_{Ru}(1 + O(1/E)).$$

Finally, we show that most results become wrong if the NC condition is violated.
A. Knauf (Univ. Erlangen-Nürnberg).

9. **L. Erdös:** Uniform magnetic Lieb-Thirring inequality for the Pauli operator with a general potential and strong magnetic field

We estimate the sum of the negative eigenvalues E_i of the Pauli operator

$$[\vec{\sigma} \cdot (\vec{p} + \vec{A})]^2 + V$$

with a magnetic field $\vec{B} = \nabla \times \vec{A}$ and an external potential V. Based upon the semiclassical picture, the estimate should have the form

$$\sum_i |E_i| \leq (const.) \int |\vec{B}|[V]_-^{3/2} + [V]_-^{5/2}. \tag{9.1}$$

It has been known that such an estimate can only be true for regular magnetic fields with constant direction, or else extra terms are needed, which involve derivatives of $\vec{B}$ or some mollified version of $\vec{B}$. In addition, for non-constant direction field a new term $\int P(x)|[V(x)]_- \, dx$ has to be added, where $P(x) = \sum_i |\psi_i(x)|^2$ and the summation is over an orthonormal basis in ker $\left(\vec{\sigma} \cdot (\vec{p} + \vec{A}\right)$. (These are the famous zero modes, first found by Loss-Yau).

Under smoothness assumptions on the magnetic field, there have been various bounds similar to (9.1) but with a $|\vec{B}|$-power higher than 1 (in the strong field regime). The essential reason for these overestimated powers was that $P(x)$ has not been estimated sharply.

Bugliaro-Fefferman-Graf obtained (9.1) with $|\vec{B}|^{17/12}$, an improvement over the earlier results scaling with the 3/2-power of $|\vec{B}|$. In our earlier work we first managed to obtain an estimate similar to (9.1) that scaled as $|B|^{5/4}$, later we even proved the correct linear behaviour $|\vec{B}|$, but with an additional unphysical term involving $\int |\nabla V|$.

Recently we proved (9.1) with the natural additional term $\int |\vec{B}|[V]_-$ (coming from the zero modes) and with some smoothness assumption on $\vec{B}$. No assumption on V is needed and the $|\vec{B}|$-power is the expected linear one.

L.Erdös (Georgiatech, Atlanta, USA): Joint work with J.P. Solovej (Univ. of Copenhagen).

10. **F. Hiroshima:** Effective mass producing ground states

The Pauli-Fierz Hamiltonian ($N = 1$ spinless) is defined by

$$H = \frac{1}{2m}(-i\vec{\nabla} - \frac{e}{c}\vec{A}(x))^2 + V + H_f,$$

where

$$H_f = \sum_{r=1}^{2} a^{*r}(k)\omega(k)a^r(k)\, dk,$$

$\omega(k) = \sqrt{k^2 + \mu^2}$, $\mu \geq 0$,

$$\vec{A(x)} = \frac{1}{\sqrt{2}} \sum_{r=1}^{2} \int a^{*r}(k) e^{-ikx} \pi(-k) e_\mu^r(k)\, dk + h.c.$$

'Assumption': $\vec{A}(x) \to \vec{A}(0)$ (dipole approximation). $V \in C_0^\infty(\mathbb{R}^3), V < 0, V \neq 0, a \int |V(x)|^{3/2} \, dx < 1$. Then $H_0 = \frac{1}{2m}(-\Delta) + V + H_f$ has no ground states!

Theorem 10.1. *$\exists \frac{e}{c} = \alpha \in \mathbb{R}$ s.t. H has a ground state.*

Proof. We can construct unitary operator U such that

$$U^{-1}HU = \frac{1}{2m_\alpha^*}(-\Delta) + V + H_f + R,$$

(Arai 1982) where $R = U^{-1}VU - V + \delta$, δ a constant. We can see that m_α^* is sufficiently large for some α and $R << H_f$. Thus by a Lattice Approximation method, we get the desired results. □

F. Hiroshima (Hokkaido Univ. Japan and TU-München): Joint work with H. Spohn.

11. **M. Hirokawa:** Some problems on the generalized Spin-Boson model

We consider some problems about the generalized spin-boson model. Namely:

- Characterize the existence or absence of ground states of the Hamiltonian of GSB model in terms of the ground state and excited state energies, and correlation functions by method of functional analysis.
- Investigate an expression or estimation of the ground state energy of GSB model without the infrared cutoff.
- Check whether there is an unusual counter-example, but familiar to us in physics, for our expectation concerning resonances. And if such an unusual example exists, investigate the reason why it has the unusual property contrary to our expectation. Then we will know when our expectation occurs.

For further details, please see our preprints in:
http://www.math.okayama-u.ac.jp/∼hirokawa
M. Hirokawa (Okayama Univ.)

12. **N. Röhrl:** The sharp bound on the stability of the relativistic electron-positron field in Hartree-Fock approximation

An operator $\gamma \in L^2(\mathbb{R}^3) \otimes \mathbb{C}^4 \to L^2(\mathbb{R}^3) \otimes \mathbb{C}^4$ is called a charge density operator if:

- γ is selfadjoint.
- γ is trace class.
- $-P_- \leq \gamma \leq P_+$, where P_+ and P_- denote the positive and negative energy subspaces of the free Dirac-Operator $\mathcal{D}$.

The energy of γ is given by

$$\mathcal{E}_\alpha(\gamma) = \mathrm{tr}(\mathcal{D}\gamma) + \alpha D(\rho_\gamma, \rho_\gamma) - \frac{\alpha}{2}\int_{G\times G} dxdy \frac{|\gamma(x,y)|^2}{|x-y|}.$$

Then there is a theorem by V. Bach, J.-M. Barbaroux, B. Helffer and H. Siedentop, that $\mathcal{E}_\alpha(\gamma) \geq 0$ if $\alpha \in [0, \frac{4}{\pi}]$. Here is was shown, that the energy per particle is not bounded from below, if $\alpha > \frac{4}{\pi}$.

N. Röhrl (Regensburg): Joint work with D. Hundertmark and H. Siedentop.

13. **D. Hundertmark:** New bounds on the Lieb-Thirring constants

Given a one-particle Schrödinger operator $H = -\Delta + V$ on $L^2(\mathbb{R}^d)$ the Lieb-Thirring estimate is the bound

$$\mathrm{tr}H_-^\gamma = \sum_j E_j^\gamma \leq L_{\gamma,d} \int_{\mathbb{R}^d} V_-(x)^{\mu+\frac{d}{2}}\,dx, \tag{13.1}$$

for the γ'th moment of negative eigenvalues $\{-E_j\}_j$ of H.

The inequality (13.1) is known to hold if $\gamma \geq \frac{1}{2}$ $(d=1)$, $\gamma > 0$ $(d=2)$, $\gamma \geq 0$ $(d \geq 3)$. The Lieb-Thirring constants $L_{\gamma,d}$ have the natural lower bound

$$L_{\gamma,d} \geq L^{cl}_{\gamma,d} \equiv \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} (p^2-1)^\gamma \, dp = \frac{\Gamma(\mu+1)}{2^d \pi^{d/2} \Gamma(\mu + \frac{d}{2} + 1)},$$

$\gamma \geq 0$. $L^{cl}_{\gamma,d}$ is the so-called classical constant.

Lieb and Thirring conjectured that for $\gamma \geq 1$ and $d \geq 3$, $L_{\gamma,d} = L^{cl}_{\gamma,d}$. This has recently been shown by A. Laptev and T. Weidl for $\gamma \geq \frac{3}{2}$. For the physically most important case $d=3$, $\gamma = 1$ the best known bound so far was $L_{1,3} \leq 5.129 L^{cl}_{1,2}$.

Based on the 'induction in the dimension' idea of Laptev and Weidl together with the recent result $L_{\frac{1}{2},1} = 2L^{cl}_{\frac{1}{2},1} = \frac{1}{2}$, we give the bound:

$$\begin{aligned} L_{\gamma,d} &\leq 2L^{cl}_{\gamma,d} \quad \text{for} \quad 1 \leq \gamma \leq 3/2, \ d \in \mathbb{N} \\ L_{\gamma,d} &\leq 4L^{cl}_{\gamma,d} \quad \text{for} \quad \frac{1}{2} \leq \gamma \leq 1, \ d \geq 2. \end{aligned}$$

This leads to certain improvements in the stability of matter bound for fermionic N-particle Coulomb systems.

D. Hundertmark (Princeton): Joint work with T. Weidl and A. Laptev (Royal Institute of Technology, Stockholm).

14. **V. Ivrii:** Sharp eigenvalue asymptotics for periodic operators

We recover sharp asymptotic for a number $N(\tau)$ of eigenvalues of operator $A - tW$ as t runs from 0 to τ, where A is a periodic operator and W is decaying at infinity potential, crossing level E which lies either in the spectral gap or on its boundary.

V. Ivrii (Univ. of Toronto).

15. **G. Scharf:** Quantum gauge theories

Until now these theories in four dimensions can only be understood as formal power series by means of perturbation theory. In this situation one would like to see the gauge structure directly in the power series. Considering the S-matrix given by the time-ordered products T_n, perturbative gauge invariance to first order means:

$$d_Q T_1 = \partial_\mu T^\mu_{1/1}, \tag{15.1}$$

where d_Q is the infinitesimal gauge variation (defined by a gauge charge Q on free fields) and the right side is a divergence, and similarly for T_n. Making a general ansatz for T_1 and $T^\mu_{1/1}$, the theory is strongly constrained by (15.1): In case of massless self-coupled spin-1 fields one gets Yang-Mills coupling. In the massive case unphysical and physical (=Higgs) scalar fields are required by 1st and 2nd order gauge invariance. For spin-2 there are more solutions: one is quantum gravity. Whether the others are gauge invariant in higher orders remains to be seen.

Papers can be found under hep-th on the net.

G. Scharf (Zürich)

16. **E. Lieb:** The ultraviolet problem in quantum electrodynamics

Various models of charged particles interacting with a quantized radiation field (but not with each other) are discussed. Upper and lower bounds for the self- or ground state-energies (without mass renormalization) are presented. For N fermions the bounds are proportional to N (as they should be) but for bosons the bounds are sublinear (which implies binding) and hence that 'free bosons' are never free. Both relativistic and nonrelativistic kinematics are considered. The bounds are non-perturbative. Indeed, in the nonrelativistic case they disagree strongly with ordinary perturbative theory.

E. Lieb (Princeton): Joint work with M. Loss.

17. **M. Loss:** A simple proof of a theorem of Laptev and Weidl

Consider the Schrödinger operator

$$H = -\frac{d^2}{dx^2} \otimes I - V(x),$$

on $L^2(\mathbb{R}; \mathbb{C}^N)$. Here, I is the $N \times N$ identity matrix and $V(x)$ is a non-negative hermitean $N \times N$ matrix with smooth, compactly supported matrix elements. This operator has finitely many negative eigenvalues, which we denote by

$$-\lambda_1 \leq -\lambda_2 \leq \cdots \leq -\lambda_L.$$

The following Lieb-Thirring inequality was proved by Laptev and Weidl using scattering theory:

$$\sum_{j=1}^{L} \lambda_j^{3/2} \leq \frac{3}{16} \int_{\mathbb{R}} \operatorname{tr}[V(x)^2]\, dx.$$

The constant $\frac{3}{16}$ is best possible.

We give an elementary proof of this result using the classical commutation method.

M. Loss (Georgia Tech.): Joint work with R. Benguria.

18. **J.P. Solovej:** The ground state energy of the charged Bose gas

The model studied here is the 'Jellium' model in which there is a uniform, fixed background with charge density ρ and in which there move charged particles of unit charge — the whole system being neutral. In 1961 Foldy used Bogolubov's 1947 method to investigate the ground state energy of this system for bosonic particles in the large ρ limit. He found that the energy per particle is $-0.803\rho^{1/4}$ in this limit. Here, we prove that this formula is correct, thereby validating, for the first time, at least one aspect of, Bogolubov's pairing theory of the Bose gas.

J.P. Solovej (Copenhagen): Joint work with E. Lieb.

19. **G.M. Graf:** Extended edge states in quantum Hall systems

A classical electron in a 2-dimensional domain Ω under the influence of a magnetic field moves in a circle about some fixed center - the guiding center - as long as it does not hit the boundary $\partial\Omega$. If it does, the electron follows the boundary by repeatedly bouncing at it. The quantum mechanical counterpart should be the existence of extended edge states. This is of some importance in connection with the quantum Hall effect. We show the existence of absolutely continuous edge spectrum of energies away from the Landau levels, first for Ω a half-plane and then for more general domains. The result is stable if some disorder potential is included. The proof is based on Mourre theory. The conjugate operator, i.e., the observable increasing in time, is related to the position of the guiding center.

G.M.Graf (Zürich).

20. **M. Kiessling:** 100 YEARS ABRAHAM-LORENTZ ELECTRON

At the dawn of relativity, Abraham and Lorentz introduced a model of an extended charged particle coupled to its own electromagnetic field. It is this semi-relativistic, pre-quantum model which lead to our first ideas of mass renormalization through the works of Kramers, Dirac and others, and which in a modern version are implemented in QED. Only recently, however, was the first rigorous study of the semi-relativistic AL-model conducted (Spohn, Kunze, Komerk), which has finally clarified a number of troubling questions. The extension of the old AL-model into a fully relativistic theory was achieved most recently only (M.K and W.A), and first rigorous results include the following:

- The Cauchy problem for a purely spinning particle coupled to its radiation field has a unique global solution provided the bare inertia does not vanish.
- With vanishing bare inertia the structure of the Cauchy problem is lost - a fact that has been overlooked since Abraham-Lorentz's original papers.
- A spin (initially not in a stationary state) with fixed axis (achievable through symmetric initial conditions) and strictly positive bare inertia exponentially fast approaches a stationary state with finite magnetic moment, giving a fraction of its initial angular momentum in the radiation field.

Future work will address the question of global well-posedness of the full dynamics as Cauchy problem and the status of Lorentz-Dirac and Barjunan-Michel-Telejoli equations as regards their relation to the relativistic AL theory.

M. Kiessling (Rutgers Univ. New Brunswick, NJ): Joint work with W. Appel (ENS-Lyon).

21. **A. Arai:** SPECTRAL ANALYSIS FOR A QUANTUM SYSTEM OF A DIRAC PARTICLE COUPLED TO THE QUANTIZED RADIATION FIELD

We consider a quantum system of a Dirac particle minimally coupled to the quantized radiation field and study mathematical properties of the Hamiltonian of the system.

The Hilbert space of the quantum system is $\mathcal{H} = [\oplus^4 L^2(\mathbb{R}^3)] \otimes \mathcal{H}_{rad}$, where $\mathcal{H}_{rad} = \oplus_{n=0}^{\infty} \otimes_s^n (L^2(\mathbb{R}^3) \oplus L^2(\mathbb{R}^3))$, the boson Fock space over $(L^2(\mathbb{R}^3) \oplus L^2(\mathbb{R}^3))$ (one-photon space). The total Hamiltonian of the system is defined by

$$H(V) = H_D(V) \otimes I + I \otimes d\Gamma(\omega) - q \sum_{j=1}^{3} \alpha_j A_j^{\nu}(x),$$

where $H_D(V) = \alpha \cdot (-i\nabla) + m\beta + V$ is the one-particle Dirac operator with V a 4×4 Hermitian matrix valued function on $\mathbb{R}^3$, $d\Gamma(\omega)$ is the second quantization of the one-photon energy function $\omega : \mathbb{R}^3 \to [0, \infty)$, q is the charge of the Dirac particle, $A_j^{\nu}(x)$ is the quantized radiation field with momentum cutoff $\nu : \mathbb{R}^3 \to \mathbb{R}^3$.

We report on some results about the following aspects:

- Self-adjointness of $H(V)$.
- Spectral analysis in the case $V = 0$: In this case we have

$$UHU^{-1} = \int_{\mathbb{R}_p^3}^{\oplus} H(p)\, dp \quad (H = H(0)),$$

  with $H(p) = \alpha \cdot p + m\beta + d\Gamma(\omega) - \sum_{j=1}^3 \alpha_j d\Gamma(k_j) - q \sum_{j=1}^3 \alpha_j A_j^{\nu}(0)$.

A. Arai (Hokkaido University, Sapporo, Japan).

22. **R. Benguria:** Stability of positive diatomic molecules

Considering the nonrelativistic Schrödinger operator for homonuclear diatomic molecular ions within the Born-Oppenheimer approximation, we study the stability problem for increasing ratio Z/N of nuclear charge Z to number N of electrons. In particular, we derive improved bounds on the critical parameters that imply instability. That is, parameters that lead to dissociation of the molecular system into atomic fragments. The principal qualitative advantage of our estimates is the inclusion of electronic correlation; i.e., taking into account the effect of electron-electron repulsion on the molecular bond. Comparing our rigorous results with empirical of computed data, we formulate a conjecture that should quantify the actual stability behaviour of realistic molecular species.

R. Benguria (P.U. Católica de Chile): Joint work with H. Alancõn, P. Duclos and H. Hograve.

23. **S. Wugalter:** Atoms in a homogeneous magnetic field

Let

$$H = M_0^{-1}(i\nabla_0 + A_0)^2 + \sum_{j=1}^{N}(i\nabla_j + A_j)^2 - \sum_{j=1}^{N} N|r_j - r_0|^{-1} + \sum_{s,t,s<t} |r_s - r_t|^{-1},$$

$r_j = (x_j, y_j, z_j)$, $A_0 = \frac{B}{2}(-Ny_0, Nx_0, 0)$, $A_j = \frac{B}{2}(y_j, -x_j, 0)$, be the Schrödinger operator of an N electron atom in a homogeneous magnetic field. Let $P = (P_x, P_y, P_z) = \sum_{j=0}^{N}(i\nabla_j + A_j)$, be the operator of pseudomomentum.

By H_ν denote the operator H reduced to the states with fixed values of pseudomomentum $\nu = (\nu_1, \nu_2, \nu_3)$.

Theorem 23.1. *For all $\nu = (\nu_1, \nu_2, \nu_3)$ we have $\sigma_{disc}(H_\nu) \neq \emptyset$. Moreover, let $N(\lambda)$ be the number of eigenvalues of the operator H_ν, which are less than $(\mu - \lambda)$; $\mu = \inf \sigma_{ess}(H_\nu)$. Then $N(\lambda)\lambda^{1/2} \to const$ as $\lambda \to +0$.*

S. Wugalter.

24. **K. Yajima:** L^p-boundedness of wave operators

Let $H = -\Delta + V$ and $H_0 = -\Delta$ on $L^2(\mathbb{R}^d)$. If V is short range the wave operator $W_\pm = s - \lim_{t\to\pm\infty} e^{itH}e^{-itH_0}$ exist and are complete, i.e. $W_\pm$ is a partial isometry from $L^2(\mathbb{R}^d)$ to $L^2_{ac}(H)$, the absolutely continuous subspace for H.

We prove that wave operators $W_\pm$ are bounded in $L^p(\mathbb{R}^d)$ for all $1 \le p \le \infty$ for $d \ge 3$ and for $1 < p < \infty$ for $d \ge 1, 2$ under suitable decay at infinity conditions on $V(x)$ and the additional spectral condition on H, viz: 0 is not an eigenvalue or a resonance of H. Because $W_\pm$ intertwine H_0 and H_{ac}, the absolutely continuous part of H; viz $f(H)P_{ac} = W_\pm f(H_0)W_\pm^*$, this result reduces $L^p - L^p$ estimates for $f(H)P_{ac}$ to that of $f(H_0)$. In this way, we can extend, e.g. the previously known results $\|e^{-itH}P_{ac}\|_{L^p\to L^{p'}} \le ct^{2p(\frac{1}{2}-\frac{1}{p'})}$ to lower dimensions. The result for the case $d = 1$ is also proven by R. Weder, and is a joint work with Galthayer.

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