Václav Janiš

Na Slovance 2 Praha, Czech Republic CZ-18221
Phone: +420 266052153 Fax: +420 286588605 E-Mail: janis@fzu.cz

Professional History and Future Research Plan

Research History

I started my research career of a condensed matter theorist in 1983 after finishing my PhD program on mathematical methods in quantum physics with the emphasis on the path-integral technique. Since then I have been following five principal areas of research:

I. *Development of many-body Green function and diagrammatic techniques*
II. *Transport properties of disordered electron systems and Anderson localization*
III. *Falicov-Kimball model and X-ray edge problem*
IV. *Strongly correlated electrons and Dynamical Mean-Field Theory*
V. *Mean-field theory of spin glasses and replica symmetry breaking*

My most significant contributions to these fields are summarized below.

I. Many-body Green functions and diagrammatic techniques

A way towards application of field-theoretical many-body and functional integral techniques in condensed matter problems can goes via Feynman diagrams in statistical mechanics and many-body problems. My first task in condensed matter was to understand the Coherent Potential Approximation (CPA) in describing the motion of an electron scattered on random lattice potential in terms of many-body Feynman diagrams. I succeeded to find a common functional-integral representation for the grand potential of disordered lattice electrons and free energy of classical spin (Heisenberg) models giving the CPA a more general meaning [1]. Further on, I was able to extend this functional-integral representation of CPA also to spin-glass and fully interacting quantum models [2]. This paper was later used as a possible understanding of the Dynamical Mean-Field Theory (DMFT) of correlated electrons. Most of my further methodological studies were connected with local approximations, the limit to high spatial dimensions. Important was an observation I made that the limit to high spatial dimensions (mean-field limit) is consistent only for the self-energy and one-particle functions. The two-particle functions cannot be consistently determined from one-particle ones via functional differentiation with only local perturbations [3]. This fact led me to shift the focus from one-particle to two-particle Green functions. I realized that the most appropriate way to treat two-particle vertices self-consistently is the parquet approach [4]. Soon after this I extended the parquet approach from interacting to disordered non-interacting electrons [5]. The parquet equations, being nonlinear integral equations, are not fully solvable. Simplifications thereof I introduced in specific physical situations are discussed below.

II. Transport properties of non-interacting disordered electrons and Anderson localization

The principal defect of the CPA and DMFT is that they, due to their local character, do not include backscatterings and quantum coherence in the electrical conductivity. One has to go beyond local approximations to assess these effects. I used the asymptotic limit to high spatial dimensions to assess the leading vertex corrections in the Kubo formula for the electrical conductivity [6]. The electrical conductivity, due to gauge invariance, can be calculated also from the density-density correlation function. We analyzed the impact of conservation laws and gauge invariance on the electrical conductivity and diffusion in disordered systems in [7]. We, however, soon discovered that the full conservation of probability expressed as a Ward identity is not compatible with causality of the self-energy within the standard diagrammatic approach in the thermodynamic limit [8,9]. The full, dynamical Ward identity leads to a non-integrable diffusion pole in the Anderson localization phase. I showed that only an integrable pole in the electron-hole vertex is admissible so that Bethe-Salpeter equations can be obeyed [10].

One of the most intriguing problems in condensed matter theory is the Anderson metal-insulator transition and vanishing of diffusion due to backscatterings of electrons (particles) on a random atomic potential. A number of approaches have been developed to treat the Anderson localization transition but no one had been able to make vanishing of diffusion compatible with the standard diagrammatic theory of disordered electrons and its mean-field solution, CPA. We were the first who noticed that the CPA fails to ensure electron-hole symmetry on the two-particle level and consequently Anderson localization cannot be reached. We used the two-particle self-consistency of the parquet approach to the nonlocal part of the electron-hole vertex and utilized a simplification in momentum convolutions induced by the limit to high spatial dimensions and derived a numerically solvable “mean-field approximation” for the Anderson localization transition and the localized phase [11,12]. Similarities and differences to the self-consistent diagrammatic construction based on the Ward identity of Vollhardt and Wölfle were presented recently in [13].

III. Falicov-Kimball model and X-ray edge problem

The simplest model of interacting electrons is the so-called Falicov-Kimball model (FKM), a simplification of the Hubbard model with localized one spin species. Its equilibrium mean-field solution is exactly known and is equivalent to the CPA, which I proved in Ref. [14]. A non-equilibrium situation with an abrupt switching on the particle interaction, relevant for the X-ray edge singularity in alkali metals, has, however, no longer a complete analytic solution [15]. A diagrammatic analysis of the spectral function of the localized electrons in equilibrium revealed a breakdown of perturbation theory at low frequencies [16]. A relation between this equilibrium Green function and the non-equilibrium dynamics of X-ray spectra was demonstrated in Ref. [17]. In particular, I was able to find dependence of the critical edge exponents of the relevant spectral functions of FKM on time scales when the system approaches a new equilibrium after switching the Coulomb interaction on. An extensive discussion of the quantum-mechanical non-equilibrium problem of the X-ray edge singularity by means of the Wiener-Hopf method was presented in Ref. [18].

IV. Strongly correlated electrons and Dynamical Mean-Field Theory

The fundamental model of interacting electrons is the Hubbard model with a local Coulomb interaction in the tight-binding description. A new wave of effort to find its comprehensive solution was revived by the introduction of the limit to infinite spatial dimensions, the solution of which is called Dynamical Mean-Field Theory. The grand potential of he Hubbard model within DMFT was already outlined via a functional-integral representation in Ref. [2] but fully exploited later in Refs. [14,19] as a generalization of the CPA from non-interacting disordered electrons. We soon also generalized the DMFT to disordered Hubbard model [20]. Using Monte-Carlo numerical simulations we obtained a first phase diagram of this model [21]. Apart from a few limiting situations [22], the Hubbard model in infinite dimensions is not analytically solvable, hence we used a variational approach and the solution of FKM in infinite dimensions to construct a generalization of the Hubbard III approximation [23,24]. This solution does not, however, lead to a Fermi liquid in the metallic state. We hence tried to improve weak-coupling approximations so that they would describe in a sense reliably intermediate and strong coupling [25,26]. From this reason we started to construct an impurity solver from an improved solution of the Single-Impurity Anderson model (SIAM). We succeeded in this by identifying the dominant contributions to the parquet equations in the vicinity of the pole in the electron-hole vertex. We were able to turn the nonlinear integral parquet equations into a semi-analytic self-consistent theory for two-particle vertices determined from simplified algebraic equations. We showed that a solution of these simplified parquet equations reproduces correctly the Kondo asymptotics as well, as the salient features of the satellite Hubbard bands in the spectral function of SIAM [27,28]. Very recently we succeeded to extend the concept of the simplification of the parquet equations also to a multiorbital Hubbard model [29].

V. Mean-field theory of spin glasses

Spin glass models are uncommon in the way ergodicity is broken there in the low-temperature phase. This ergodicity breaking, where it is impossible to circumvent the critical point by a distribution of the external magnetic field on individual lattice sites, is caused by a frustration in the spin exchange that makes it difficult to find the appropriate phase space of order parameters. I found that the spin-glass instability in the mean-field model can be generated by symmetry breaking magnetic fields only when real replicas of the spin system is introduced [30]. I returned to the spin-glass problem after some years when I noticed that real replicas can be used to test thermodynamic homogeneity and thereby disclosed that the latter is the physical principle being broken in the replica symmetric solution [31]. A simple conclusion followed, namely, one has to get rid of the dependence of the free energy on the number of real replicas to restore thermodynamic homogeneity. Our analysis proved that integer number of replicas, do not recover thermodynamic homogeneity [32]. Analytic continuation to a real (non-integer) replication number was to be done. We did it in the thermodynamic approach of Thouless, Anderson, and Palmer and showed that that the replica-symmetry breaking order parameters are to be introduced even without using the replica trick [33]. We used the real-replica method to construct solutions with hierarchies of spin replica generations and explicitly calculated their asymptotics below the transition to the glassy phase [34,35]. There had not been an explicit representation of the free energy with the full replica-symmetry breaking until I was able to find a representation via a time-ordering evolution operator for the free energy of the Parisi solution [36]. This representation opened new possibilities to study and understand low-temperature glassy phases in spin-glass models and their generalizations.

Recent and Present Research Activities with Future Plans

I am actively working and going to continue the research on four main topical problems in condensed matter theory:

- **A.** *Strongly correlated electrons and quantum phase transitions*
- **B.** *Charge diffusion and Anderson localization in disordered and interacting electron systems*
- **C.** *Mean-field theory of spin and other glass models with replica symmetry breaking*
- **D.** *Quantum dot attached to superconducting leads*

A. Strongly correlated electrons and quantum phase transitions

Low-temperature behavior of strongly correlated electrons is still a vivid topic, since there are a number of effects that have not yet been fully understood. In particular, non-Fermi liquid behavior and correlation-induced (quantum) criticality and phase transitions are among the most important ones. Little has been understood the way Fermi liquid may become unstable in the strong coupling regime. Even the Mott-Hubbard transition in DMFT has not yet been explained within a consistent analytic theory. Nonexistence of such a theory is generally related to the nonexistence of a description of quantum critical behavior that would match consistently emergence of the order parameter in terms of one-particle Green functions with the singularity in the response function, or equivalently a two-particle vertex.

My research in this field concentrates on the behavior of equations for the vertex functions in a Fermi liquid regime. First of all, a consistent approximation free of unphysical behavior and spurious poles must contain a two-particle self-consistency. It is introduced in the most straightforward way via a parquet construction with external perturbations that allow for quantum phase transitions, that is transitions to phases with anomalous order parameters [4]. The full set of the parquet equations ids not solvable analytically and does not provide a way to control quantum critical behavior. That is why we introduced a reduced asset of parquet equations and introduced a static effective-interaction approximation that allows for an analytic control of quantum criticality [37]. The major novelty and also asset of this approach is thermodynamic consistency of between the emergence of the order parameter in the one-particle self-energy and the two-particle singularity, not existing in the present approaches. We achieved it by a new form of the one-particle self-consistency via a linearized form of the Ward identity. This partially self-consistent approach opens new ways to reach affordable thermodynamically consistent approximations producing qualitatively the same quantum critical behavior in the spectral and thermodynamic functions. It seem to be the proper systematic way to introduce the necessary consistency between the pole in the response function and opening of the gap at the paramagnet-antiferromagnet and metal-superconductor transitions.

B. Charge diffusion and Anderson localization in disordered systems

Basic tool to investigate vanishing of charge diffusion in disordered electron systems is a diagrammatic expansion for the vertex functions determining the non-local corrections to the semi-classical Drude conductivity. There are, however, a number of problems to extract the relevant physical data from the perturbation expansion. The first problem is to guarantee non-negativity of the electrical conductivity calculated from the Kubo formula. We succeeded to reformulate the perturbation expansion in such a way that the negative vertex corrections do not turn the overall sign of the conductivity negative [38,39]. It is a first step towards a more comprehensive approach including a two-particle self-consistency via e. g. the parquet equations.

There is a more severe problem when trying to introduce self-consistent approximations beyond the local mean-field theory. One has to obey the Ward identity matching the one-electron self-energy with the two-particle vertex so that to guarantee macroscopic conservation laws. As we showed earlier, it is not possible in approximate treatments [9,10]. We made a fundamental step in resolving incompatibility of the microscopic perturbation theory and the macroscopic conservation laws. We found that the vertex functions derived from the microscopic perturbation theory must be corrected in the subspace where their values are determined by the global Ward identity [40]. We thereby made perturbation theories compatible with the conservation laws and opened a new way to study charge diffusion and Anderson localization without breaking underlying physical principles. The next is to see the impact of the introduced corrections to the vertex functions on the two-particle self-consistency in the parquet equations.

C. Mean-field theory of spin and other glass models

The explicit representation of the free energy of spin-glass models with full continuous replica symmetry breaking from Ref. [36], due to its generality, offers a new way of investigating spin and other glass and frustrated systems. We recently demonstrated that, against expectations, there is a solution with continuous replica-symmetry breaking in the Potts glass where the one-step replica symmetry breaking was considered to be stable [41,42]. Similarly one can use this representation and find a low-temperature solution for e. g. p-spin or quadrupolar glasses. Major prospect of the free energy functional from [36], however, lies in a possibility to rescale the variables in such a way that one can derive an explicit free energy down to zero temperature. It is hence possible to study the low-temperature behavior of these glassy models, disclose the reason why entropy turns negative in incomplete solutions and which conditions are to be fulfilled so that entropy stays non-negative. We are now developing a perturbation scheme in which the deviation of the continuous order-parameter function from a constant (one-step replica-symmetry breaking) serves as a small expansion parameter. At least first order perturbation is fully numerically manageable for most of the models of interest [43]. The problem to be resolved remains to find an approximate scheme converging to the full Parisi solution and does not lead to negative entropy in the low-temperature limit. A prospective way seems to be the real-replica approach we developed earlier that enables to treat simultaneously quenched and annealed types of disorder and track the origin of negativity of entropy in approximate solutions [44].

C. Quantum dot attached to superconducting leads

Quantum dot, experimentally realized via a carbon nanowire and modeled by Anderson impurity, attached to superconducting leads displays nontrivial quantum critical behavior. Interplay between the

Kondo effect and pairing mechanism of superconductivity leads to a so-called 0-π transition from a spin singlet (0) to a spin doublet (π) ground state of the impurity. Full microscopic understanding of this quantum phase transition, manifested by a change of sign of the Josephson current through the dot, is still missing.

We introduced a reduced set of parquet equations for systems with anomalous propagators due to the existence of superconducting condensates [45]. Parquet equations with anomalous propagators, in their simplified form, can be helpful in this problem but also in better understanding the weak-to-strong coupling superconducting transition (BCS superconductor to BEC of bound pairs) in extended systems with the attractive electron coupling. The two-particle self-consistency of the parquet equations is not, however, necessary In the weak-coupling regime. We applied a modified second-order perturbation theory to determine the phase boundary of the spin-singlet phase [46,47]. Our solution in the weak-coupling regime with no Kondo behavior showed unprecedented accuracy compared to the more demanding numerically exact solution. Moreover, we were able to predict the existence of the critical boundary of the spin-singlet phase at zero temperature non-perturbatively [48]. The real boundary of between the phases of the superconducting dot must be confirmed by a stability analysis. It can be done only if a spin-resolved state is assumed and the perturbation theory, including the parquet equations, is extended to models with an applied external magnetic field. The work in this direction is in progress.

References

[1] V. Janiš, *Renormalized expansions for functional integrals: Generalized coherent-potential approximation*, Czech. J. Phys. B 36 (1986) 1 107-29.

[2] V. Janiš, *Free-energy functional in the generalized coherent-potential approximation*, Phys. Rev. B 40 (1989) 11 331-4.

[3] V. Janiš, *Asymptotic limit of high spatial dimensions and thermodynamic consistence of mean-field theories*, Phys. Rev. Lett. 83 (1999) 2781-4.

[4] V. Janiš, *Stability of self-consistent solutions for the Hubbard model at intermediate and strong coupling*, Phys. Rev. B 60 (1999) 11345-60.

[5] V. Janiš, *Parquet approach to nonlocal vertex functions and electrical conductivity of disordered electrons*, Phys. Rev. B 64 115115 (2001) 1-16.

[6] V. Janiš and D. Vollhardt, *Conductivity of disordered electrons: mean-field approximation containing vertex corrections*, Phys. Rev. B 63 125112 (2001) 1-7.

[7] V. Janiš, J. Kolorenč, and V. Špička, *Density and current response functions in strongly correlated electron systems: diffusion, electrical conductivity and Einstein relation*, Eur. Phys. J. B 35 (2003) 77-91.

[8] V. Janiš and J. Kolorenč, *Conservation laws in disordered electron systems: Thermodynamic limit and configurational averaging*, Phys. stat. sol. (b) 241 (2004) 2032-42.

[9] V. Janiš and J. Kolorenč, *Causality versus Ward identity in disordered electron systems*, Mod. Phys. Lett. B 18 (2004) 1051-8.

[10] V.Janiš, *Integrability of the diffusion pole in the diagrammatic description of noninteracting electrons in a random potential*, J. Phys.: Condens. Matter 21, 485501 (2009) 1-8.

[11] V. Janiš and J. Kolorenč, *Mean-field theory of Anderson localization: Asymptotic solution in high spatial dimensions*, Phys. Rev. B 71, 033103 (2005) 1-4.

[12] V. Janiš and J. Kolorenč, *Mean-field theories for disordered electrons: Diffusion pole and Anderson localization*, Phys. Rev. B 71, 245106 (2005) 1 -11.

[13] V. Janiš and V. Pokorný, *Renormalized perturbation theories of Anderson localization: Self-consistent two-particle vertices*, Ann. Phys. (Berlin) 523 (2011) 715-23.

[14] V. Janiš, *A new construction of thermodynamic mean-field theories of itinerant fermions: Application to the Falicov-Kimball model*, Z. Physik B 83 (1991) 227-35.

[15] V. Janiš, *A lattice model for x-ray emission and absorption of metals: the edge singularity*, J. Phys.: Condens. Matter 5 (1993) L425-32.

[16] V. Janiš, *Green's function of the core electrons in a lattice model for x-ray spectra: Breakdown of perturbation theory in the long-time limit*, Phys. Rev. B 49 (1994) 1612-26.

[17] V. Janiš, *Theory of soft x-ray spectra: Nonequilibrium dynamics of many electrons*, Acta Physica Slovaca 44 (1994) 391-402.

[18] V. Janiš, *Wiener-Hopf method applied to the x-ray edge problem*, Int. J. Mod. Phys. B 11 (1997) 3 433-53.

[19] V. Janiš and D. Vollhardt, *Comprehensive mean-field theory for the Hubbard model*, Int. J. Mod. Phys. B 6 (1992) 731-747.

[20] V. Janiš and D. Vollhardt, *Coupling of quantum degrees of freedom in strongly interacting, disordered electron systems*, Phys. Rev. B 46 (1992) 15 712-15.
[21] M. Ulmke, V. Janiš, and D. Vollhardt, *Anderson-Hubbard model in d = 0*, Phys. Rev. B 51 (1995) 10 411-26.
[22] P. G. J. van Dongen and V. Janiš, *Mott transition near the ferromagnetic state*, Phys. Rev. Lett. 72 (1994) 3 258-61, Phys. Rev. Lett. 73 (1994) 912.
[23] V. Janiš and D. Vollhardt, *Construction of analytically tractable mean-field theories for quantum models. I General formalism with application to the Hubbard model at strong coupling*, Z. Physik B 91 (1993) 317-23.
[24] V. Janiš, J. Mšek, and D. Vollhardt, *Construction of analytically tractable mean-field theories for quantum models. II Susceptibilities and energy bounds on the Hubbard model*, Z. Physik B 91 (1993) 325-36.
[25] V. Janiš and J. Schlipf, *Linked-cluster expansion around mean-field theories of interacting electrons*, Phys. Rev. B 52 (1995) 17 119-34.
[26] V. Janiš, *Hubbard model at intermediate coupling: Renormalization of interaction strength*, J. Phys: Condens. Matter 10 (1998) 2 915-32.
[27] V. Janiš and P. Augustinský, *Analytic impurity solver with Kondo strong-coupling asymptotics*, Phys. Rev. B 75, 165108 (2007) 1-7.
[28] V. Janiš and P. Augustinský, *Kondo behavior in the asymmetric Anderson model: Analytic approach*, Phys. Rev. B 77, 085106 (2008) 1-11.
[29] P. Augustinský and V. Janiš, *Multiorbital simplified parquet equations for strongly correlated electrons*, Phys. Rev. B 83, 035114 (2011)1 -13.
[30] V. Janiš, *On the mean-field spin-glass instability at finite fields*, J. Phys. A: Math. Gen. 20 (1987) L1017-22.
[31] V. Janiš, *Stability of solutions of the Sherrington-Kirkpatrick model with respect to uniform scalings of extensive variables*, Phys. Rev. B 71, 214403 (2005) 1 -9.
[32] V. Janiš and L. Zdeborová, *Thermodynamic origin of order parameters in mean-field models of spin glasses*, Phys. Stat. Sol. 243 (2006) 716-31.
[33] V. Janiš, *Incompleteness of the Thouless, Anderson, and Palmer mean-field description of the spin-glass phase*, Phys. Rev. B 74, 054207 (2006) 1-12.
[34] V. Janiš and A. Klíč, *Hierarchical solutions of the Sherrington-Kirkpatrick model: Exact asymptotic behavior near the critical point*, Phys. Rev. B 74, 054410 (2006) 1-9.
[35] V. Janiš, A. Klíč, and M. Ringel, *Replica-symmetry breaking: discrete and continuous schemes in the Sherrington-Kirkpatrick model*, J. Phys. A: Math. Theor. 41, 324004 (2008) 1 -14.
[36] V. Janiš, *Free-energy functional for the Sherrington-Kirkpatrick model: The Parisi formula completed*, Phys. Rev. B 77, 104417 (2008) 1 -5.
[37] V. Janiš, A. Kauch, and V. Pokorný, *Thermodynamically consistent description of quantum criticality of correlated electrons*, E-print arXiv:1604.01678v2, submitted for publication.
[38] V. Janiš and V. Pokorný, *Vertex corrections to the electrical conductivity in models with elastically scattered electrons*, Phys. Rev. B 81, 165103 (2010) 1-9.
[39] V. Pokorný and V. Janiš, *Vertex corrections to the mean-field electrical conductivity in disordered electron systems,* J. Phys.: Condens. Matter 25, 175502 (2013).
[40] V. Janiš and J. Kolorenč, *Conserving approximations for response functions of the Fermi gas in a random potential*, Eur. J. Phys. B 89, 170 (2016)1- 12.
[41] V. Janiš and A. Klíč, *Equilibrium state of the mean-field Potts glass*, J. Phys.: Condens. Matter 23, 022204 (2011) 1 -5.
[42] V. Janiš and A. Klíč, *Mean-field solution of the Potts glass near the transition temperature to the ordered phase*, Phys. Rev. B 84, 064446 (2011) 1-10.
[43] V. Janiš, A. Kauch, and A. Klíč, *Free energy of mean-field spin-glass models: Evolution operator and perturbation expansion*, Phys. Rev. B 84, 054201 (2013)1-11.
[44] V. Janiš, A. Kauch, and A. Klíč, *Ergodicity breaking in frustrated disordered systems: Replicas in mean-field spin-glass models*, Phase Transitions 98, 4711 (2015)1-19.
[45] V. Janiš and V. Pokorný, *Vertices for correlated electron systems with anomalous propagators*, Science Letters 3:66 (2014)1-10.
[46] M. Žonda, V. Pokorný, V. Janiš, and T. Novotný, *Perturbation theory of a superconducting 0-π impurity quantum phase transition,* Scientific Reports 5, 8821 (2015)1-6.
[47] M. Žonda, V. Pokorný, V. Janiš, and T. Novotný, *Perturbation theory for an Anderson quantum dot asymmetrically attached to two superconducting leads*, Phys. Rev. B 93, 024523 (2016)1-18.
[48] V. Janiš, V. Pokorný, and M. Žonda, *Spin-symmetric solution of an interacting quantum dot attached to superconducting leads: Andreev states and 0-π transition,* Eur. Phys. J. B 89, 197 (2016)1-12.