

Report No. 36/2001

## Relativistic Quantum Systems and Quantum Electrodynamics

August 12th - August 18th, 2001

The conference was organized by VOLKER BACH (MAINZ), HEINZ SIEDENTOP (MUNICH), and JAN-PHILIP SOLOVEJ (COPENHAGEN). Forty-four mathematicians and physicists from universities and research institutes in Austria, Canada, Chile, Denmark, France, Germany, Great Britain, Italy, Japan, Poland, Sweden, Switzerland, and the USA participated in the conference. Twenty-two participants presented their recent results obtained in the mathematical study of (relativistic) quantum systems and quantum electrodynamics. The topics discussed include scattering theory, stability of matter, quantum statistical mechanics, among other things. Another highlight of the scientific part of the program was a book and software presentation.

Special thanks go to the MFO staff for their hospitality, efficiency in organizing the meeting and running the institute.

*Edited by Oliver Matte*

# Abstracts

## A Remark on $L^1$ -Asymptotic Abelianness for a Spin-Fermion System

ZIED AMMARI

(joint work with C. Gérard)

We consider a spin system interacting with a Fermion system. The free and perturbed dynamics is given by a one-parameter group  $\tau_t^0, \tau_t^P$  of automorphisms on a  $C^*$ -algebra  $\mathcal{U}$  of observables of the coupled system.  $P$  is the perturbation and it is a bounded even operator in  $\mathcal{U}$ . In this framework we explore the validity of certain dynamical and statistical properties of the model. We prove the asymptotic completeness for the Hamiltonian of the system in the Fock space representation. We show the non-existence of the Møller morphisms (i.e.,  $\lim_{t \rightarrow \pm\infty} \tau_t^P \circ \tau_{-t}^0$  in  $\mathcal{U}$ ). In particular, the property of  $L^1$ -asymptotic abelianness, i.e.,

$$\int_{-\infty}^{\infty} \|[A, \tau_t^0(B)]\| dt < \infty, \quad \text{for all } A, B \in \mathcal{U},$$

does not hold.

## Nonlinear Equations with Critical Sobolev Exponent

RAFAEL BENGURIA

(joint work with C. Bandle, J. Dolbeault and M. J. Esteban)

We consider the Brézis-Nirenberg problem on a geodesic ball on  $S^3$ :  $-\Delta u = u^5 + \lambda u$  on  $D \subset S^3$ ,  $u = 0$  on  $\partial D$ . Here  $D$  is a geodesic ball contained in  $S^3$  of geodesic radius  $\theta_1$ . We determine the range of values of  $\lambda$  and  $\theta_1$  for which this equation has a non-trivial, positive, bounded solution. For  $\theta_1 > \frac{\pi}{2}$ , i.e. for geodesic balls that exceed the hemisphere of  $S^3$  there are two branches of positive solutions. This is in contrast with the situation of the Brézis-Nirenberg problem on  $\mathbb{R}^3$ . We also consider the Brézis-Nirenberg problem on a unit ball of  $\mathbb{R}^n$ ,  $n \geq 3$ , and classify all radial solutions for the equation  $-\Delta u = |u|^{p-1}u + \lambda u$  on  $B_1$ ,  $u = 0$  on  $\partial B_1$ , as a function of the exponent  $p$ .

## Return to Equilibrium for Pauli-Fierz Systems

JAN DEREZIŃSKI

(joint work with V. Jakšić)

I present recent work of V. Jakšić and myself based on the ideas of V. Jakšić and C. A. Pillet about Pauli-Fierz systems at temperature  $T \geq 0$ . Pauli-Fierz systems describe the interaction of a small quantum system with a bosonic field.  $W^*$ -algebraic formalism is used. Ergodic properties are studied by considering spectral properties of the corresponding Liouvillean. Using the assumption of the differentiability w.r.t. the generator of translations, return to equilibrium is proven under some relatively weak generic assumptions, uniformly in the temperature.

# Linear Boltzmann Equation as the Long Time Dynamics of an Electron Weakly Coupled to a Phonon Field

LASZLO ERDÖS

We consider the long time evolution of a quantum particle (electron) weakly interacting with a phonon field. We show that in the weak coupling limit the Wigner distribution of the electron density matrix converges to the solution of the linear Boltzmann equation globally in time. The collision kernel is identified as the sum of an emission and an absorption term that depend on the equilibrium distribution of the free phonon modes.

## On the Scattering Theory of Massless Nelson Models

CHRISTIAN GÉRARD

We consider the Nelson model describing an atom interacting with a quantized field of massless scalar bosons. We assume for simplicity that the atom is confined by a potential well. The Nelson Hamiltonian has the form:

$$H = -\Delta_{\mathbf{x}} + V + \int \omega a^* a + \sum_{j=1}^P \frac{1}{\sqrt{2}} \int (v_j(\mathbf{k}) e^{i\mathbf{k} \cdot \mathbf{x}_j} a^*(\mathbf{k}) + \bar{v}_j(\mathbf{k}) e^{-i\mathbf{k} \cdot \mathbf{x}_j} a(\mathbf{k})) dk,$$

where  $\mathbf{x} = (\mathbf{x}_1, \dots, \mathbf{x}_P) \in \mathbb{R}^{3P}$  are the electron positions,  $\omega(\mathbf{k}) = |\mathbf{k}|$ , and  $v(\mathbf{k})$  is a form-factor of compact support.  $H$  acts on the Hilbert space  $\mathcal{H} = L^2(\mathbb{R}^{3P}, d\mathbf{x}) \otimes \Gamma(L^2(\mathbb{R}^3, dk))$ . A typical assumption on  $v(\mathbf{k})$  is  $v(\mathbf{k}) = |\mathbf{k}|^\rho \chi(|\mathbf{k}|)$ ,  $\chi \in C_0^\infty(\mathbb{R})$ ,  $\rho > 0$ .

**Results:**

- We construct the asymptotic Weyl operators,

$$W^\pm(f) = s - \lim_{t \rightarrow \pm\infty} e^{itH} e^{i\phi(f_t)} e^{-itH},$$

where  $f \in h_0$ ,  $h_0 = \mathcal{D}(\omega^{-1/2})$ ,  $f_t = e^{-it\omega} f$ .

- We construct, for each  $0 < c < 1$ , non-trivial  $H$ -invariant spaces  $\mathcal{H}_c^\pm$  containing a finite number of particles in  $\{|\mathbf{x}| \geq ct\}$ .
- We show that the spaces  $\mathcal{H}_c^\pm$  are invariant under the asymptotic Weyl operators  $W^\pm(f)$ , and that the CCR representation is of Fock type on  $\mathcal{H}_c^\pm$ .
- We give a geometric description of the asymptotic vacua in  $\mathcal{H}_c^\pm$ , denoted by  $\mathcal{K}_c^\pm$ , which says that  $u \in \mathcal{K}_c^\pm \Leftrightarrow e^{-itH} u = \Gamma(f(\{\frac{|\mathbf{x}|}{t} \leq c + \varepsilon\})) e^{-itH} u + o(1) \forall \varepsilon > 0$ , where  $f$  is a smoothed characteristic function of the set indicated in its argument.
- Assuming that a Mourre estimate holds in an energy interval  $\Delta \subset \sigma(H)$ , we show using this description that  $\mathbf{1}_\Delta(H) \mathcal{K}_c^\pm = \mathbf{1}_\Delta(H) \mathcal{H}_{pp}(H)$ , for  $c < c_0$ , i.e. the asymptotic vacua in  $\mathcal{K}_c^\pm$  coincide with the bound states.

## A Generalization of the Electromagnetic Field Leading to Local Relativistic Quantum Field Theories with Indefinite Metric and Non-Trivial Scattering

HANNO GOTTSCHALK

(joint work with S. Albeverio and J.-L. Wu)

The free electromagnetic vector potential in the Euclidean space-time ( $d = 4$ ) can be obtained as the solution of the stochastic partial differential equation  $\partial A = \eta$ , where  $\eta$  is a suitable, vector-valued, covariant and stationary Gaussian noise field, and  $\partial$  is the quaternionic Cauchy-Riemann differential operator. Generalizing this equation to noise

fields with also Poisson component, one obtains new Euclidean models. The Schwinger functions (moments) can be calculated explicitly and can also be continued analytically to real, relativistic times (Wightman functions). All Wightman axioms are fulfilled with the exception of positivity. The Wightman functions can however be represented as vacuum expectation values of a quantum field theory with indefinite metric in the sense of Marchio and Stracchi. One can construct asymptotic fields and states such that the LSZ asymptotic condition is fulfilled. The S-matrix is calculated explicitly and found to be non-trivial. The theory only permits an asymptotic gauge yielding  $\mathcal{H}_{\text{phys}}^{\text{in}}$  and  $\mathcal{H}_{\text{phys}}^{\text{out}}$  with positive semi-definite inner product. Formally,  $\mathcal{H}_{\text{phys}}^{\text{in}}$  is mapped into  $\mathcal{H}_{\text{phys}}^{\text{out}}$  by the S-matrix, which thus exhibits gauge invariance.

### Quantum Pumps

GIAN MICHELE GRAF

(joint work with J. Avron, A. Elgart and L. Sadun)

Quantum pumps are time dependent scatterers operating between different reservoirs having common temperature and chemical potential. As a result of the operation charge and energy is transported between the reservoirs and noise and entropy are produced. These phenomena can be described in terms of the energy shift - a dual to Wigner's time delay - which is in turn determined by the (static) scattering matrix and its change. Optimal pump operations can be characterized either by the property of transporting a current with minimal dissipation or by the absence of noise or entropy production. In a geometric description, where the pump operation is represented as a path in a distinguished fibre bundle, optimality occurs if the path is along a fibre. In this case, the charge transported along a cycle is quantized.

### Asymptotic Completeness for Rayleigh Scattering

MARCEL GRIESEMER

(joint work with J. Fröhlich and B. Schlein)

It is expected that the state of an isolated atom or molecule, initially put into an excited state with energy *below* the ionization threshold, relaxes to a ground state by spontaneous emission of photons which propagate to spatial infinity. I explain how this picture is established for a large class of models of non-relativistic atoms and molecules coupled to quantized radiation field, but with the simplifying feature that an (arbitrary tiny, but positive) *infrared cutoff* is imposed on the interaction Hamiltonian. This result relies on a proof of asymptotic completeness for Rayleigh scattering of light on an atom. We establish asymptotic completeness for a class of model Hamiltonians with the features that the atomic Hamiltonian has point spectrum *coexisting* with absolutely continuous spectrum, and that either an infrared cutoff is imposed on the interaction Hamiltonian or the photons are treated as massive particles. We show that, for models of *massless* photons, the spectrum of the Hamiltonian strictly below the ionization threshold is *purely continuous*, except for the ground state energy.

# Stability of a Model of Relativistic Quantum Electrodynamics

ELLIOTT LIEB

(joint work with M. Loss)

We investigate the Hamiltonian for  $N$  electrons,  $H_N = \sum_{i=1}^N D_i + \alpha V_C + H_f$ , where  $D_i(\mathbf{A}) = \boldsymbol{\alpha} \cdot \mathbf{p}_i + \boldsymbol{\alpha} \cdot \mathbf{A}(\mathbf{x}_i) + m\beta$  is the Dirac operator,  $\alpha \approx 1/137$ ,  $V_C$  is the Coulomb potential for  $N$  electrons and  $K$  nuclei of charge  $Z$ ,  $H_f$  is the field energy for the quantized electromagnetic field,  $H_f = \sum_{\lambda=1}^2 \int |\mathbf{k}| a_{\mathbf{k},\lambda}^\dagger a_{\mathbf{k},\lambda} dk$ , and  $\mathbf{A}(\mathbf{x})$  is the ultraviolet cutoff vector potential,

$$\mathbf{A}(\mathbf{x}) = \sum_{\lambda=1}^2 \int_{|\mathbf{k}| < \Lambda} \frac{1}{\sqrt{|\mathbf{k}|}} \boldsymbol{\varepsilon}_{\mathbf{k},\lambda} \left( a_{\mathbf{k},\lambda} e^{i\mathbf{k} \cdot \mathbf{x}} + a_{\mathbf{k},\lambda}^\dagger e^{-i\mathbf{k} \cdot \mathbf{x}} \right) dk .$$

We show that this model is stable of the second kind,  $H_N \geq \text{const} (N + K)$ , when  $Z \leq 42$ , when restricted to functions that lie in the positive spectral subspace of the Dirac operator  $D_i(\mathbf{A})$ , for all  $i$ , and *not*  $D_i(0)$  (which is unstable).

## Ground States in Non-Relativistic QED

MICHAEL LOSS

(joint work with M. Griesemer and E. Lieb)

We consider a model of charged particles interacting with the ultraviolet cutoff radiation field and an external potential (due, e.g. to the nuclei fixed in space). The parameters of the model are the finestructure constant  $\alpha$ , the gyromagnetic factor  $g$  and the ultraviolet cutoff  $\Lambda$ . We show that for any choice of these parameters a ground state exists in this model. The main ingredients are a binding condition and a new infrared bound.

## Existence of Ground States for the Brown-Ravenhall Model Coupled to the Quantized Electromagnetic Field

OLIVER MATTE

(joint work with V. Bach)

In their mathematical study of the standard model of non-relativistic QED, Bach, Fröhlich and Sigal proved the existence of a ground state of the corresponding Hamiltonian. In this talk, we present an extension of this result to a semi-relativistic setting, the so called Brown-Ravenhall model coupled to the quantized radiation field. Our Hamiltonian has the form

$$H = \Lambda_+ \otimes \mathbf{1} [ D_0 - V + d\Gamma(|\mathbf{k}|) + gW ] \Lambda_+ \otimes \mathbf{1} , \quad \Lambda_+ = \mathbf{1}_{[0,\infty)}(D_0) .$$

Here,  $D_0$  denotes the free one-particle Dirac operator,  $V$  is the potential of a static nucleus, and  $g$  is a coupling parameter for the interaction  $W$ . The main new problem is posed by the non-locality of  $\Lambda_+$  in the derivation of exponential localization of spectral subspaces corresponding to the bottom of  $\sigma(H)$ , which is required to prove the existence of a ground state of  $H$ . We show how to overcome this problem by using an explicit integral kernel representation of  $\Lambda_+$ . We obtain our results for small values of  $g$ , employing an ultraviolet cutoff and a mild infrared regularization in the interaction.

## Positive Commutators and Return to Equilibrium

MARCO MERKLI

We show that a system of an atom coupled to the quantized electromagnetic field exhibits the property of return to equilibrium. This property says that if the system is slightly perturbed from its equilibrium state, then it converges back to it as time goes to infinity (asymptotic stability). We tackle the problem by developing the method of positive commutators in the framework of non-equilibrium quantum statistical mechanics.

## General Properties of Non-Equilibrium Steady States in QSM

CLAUDE-ALAIN PILLET

(joint work with V. Jakšić)

The framework of  $C^*$ -dynamical systems has been extremely successful in our understanding of the structure of equilibrium states in quantum statistical mechanics. In my talk I will report on the results of recent works with V. Jakšić on non-equilibrium steady states of  $C^*$ -dynamical systems. Some basic properties of NESS, including entropy production will be discussed. I will also explain how one can hope to obtain a spectral characterization of NESS, and present the results of a study of a simple model where this characterization can actually be proved rigorously: a quantum spin coupled to two fermionic fields at equilibrium at different temperatures.

## One-Particle (Improper) States in Nelson's Massless Model

ALESSANDRO PIZZO

In the one-particle sector of Nelson's massless model, with an ultraviolet cutoff and no infrared regularization, one-particle states are constructed. They are obtained by iterating the analytic perturbation of isolated eigenvalues.

## Migdal's World

MANFRED SALMHOFER

In this talk I discuss several versions of Migdal's theorem, which at present has the status of a conjecture, about vertex corrections in the electron-phonon system. This quantum field theory is the standard model for the description of ordinary superconductors. The model with acoustic phonons contains a small parameter, the velocity of sound,

$$c \sim \sqrt{\frac{\text{electron mass}}{\text{ion mass}}}.$$

Migdal's theorem states that the vertex function  $\Gamma(p, q)$ , which describes the irreducible interaction of an electron with momentum  $p$  and a phonon with momentum  $q$ , satisfies

$$|\Gamma(p, q) - g| \leq \text{const } c,$$

even if the bare coupling constant  $g$  is not small. This smallness of the vertex correction is the basis of the Migdal-Eliashberg theory of superconductors. I discuss the reasons why this is expected to hold and sketch a proof of a weaker bound, by  $\text{const } c^{1-\varepsilon}$ , for any  $\varepsilon > 0$ , to all orders in an expansion in  $g$ .

# General Decomposition of Radial Functions on $\mathbb{R}^n$ and Infrared Conditions for Positive Definiteness

ROBERT SEIRINGER

(joint work with Ch. Hainzl)

We present a generalization of the Fefferman-de la Llave decomposition of the Coulomb potential to quite arbitrary radial functions  $V$  on  $\mathbb{R}^n$  going to zero at infinity. That is, we show that

$$V(x - y) = \int_{\mathbb{R}^n} dz \int_0^\infty dr g(r) \chi_{\lambda,z}(x) \chi_{\lambda,z}(y),$$

where  $\chi_{\lambda,z}$  is the characteristic function of a ball of radius  $\lambda$  centered at  $z$ , and  $g(r)$  is some weight function related to the  $[\frac{n}{2}] + 2$ 'nd derivative of  $V$ . As a byproduct, we see from this decomposition that  $V$  is positive definite if the corresponding  $g(r)$  is positive, yielding conditions on  $V$  which are less restrictive than the ones obtained before by Askey.

## The Ionization Conjecture in Hartree-Fock Theory

JAN-PHILIP SOLOVEJ

The ionization conjecture for atoms states that the maximal ionization, the radius, and ionization energy are bounded independently of the nuclear charge of the atom. There are several mathematical models of atoms in which this conjecture can be formulated as a purely mathematical statement. In this talk we discuss the Thomas-Fermi model, the Hartree-Fock model, and the full quantum mechanical Schrödinger model. The ionization conjecture is known in the Thomas-Fermi model mainly due to the work of Lieb and Simon. Using the result in the Thomas-Fermi model we sketch how to prove the conjecture in the much more complicated Hartree-Fock model. We also explain why the presented method does not work in the full many body quantum mechanical theory.

## Magnetic Moment of the Electron on the Basis of the Pauli-Fierz Model

HERBERT SPOHN

(joint work with S. Teufel)

In non-relativistic quantum electrodynamics one considers a single electron with spin minimally coupled to the quantized photon field in the Coulomb gauge. We are interested in the effective motion of the electron subject to slowly varying external potentials. This is the space-adiabatic problem of non-relativistic QED. Of particular interest is the spin precession and possibly higher corrections for the back coupling to the orbit. Our problem can be rephrased as an adiabatic limit for operator-valued symbols. As described in the talk by S. Teufel we have developed a general scheme under which subspaces can be adiabatically decoupled and effective Hamiltonians can be computed, in principle to any order. Applied to the Pauli-Fierz model one has to check that the ground state band is separated by a gap and two-fold degenerate, see F. Hiroshima, for the principal symbol. There is also a subleading symbol which together with the first order correction determines the spin motion. As a result we obtain a non-perturbative definition of the  $g$ -factor of the electron within the Pauli-Fierz model.

# The Ground State Energy of Relativistic One-Electron Atoms According to Jansen and Heß

EDGARDO STOCKMEYER

(joint work with R. Brummelhuis and H. Siedentop)

Jansen and Heß - correcting an earlier paper of Douglas and Kroll - have derived a (pseudo)-relativistic energy expression which is very successful in describing heavy atoms. It is an approximate no-pair Hamiltonian in the Furry picture. We show that their energy in the one-particle Coulomb case, and thus the resulting self-adjoint Hamiltonian and its spectrum, is bounded from below for  $\alpha Z \leq 1.006$ .

## Adiabatic Decoupling and Effective Dynamics for the Dirac Equation

STEFAN TEUFEL

(joint work with H. Spohn)

We present a general scheme for constructing effective Hamiltonians on almost invariant subspaces, which are related to isolated parts of the spectrum of the principal operator-valued symbol of some Hamiltonian. The scheme is applied to the Dirac Hamiltonian with slowly varying external potentials, i.e. to  $H_D^\varepsilon = c \boldsymbol{\alpha} \cdot (-i\hbar \nabla_{\mathbf{x}} - \frac{e}{c} \mathbf{A}(\varepsilon \mathbf{x})) + mc^2 \beta + e V(\varepsilon \mathbf{x})$  on  $\mathcal{H} = L^2(\mathbb{R}^3; \mathbb{C}^4)$ , where  $\varepsilon$  is small. Following a construction of Nenciu and Sordani (2001) one can construct projectors  $\Pi_\pm^\varepsilon$  such that  $\Pi_+^\varepsilon + \Pi_-^\varepsilon = 1$  and  $\|[H_D^\varepsilon, \Pi_+^\varepsilon]\| + \|[H_D^\varepsilon, \Pi_-^\varepsilon]\| = \mathcal{O}(\varepsilon^0)$  in  $\mathcal{B}(\mathcal{H})$ . The subspaces  $\text{Ran } \Pi_\pm^\varepsilon$  have no simple characterization and thus a unitary  $U^\varepsilon$  is constructed, such that

$$U^{\varepsilon*} \Pi_\pm^\varepsilon U^\varepsilon = \Pi_\pm \quad \text{with} \quad \Pi_\pm = \begin{pmatrix} \mathbf{1}_{2 \times 2} & 0 \\ 0 & 0 \end{pmatrix}.$$

Hence  $U^{\varepsilon*} H_D^\varepsilon U^\varepsilon =: h^\varepsilon$  is almost block diagonal and an asymptotic expansion  $h^\varepsilon \asymp h_0 + \varepsilon h_1 + \dots$  can be computed explicitly. From  $h_0 + \varepsilon h_1$  we derive the BTM-equation in the limit  $\varepsilon \rightarrow 0$ .

## On the Discrete Spectrum of a Two-Body Pseudo-Relativistic Pair Operator

TIMO WEIDL

(joint work with S. Wugalter)

Let  $\sqrt{k_1^2 + m^2} + \sqrt{k_2^2 + m^2} - V(x_1 - x_2)$  be the pseudo-relativistic Hamiltonian for the motion of two interacting particles without external field. Separation of variables due to translation invariance yields a pair operator of the type  $\sqrt{(p+q)^2 + m^2} + \sqrt{(p-q)^2 + m^2} - V(y)$ , where  $q$  is the momentum and  $p$  acts as parameter. We show that the number of eigenvalues of this operator below the essential spectrum depends on  $p$ . We give CLR and Lieb-Thirring type bounds and calculate the spectral asymptotics as  $p \rightarrow \infty$ .



# Mathematical Analysis of the Photoelectric Effect

HERIBERT ZENK

(joint work with V. Bach and F. Klopp)

The talk reports on joint work with Volker Bach and Frédéric Klopp on a model of the photoelectric effect. We adapt the model of Bach, Fröhlich, Sigal of non-relativistic particles coupled to the quantized electromagnetic field and look at a single electron bound in a potential well of depth  $e_0 < 0$ . So the Hamiltonian is of the form  $H_g = H_0 + gW$ , where  $H_0$  describes the uncoupled electron-photon system and  $g$  is a small coupling parameter for the interaction  $W$ . We define transported charges, and for photon clouds added to the ground state  $\phi_{gs}$  of  $H_g$ , we give an asymptotic expansion of the time evolution, which neglects higher orders in  $g$ . Using this expression, we show that the first non-vanishing term of the transported charges is additive in the involved  $N$  photons. If the photon cloud is approaching the atom from large distance or if it is monochromatically, we prove that Einstein's prediction for the photoeffect is correct - qualitatively and quantitatively - to this leading order.

# Software Presentation

## Visual Quantum Mechanics

BERND THALLER

Visual Quantum Mechanics is a systematic effort to use computer generated animations in order to push the teaching in theoretical quantum mechanics to an even higher level. This goal is reached because the visualization makes complicated results more understandable and motivates the inclusion of topics that are often ignored or mystified. Another consequence of this approach is a shift in emphases towards the dynamics of quantum systems. The presented CD-ROM - a cover CD for a book about quantum mechanics - contains 320 QuickTime movies showing quantum mechanical wave packets. The movies are presented in a multimedia framework together with explanatory text (full documentation), graphics, and about 16000 lines of Mathematica code for own experiments. Complex-valued wave functions are visualized by a new method, using a color for the complex phase and lightness for the absolute value of the wave function. Some phenomena are shown for the first time. The CD includes special Mathematica packages for visualization and numerical solutions of the Schrödinger equation. Another part of the project is a platform-independent OpenGL-based software that is especially useful for the visualization of complex-valued functions in three dimensions. A large part of the presentation was devoted to relativistic systems. Movies showing negative-energy wave packets, Zitterbewegung, and transitions to positronic states (Klein's paradox) were shown for the first time.

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