I. General Themes:

Many-Body Physics in Condensed-Matter Systems oriented towards a deeper understanding of electronic structure, optical, magnetic, etc. excitations. Interplay of electronic correlations and superconductivity.

Topological Superconductivity as a new quantum-state of matter.

II. Scientific Developments:

1. **Thesis:** Techn. Univ. Munich 1970 – 72 (Electron-Phonon Interaction in Transition Metals), Refs [5, 6]
2. **Postdoc:** UCSD 1972 – 74 with L. J. Sham and W. Kohn, University of California (San Diego)
   - Formulation of optical excitations taking local-field effects into account. In the, at that time, exclusively used "Jellium Model" of optical (or, more generally electro-magnetic) excitations, these effects were neglected and, thus, peaks in the experimental optical absorption directly identified with peaks in the interband density of states (DOS). In a series of papers with L. J. Sham (University of California, San Diego), we showed that the local field contains not just the induced field with the wavelength of the applied (q → 0, long wavelength) field, but in addition rapidly oscillating components due to the local, short-range interactions of the excited electron-hole pairs. The latter can be viewed as being due to the Bragg reflections of the electro-magnetic field from the lattice sites. This induces sizeable shifts (~eV in semiconductors and insulators, Ref. [7, 10, 34]) between the DOS peaks from interband transitions and the experimental spectra. This finding has, e.g. important consequences for (and invalidates) the still much-used determination of optical absorption in this interband picture.
   - Technically, this achievement was made possible by the solution of the Bethe-Salpeter equation in real space (overlap of Wannier Functions → matrix inversion), a technique, which is nowadays much used in extracting charge-, spin- and pairing-susceptibilities (Ref [34]) .

3. **Associate Professor:** Max-Planck Institute Stuttgart 1975 – 1984
   - Motivated by these postdoc studies, I formulated a more general theory of the Microscopic Electrodynamics in Solids beyond the Jellium Model. This allows for a description of elementary excitations including local-field and leading many-body corrections such as excitonic effects [24]→ Influence e.g. on charge and magnetic excitations in solids with more or less localized electrons (Adv. in Physics, Review, Ref [22]) such as insulators, semiconductors and transition metals.
   - We formulated and carried out the first "GW"-calculations of quasi-particle properties in semiconductors and insulators in a series of PRL and PRB papers from 1980 – 1982 [e.g. 32, 44]. The theory took into account many-body effects (local-field, excitonic) in the screening W of a quasiparticle described by a propagator G. In the meantime, these effects have also been established- using e.g. extensions of density-functional theory (time-dependent DFT) – by different techniques to have a sizeable influence.
   - With W. Kohn (Ref. [13] and [28]), I worked on non-local corrections to the exchange and correlation energy of an inhomogeneous Electron Gas. The results played later an important

role for our studies of non-local effects within DFT, induced e.g. by the image tail of a surface barrier [124, 127].

- With M. J. Kelly (Oxford, England), I suggested a purely electronic mechanism of superconductivity (SC) in interface (MOSFET) systems, based on the existence of quasi-two dimensional charge (plasmon) excitations [33, 38]. New interface systems, e.g. fabricated by J. Mannhards group at the MPI Stuttgart (Germany) displaying the field-effect transistor (FET) effect as well as superconductivity, are nowadays investigated along similar lines.
- During my MPI years, I developed more and more interest in superconductivity (SC). For example, we gave an argument [14] how phonon anomalies (like in NbC) influence the pairing interaction and eventually T_c.

4. **Chair for Theoretical Physics;** Physics Department University of Würzburg (1985 – present)

Many-body aspects of density-functional theory:

- Papers with L. J. Sham (for example [83]) on why a LDA exchange-correlation potential $\sim\rho^{1/3}$, originally constructed for metals, physically also makes sense in insulators and semiconductors.
- Microscopic picture for the image-potential effect: based on the earlier work with W. Kohn, we showed that [124, 127], when a quasi-electron with its exchange + correlation (x-c) hole is moved towards a metallic surface and eventually beyond, this x-c hole (+e charge) is left behind. The +e-charge spreads into a δ-fct layer and creates the image potential for the outgoing -e-charge. Todays much-used surface-sensitive techniques are influenced by the image-tail of the surface barrier, such as photoemission and tunneling currents in STM. We verified this influence introducing the corresponding non-local potential effects in DFT.

Microscopic Theory of high-T_C superconductivity:

- Numerical (mostly QMC) as well as analytical studies were carried out of the low-energy competing phases in Hubbard-type of models, in particular, of antiferromagnetic (AF) and SC phases. We concentrated especially on the 3-band "charge-transfer" model accounting for the oxygen degrees of freedom and the question to what extent we need a multi-orbital description in the SC properties of the cuprates (see, e.g. Refs. [95, 122, 123, 140, 158, 231, 253, 256]). Here, an important development, put forward in terms of the "Maximum Entropy" method by W. v. d. Linden (TU Graz) during his time as a postdoc in Würzburg, played a decisive role, [140, 141, 143, 146, 147], facilitating a controlled translation of QMC imaginary frequency data to real frequencies.
- These investigations led to a very fruitful collaboration, starting out around 1990 and then over many years, with D. J. Scalapino´s group in Santa Barbara. Out of the many joint papers one might want to especially mention papers on a "booster mechanism" to extract the SC transition. It makes use of the "gigantic" increase of the T-derivative of the superfluid density near the transition. The corresponding QMC numerical studies determined T_c very accurately in a variety of situations (e.g. negative U models) [128, 131, 135].
- Motivated by one of the most important supporting arguments developed for electron-phonon driven BCS superconductivity in metals (McMillan-Rowell), our two groups, together with leading experimentalists, have recently carried out a similar combined theoretical and experimental study for high-T_c cuprates (Nature Physics 2010 [248]). Here, the experimental

spin-excitation and photoemission experiments were used to extract the spin-fluctuation-electron coupling constant. In the end, this allowed for an estimation (Eliashberg Theory) that spin fluctuations do have enough strength for pairing in the high-T_C cuprates.

- Aspects of spin-charge separation and, in particular, how to measure in a photoemission type of process, the different holon and spinon velocities in a quasi-1D system were studied and published with J. R. Schrieffer (Ref. [163]), University of Florida (Tallahassee).
- With S. A. Kivelson (Stanford) we embarked in a study of inhomogenities, such as stripes, in the presence of long-range Coulomb interactions. To this, we combined t-J modeled short-range stripe physics with the LDA density-functional theory, finding a substantial enhancement of the pairing correlations (Ref. [200]). This finding is still of relevance for the recently much-discussed stripe physics in the cuprates, but also in the pnictide high-T_C SC.
- A very central effort of our group starting in 1996, documented in a large variety of papers with S. C. Zhang´s group in Stanford and partly E. Demler (Harvard), has been the development of the SO(5)-Theory for High-T_c superconductivity (e.g. Ref. [166] and Rev. Mod. Phys. 2004, e.g. [219]). Put in a very simplified picture, this theory postulates that AF and SC are "two faces of one and the same coin" unified in the SO(5)-theory, in spirit somewhat similar to the $\vec{E}$- and $\vec{B}$-field in Maxwell´s theory unified by the 4-dimensional rotation in Minkowski space. Attracted by the beauty of this symmetry concept, originally proposed by S. C. Zhang, many obstacles have been overcome and predictions made, in particular with E. Arrigoni (TU Graz), still awaiting further experimental assertions [Rev. Mod. Phys. article].
- Important numerical progress was initiated by M. Aichhorn and E. Arrigoni (both now at TU Graz), who were pivotal in the development of the Variational-Cluster Theory, originally proposed by M. Potthoff (now Professor in Hamburg) in Würzburg. We worked out, for example, the emerging orders and the details of the AF to SC phase transition in Hubbard-type models (231). The observation of a phase-separation tendency is still pertinent for recent experimental findings in a variety of strongly correlated compounds (236).

Topological Superconductivity, a New Quantum State of Matter:

- In recent years, we have concentrated with our group in Würzburg and R. Thomale (previously Princeton and Stanford, now Würzburg University) and partly S.C. Zhang (Stanford) and B.A. Bernevig (Princeton) on a common thread in multi-orbital Fermi-Surface Instabilities. In particular, we have been interested in high-T_C superconductivity in the pnictides, and in topological superconductivity.
- In a variety of recent contributions, summarized in the Advances in Physics Review Article [275], we propagate the functional renormalization group (FRG) as a suited approach to investigate multi-band Fermi surface instabilities. This summary of our work includes exemplary illustrations of magnetism and, in particular, superconductivity for the iron pnictides (also the possibility of time-reversal symmetry breaking) from the viewpoint of FRG [260-261,263, 2656, 268]. Furthermore, it discusses candidate scenarios for topological bulk singlet superconductivity on hexagonal lattices such as sodium-doped cobaltates [271] and graphene doped to a van Hove filling [269].
- In recent work, again employing the multi-band FRG, we have studied with the Zhang-Rice group (Zürich, Hongkong) Sr_2RuO_4, which has been heralded as the solid-state analogue of

^{3}He. Indeed, we have found evidence for p-wave symmetry of its SC phase, as in superfluid ^{3}He [274].

- With the M. Sigrist group (again Zürich), we have investigated [278] the possibility of an unconventional SC state in the recently much-discussed pnictide SrPtAs, where spin-orbit coupling and inversion-symmetry breaking conspire to an unusual topological SC state: Our theoretical findings, together with the experimental evidence suggest that SrPtAs is the first example of a topological chiral d-wave SC, which, in addition, displays topological bulk properties (Weyl SC).
- A rather different subject concerns a paper, we have recently published together with experimentalists (L. Molenkamp's group) from our University (Nature Phys. 2010 [254]). It made predictions of how to measure the Spin-Hall effect which, due to its spin manipulation aspect is of relevance in spintronics. These predictions were confirmed in corresponding studies in L. Molenkamp's group, which has experimentally discovered the Quantum Spin-Hall effect.
- Another fruitful interaction we have with an experimental group in Würzburg (R. Claessen), is studying metal adatom systems on semiconductor surfaces. The adatoms can be arranged in 2D-layers, with or without frustration and, in terms of many-body physics present a beautiful playground for studies ranging from exotic magnetic to exotic SC phases. Out of the projects, an article on magnetic order in a frustrated 2D atom lattice (Sn/Si (111) (Nature Com. 2013 [264]) should be especially mentioned, which verified that a magnetically ordered state appears despite the frustration, and not the much-discussed spin-liquid phase.
- Last not least, a scheme was proposed together with E. Hankiewicz (Würzburg) which links as directly as possible the experimental search for topological superconductivity to a material-based microscopic theory [277]. To this, the scanning tunneling microscopy (STM), which typically uses a phenomenological Ansatz for the SC gap functions is elevated to a theory, where a multi-orbital functional RG (fRG) analysis allows for an unbiased microscopic determination of the material-dependent pairing potentials. The strength of the combined approach was demonstrated for hexagonal systems, i.e. doped graphene and water-intercalated sodium cobaltates, where the lattice symmetry and electronic correlations can lead to a time-reversal symmetry breaking (chiral) topological SC state.
- Quantum spin Hall materials hold the promise of revolutionary devices with dissipationless spin currents but have required cryogenic temperatures owing to small energy gaps. In our recent Science Report [283] we show theoretically that a room-temperature regime with a large energy gap may be achievable within a paradigm that exploits the atomic spin-orbit coupling. The concept is based on a substrate-supported monolayer of a high-atomic number element and is experimentally realized as a bismuth honeycomb lattice on top of the insulating silicon carbide substrate SiC(0001). Using scanning tunneling spectroscopy, we detect a gap of ~0.8 electron volt and conductive edge states consistent with theory. Our combined theoretical [285] and experimental results demonstrate a concept for a quantum spin Hall wide-gap scenario, where the chemical potential resides in the global system gap, ensuring robust edge conductance.
- In recent years, the discovery of superconductivity in twisted bilayer graphene and infinite-layer nickelates, to only name a few, combined with revolutionary developments in seemingly established material classes such as strontium ruthenates and the overdoped cuprates, yielded an unprecedented diversification of potential material hosts for

unconventional superconductors, ranging from high-temperature superconductor candidates and topological superconductors up to the possible stabilization of Majorana fermions in half-quantum vortices or boundary states of particular spin-orbit and/or triplet superconductors. These exciting new developments moved more and more into the focus of our research, as documented by our publications from [283] on, until today.

References refer to the publication list.