1 From Gutzwiller Wave Functions to Dynamical Mean-Field Theory

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1 Introduction

Correlations between the degrees of freedom of d and f electrons lead to a wealth of fascinating phenomena, which include Mott metal-insulator transitions [1–3], the Kondo effect [4], heavy fermion behavior [5], band-ferromagnetism [6], high-temperature superconductivity [7], colossal magnetoresistance [8], and other Fermi liquid instabilities [9]. In particular, the very sensitive dependence of the properties of correlated materials on external parameters such as temperature, pressure, magnetic field, or doping make them interesting not only for fundamental research but also for future technological applications, e.g., the construction of sensors and switches, and the development of electronic devices with novel functionalities [10].
The importance of interactions between electrons in a solid was realized already at the outset of modern solid state physics. Namely, the report by de Boer and Verwey [11] on the surprising properties of materials with partially filled $3d$-bands such as NiO prompted Mott and Peierls [12] to postulate that theoretical explanations of these properties must include the electrostatic interaction between the electrons. Explicit calculations soon confirmed this conjecture. At the same time it turned out that theoretical studies of interacting many-fermion systems are highly demanding. Here the development of the dynamical mean-field theory (DMFT) marks a methodological breakthrough. Indeed, by replacing the d-dimensional lattice of a correlated-electron solid by a single quantum impurity, which is self-consistently embedded in a bath provided by the other electrons, the DMFT opened the way for comprehensive theoretical investigations of correlation phenomena in electronic lattice models and materials. The starting point for the development of this powerful new many-body approach was the discovery, 25 years ago, that diagrammatic perturbation theory for interacting lattice fermions is much simpler in infinite spatial dimensions than in finite dimensions and, in particular, that the self-energy is then purely local. The current Autumn School on Correlated Electrons *DMFT at 25: Infinite Dimensions* commemorates this anniversary. Starting with a discussion of the properties of the Gutzwiller variational wave function and the mean-field-type Gutzwiller approximation, which provides a simplistic but robust, non-perturbative theoretical approach to correlated lattice fermions, I will describe the steps which eventually led to the formulation of the DMFT.

1.1 Modeling of correlated lattice electrons

The simplest model for interacting electrons in a solid is the one-band Hubbard model, which was introduced independently by Gutzwiller, Hubbard and Kanamori [13–15]. In this model the interaction between the electrons is assumed to be strongly screened, i.e., purely local. The Hamiltonian $\hat{H}$ is the sum of two terms, the kinetic energy $\hat{H}_{\rm kin}$ and the interaction energy $\hat{H}_I$ (here and in the following operators are denoted by a hat):

$$\hat{H} = \sum_{\boldsymbol{R}_i,\boldsymbol{R}_j} \sum_{\sigma} t_{ij}\ \hat{c}^{\dagger}_{i\sigma}\hat{c}_{j\sigma} + U \sum_{\boldsymbol{R}_i} \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}\,, \tag{1}$$

where t_{ij} is the hopping amplitude, U is the local Hubbard interaction, $\hat{c}^{\dagger}_{i\sigma}(\hat{c}_{i\sigma})$ is the creation (annihilation) operator of an electron with spin σ in a Wannier orbital localized at lattice site $\boldsymbol{R}_i$,

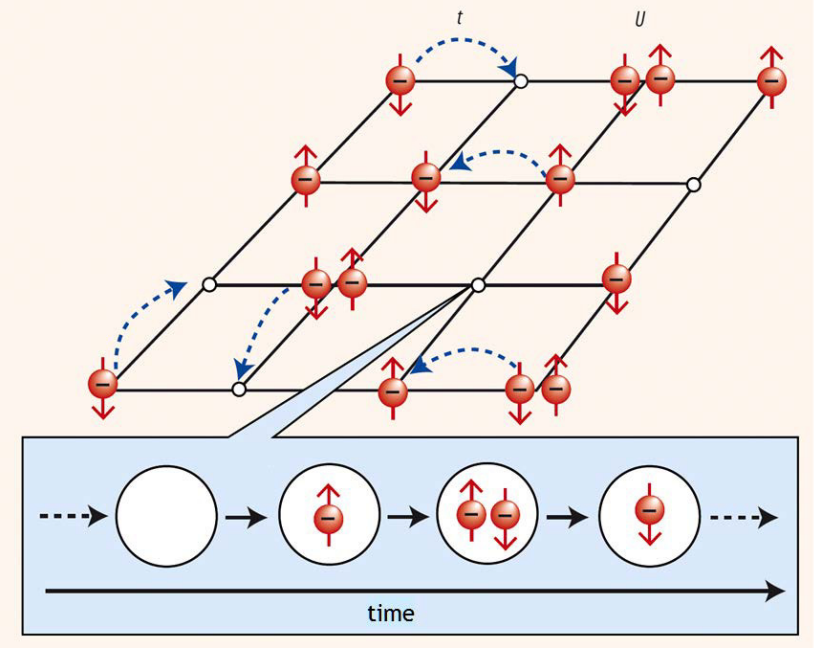

Fig. 1: *Schematic illustration of interacting electrons in a solid described by the Hubbard model. The ions enter only as a rigid lattice, here represented by a square lattice. The electrons, which have a mass, a negative charge, and a spin (↑ or ↓), are quantum particles that move from one lattice site to the next with a hopping amplitude t. The quantum dynamics thus leads to fluctuations in the occupation of lattice sites as indicated by the time sequence. A lattice site can either be unoccupied, singly occupied (↑ or ↓), or doubly occupied. When two electrons meet on a lattice site, which is only possible if they have opposite spin because of the Pauli exclusion principle, they encounter an interaction U.*

and $\hat{n}_{i\sigma} = \hat{c}^\dagger_{i\sigma}\hat{c}_{i\sigma}$. The Hubbard interaction can also be written as $\hat{H}_I = U\hat{D}$ where $\hat{D} = \sum_{\boldsymbol{R}_i} \hat{D}_i$ is the number operator of doubly occupied sites of the system, with $\hat{D}_i = \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}$ as the local operator for double occupation. The Fourier transform of the kinetic energy

$$\hat{H}_{\mathrm{kin}} = \sum_{\boldsymbol{k},\sigma} \varepsilon_{\boldsymbol{k}} \hat{n}_{\boldsymbol{k}\sigma} \tag{2}$$

is defined by the dispersion $\varepsilon_{\boldsymbol{k}}$ and the momentum distribution operator $\hat{n}_{\boldsymbol{k}\sigma}$. A schematic picture of the Hubbard model is shown in Fig. 1. For strong repulsion U double occupations are energetically unfavorable and are therefore suppressed. In this situation the local correlation function $\langle \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}\rangle$ must not be factorized, since otherwise correlation phenomena are eliminated from the beginning. Therefore Hartree-Fock-type mean-field theories, which do factorize the interaction, cannot explain the physics of strongly correlated electrons.

The Hubbard model looks deceptively simple. However, the competition between the kinetic energy and the interaction leads to a complicated many-body problem, which is impossible to solve analytically except in dimension $d = 1$ [16]. This model provides the basis for most of the theoretical research on correlated electrons during the last few decades.

2 Approximation schemes for correlated electrons

Theoretical investigations of quantum-mechanical many-body systems are faced with severe technical problems, particularly in those dimensions which are most interesting to us, namely $d = 2, 3$. This is due to the complicated quantum dynamics and, in the case of fermions, the non-trivial algebra introduced by the Pauli exclusion principle.

In view of the fundamental limitations of exact analytical approaches one might hope that, at least, modern supercomputers can provide detailed numerical insights into the thermodynamic and spectral properties of correlated fermionic systems. However, since the number of quantum mechanical states increases exponentially with the number of lattice sites L, numerical solutions of the Hubbard model and related models are limited to relatively small systems. This shows very clearly that there is still a great need for analytically tractable approximation methods [17], in particular for non-perturbative approximation schemes which are applicable for all input parameters.

2.1 Mean-field theories

In the theory of classical and quantum many-body systems an overall description of the properties of a model is often obtained within a *mean-field theory*. Although the term is frequently used it does not have a precise meaning, since there exist numerous ways to derive mean-field theories. One construction scheme is based on a factorization of the interaction, as in the case of the Weiss mean-field theory for the Ising model, or the Hartree-Fock theory for electronic models. The decoupling implies a neglect of fluctuations (or rather of the correlation of fluctuations; for details see Ref. [18]) and thereby reduces the original many-body problem to a solvable problem where a single spin or particle interacts with a mean field provided by the other particles. Another, in general unrelated, construction scheme makes use of the simplifications that occur when some parameter is assumed to be large (in fact, infinite), e.g., the magnitude of the spin S, the spin degeneracy N, the number Z of nearest neighbors of a lattice site (the coordination number), or the spatial dimension d.[1] Investigations in this limit, supplemented, if possible, by an expansion in the inverse of the large parameter, [2] often provide valuable insight into the fundamental properties of a system even when this parameter is not large. One of the best-known approximations obtained in this way is the Weiss mean-field theory for the Ising model [19]. This is a prototypical "single-site mean-field theory," which becomes exact not only in the limit $Z \to \infty$ or $d \to \infty$, but also for an infinite-range interaction. It contains no unphysical singularities and is applicable for all values of the input parameters, i.e., coupling parameters, magnetic field, and temperature.

[1] For regular lattices both a dimension d and a coordination number Z can be defined. However, there exist other lattices, such as the Bethe lattice, which cannot be associated with a physical dimension d although a coordination number Z is well-defined.

[2] In three dimensions one has $Z = 6$ for a simple cubic lattice, $Z = 8$ for a bcc lattice, and $Z = 12$ for an fcc-lattice. The parameter $1/Z$ is therefore quite small already in $d = 3$.

2.2 Variational wave functions

Another useful approximation scheme for interacting quantum many-body systems makes use of variational wave functions. They allow for approximate but explicit and physically intuitive investigations of correlations among quantum particles and are particularly valuable in situations where standard perturbation theory fails. Correlation problems where variational wave functions have been employed include such diverse examples as the quantum liquids Helium-3 and Helium-4 [20], rotons in superfluid ^{4}He [21], nuclear physics [22], and the fractional quantum Hall effect [23]. Variational wave functions received renewed attention in the study of heavy fermions [24, 25] and high-T_c superconductivity [26].
The general strategy is to construct an explicit wave function of the form

$$|\Psi_{\rm var}\rangle = \hat{C}|\Psi_0\rangle \tag{3}$$

where $|\Psi_0\rangle$ is a tractable one-particle starting wave function on which a correlation operator $\hat{C}(\lambda_1, \ldots, \lambda_n)$ acts. The latter depends on variational parameters λ_i and describes the microscopic interaction between the particles in an approximate way. This wave function is then used to calculate the expectation value of an operator $\hat{\mathcal{O}}$ as

$$\langle\hat{\mathcal{O}}\rangle_{\rm var} = \frac{\langle\Psi_{\rm var}|\hat{\mathcal{O}}|\Psi_{\rm var}\rangle}{\langle\Psi_{\rm var}|\Psi_{\rm var}\rangle}. \tag{4}$$

In particular, by calculating and minimizing the ground state energy $E_{\rm var} = \langle\hat{H}\rangle_{\rm var}$, where $\hat{H}$ is the Hamiltonian, the variational parameters contained in $\hat{C}$ (and perhaps also in $|\Psi_0\rangle$) can be determined. These parameters are used to suppress those configurations in $|\Psi_0\rangle$ which for given interaction strength are energetically unfavorable. The variational principle guarantees that $E_{\rm var}$ provides a rigorous upper bound for the exact ground state energy.

3 Gutzwiller wave functions

For the Hubbard model, (1), the simplest variational wave function of the form (3) is the so-called Gutzwiller wave function

$$|\Psi_G\rangle = g^{\hat{D}}\,|{\rm FG}\rangle \tag{5a}$$

$$= \prod_{\boldsymbol{R}_i}[1-(1-g)\hat{D}_i]\,|{\rm FG}\rangle\,, \tag{5b}$$

where $g^{\hat{D}}$, with $0 \le g \le 1$, is the correlation operator and $|{\rm FG}\rangle$ is the ground state of the non-interacting Fermi gas. Hence the correlation operator globally reduces the amplitude of those spin configurations in $|{\rm FG}\rangle$ with too many doubly occupied sites. The limit $g = 1$ corresponds to the non-interacting case, while $g \to 0$ describes the limit $U \to \infty$. Indeed, for $g \to 0$ one finds

$$g^{\hat{D}}\Big|_{g=0} = \prod_{\boldsymbol{R}_i}[1-\hat{D}_i] \equiv \hat{P}_G\,. \tag{6}$$

The projection operator $\hat{P}_G$ eliminates all configurations with doubly occupied sites (*Gutzwiller projection*). The ground state energy in terms of the Gutzwiller wave function is then given by

$$E_{\rm G} = \langle \hat{H} \rangle_G \equiv \frac{\langle \Psi_G | \hat{H} | \Psi_G \rangle}{\langle \Psi_G | \Psi_G \rangle} \,. \tag{7}$$

By replacing $|{\rm FG}\rangle$ with a more general starting wave function one can also describe states with broken symmetry; examples are the antiferromagnetic Hartree-Fock wave function (spin density wave)

$$|{\rm SDW}\rangle = \prod_{\boldsymbol{k},\sigma} \left[u_{\boldsymbol{k}} \hat{a}^\dagger_{\boldsymbol{k}\sigma} + \sigma v_{\boldsymbol{k}} \hat{a}^\dagger_{\boldsymbol{k}+\boldsymbol{Q},\sigma} \right] |0\rangle \,, \tag{8a}$$

where $\boldsymbol{Q}$ is half a reciprocal lattice vector and $|0\rangle$ is the vacuum, and the BCS wave function [27]

$$|{\rm BCS}\rangle = \prod_{\boldsymbol{k}} \left[u_{\boldsymbol{k}} + v_{\boldsymbol{k}} \hat{a}^\dagger_{\boldsymbol{k}\uparrow} \hat{a}^\dagger_{-\boldsymbol{k}\downarrow} \right] |0\rangle \,, \tag{8b}$$

which after projection leads to a resonating valence bond state (RVB) [26].

3.1 Gutzwiller approximation

In addition to introducing the wave function (5a) Gutzwiller constructed a non-perturbative approximation scheme that allowed him to obtain an explicit expression for the ground state energy of the Hubbard model [13, 28].[3] We will see in Sec. 4.1.1 that this Gutzwiller approximation yields the exact result for expectation values calculated with Gutzwiller wave functions in the limit of infinite spatial dimensions ($d = \infty$). The idea behind the Gutzwiller approximation is easily understood [29, 30] and will be illustrated below by calculating the norm $\langle \Psi_G | \Psi_G \rangle$. Working in configuration space the ground state of the Fermi gas can be written as

$$|{\rm FG}\rangle = \sum_D \sum_{\{i_D\}} A_{i_D} |\Psi_{i_D}\rangle, \tag{9}$$

where $|\Psi_{i_D}\rangle$ is a spin configuration with D doubly occupied sites and A_{i_D} the corresponding probability amplitude. The sum extends over the whole set $\{i_D\}$ of different configurations with the same D, and over all D. For a system with L lattice sites and N_σ electrons of spin σ (σ-electrons) the number N_D of different configurations in $\{i_D\}$ is given by the combinatorial expression

$$N_D = \frac{L!}{L_\uparrow! L_\downarrow! D! E!}, \tag{10}$$

where $L_\sigma = N_\sigma - D$ and $E = L - N_\uparrow - N_\downarrow + D$ are the numbers of singly occupied and empty sites, respectively. Since $|\Psi_{i_D}\rangle$ is an eigenstate of $\hat{D}$, the norm of $|\Psi_G\rangle$ reads

$$\langle \Psi_G | \Psi_G \rangle = \sum_D g^{2D} \sum_{\{i_D\}} |A_{i_D}|^2. \tag{11}$$

[3] By studying lattice electrons with a local Coulomb repulsion Gutzwiller wanted to understand the origin of ferromagnetism in metals.

The Gutzwiller approximation effectively amounts to neglecting spatial correlations between the spins of the electrons. The probability $|A_{i_D}|^2$ is then the same for all configurations of electrons on the lattice, i.e., is given by the classical combinatorial result for uncorrelated particles

$$|A_{i_D}|^2 = P_\uparrow P_\downarrow. \tag{12}$$

Here $P_\sigma = 1/\binom{L}{N_\sigma} \simeq n_\sigma^{N_\sigma}(1-n_\sigma)^{L-N_\sigma}$, with $n_\sigma = N_\sigma/L$, is the probability for an arbitrary configuration of σ-electrons. In this case (11) reduces to

$$\langle \Psi_G | \Psi_G \rangle = P_\uparrow P_\downarrow \sum_D g^{2D} N_D. \tag{13}$$

In the thermodynamic limit the sum in (13) is dominated by its largest term corresponding to a value $D = \bar{D}$, where $\bar{D} = L\bar{d}$ is determined by

$$g^2 = \frac{\bar{d}(1-n_\uparrow - n_\downarrow + \bar{d})}{(n_\downarrow - \bar{d})(n_\uparrow - \bar{d})}\,. \tag{14}$$

Equation (14) has the form of the law of mass action where, however, the correlation parameter g^2 rather than the Boltzmann factor regulates the dynamical equilibrium between the concentrations of singly occupied sites on one side of this "chemical reaction" and that of doubly occupied sites and holes on the other.[4] Eq. (14) uniquely relates $\bar{d}$ and g, such that g may be replaced by the quantity $\bar{d}$. The calculation of the expectation values of the kinetic and the interaction energy of the Hubbard model proceeds similarly [30]. The Gutzwiller approximation for quantum mechanical expectation values, which is based on the counting of classical spin configurations, belongs to the class of *quasiclassical approximations*.

3.1.1 Brinkman-Rice transition

The ground state energy per lattice site of the Hubbard model as a function of the variational parameter $\bar{d}(g)$ is then found as

$$E_G[\,\bar{d}(g)]/L = \sum_\sigma q_\sigma(\bar{d}, n_\uparrow, n_\downarrow)\varepsilon_{0,\sigma} + U\bar{d}, \tag{15}$$

which is to be minimized with respect to $\bar{d}$. Here $\varepsilon_{0,\sigma}$ is the energy of non-interacting σ-electrons and $q_\sigma \leq 1$ may be viewed as a reduction factor of the kinetic energy (or the band width) due to correlations. In particular, for $n_\uparrow = n_\downarrow$ one has $q_\sigma \equiv q = 2(1-\delta-2\bar{d})(\sqrt{\bar{d}+\delta}+\sqrt{\bar{d}})^2/(1-\delta^2)$, where $\delta = 1-n$, with $n = n_\uparrow + n_\downarrow$ as the particle density, and $\varepsilon_\uparrow = \varepsilon_\downarrow$. So one finds that within the Gutzwiller approximation the correlations only lead to a multiplicative renormalization of the non-interacting kinetic energy. Brinkman and Rice [32, 33] showed that in the special case $n_\sigma = 1/2$ (half-filled band) the minimization of (15) yields

$$q = 1 - \overline{U}^2, \tag{16a}$$

$$\bar{d} = (1-\overline{U})/4, \tag{16b}$$

$$E/L = -|\varepsilon_0|\,(1-\overline{U})^2, \tag{16c}$$

[4] It is interesting to note that (14), with g^2 replaced by the Boltzmann factor $e^{-\beta U}$, is the exact result for the Hubbard model with infinite-range hopping [31].

where $\overline{U} = U/(8|\varepsilon_0|)$ and $\varepsilon_0 = \varepsilon_{0\uparrow} + \varepsilon_{0\downarrow}$. Eq. (16c) implies that the ground state energy E, which equals $-L\,|\varepsilon_0|$ at $U = 0$, increases with U and vanishes at a finite critical value $U_c = 8\,|\varepsilon_0|$, since the density of doubly occupied sites $\bar{d}$ (and hence the reduction factor q) vanishes at this point. The fact that $E_{\rm kin} \to 0$ and $E_{\rm I} \to 0$ for $U \to U_c$ means that the particles become localized, which implies that a charge current can no longer flow. So the Gutzwiller approximation actually describes a Mott-Hubbard metal-insulator transition at a finite interaction strength (*Brinkman-Rice-transition*). It occurs only for $n_\sigma = 1/2$. A transition to a localized, paramagnetic state with $E = 0$ at a finite value of U clearly does not describe the behavior of the electrons completely. It is well known that for $U \gg t$ localized spins couple antiferromagnetically, which leads to a lowering of the energy $E = 0$ by an amount $E_{AF} \propto -t^2/U$. This effect is not included in the Gutzwiller approximation, since spatial correlations were explicitly neglected. On the other hand, the magnetic coupling is an additional effect, which can be derived within second-order perturbation theory from the localized state. Therefore, as long as one is not too close to $U = U_c$ the overall results of the Gutzwiller approximation are not invalidated by the magnetic coupling and give important insight into the correlation-induced approach to the localized state.

3.2 Connection to Fermi liquid theory

Since the results of the Gutzwiller approximation describe correlated, paramagnetic fermions with a renormalized kinetic energy one can make contact with Landau's Fermi liquid theory [32, 30]. In particular, it turns out that the reduction factor q in (15) describes the discontinuity of the momentum distribution $n_{\boldsymbol{k}}$ at the Fermi level and may thus be identified with the inverse effective mass ratio $(m^*/m)^{-1}$ of the quasiparticles. Since $m^*/m = q^{-1} < \infty$ for $U < U_c$, the system is a Fermi liquid, i.e., a metal. At $U = U_c$ the effective mass diverges and the system becomes an insulator.

One can use (15) to calculate the spin susceptibility $\chi_s = \chi_s^0\,(m^*/m)/(1 + F_0^a)$ and compressibility $\kappa = \kappa^0\,(m^*/m)/(1 + F_0^s)$ within the Gutzwiller approximation, where χ_s^0 and κ^0 are the results for the non-interacting Fermi gas [32,30]. For $n_\sigma = 1/2$, and assuming Galilei invariance, one finds [30] $m^*/m \equiv 1 + \frac{1}{3}F_1^s = 1/(1 - \overline{U}^2)$. The corresponding Fermi liquid parameters are given by

$$F_0^a = p\left(\frac{1}{(1+\overline{U})^2} - 1\right), \tag{17a}$$

$$F_0^s = p\left(\frac{1}{(1-\overline{U})^2} - 1\right), \tag{17b}$$

$$F_1^s = \frac{3\overline{U}^2}{1-\overline{U}^2}, \tag{17c}$$

where $p = 2|\varepsilon_0|N(0)$, with $N(0)$ as the density of states at the Fermi energy. For typical symmetric densities of states one finds $p \simeq 1$. Hence, for $U \to U_c$ the Landau parameter F_0^a levels off and saturates at $\simeq -3/4$, while F_0^s increases much faster than linearly and eventually

diverges. In particular, for $U \to U_c$ the Wilson ratio remains constant:

$$\frac{\chi_s/\chi_s^0}{m^*/m} = \frac{1}{1+F_0^a} \to \text{const.} \tag{18}$$

So the strong increase of χ_s as a function of U for $U \to U_c$ is mainly due to the rapid increase of the effective mass ratio m^*/m and not due to an incipient ferromagnetic instability [34], which would demand $F_0^a \to -1$.
As first pointed out by Anderson and Brinkman [35] and discussed in detail in Ref. [30], the behavior expressed by (17c) and (18) is indeed observed in the prototypical Fermi liquid Helium-3 (^{3}He). Normal-liquid ^{3}He is an isotropic, strongly correlated fermionic system. The effective mass m^* and the spin susceptibility χ_s of the quasiparticles are strongly enhanced, while the compressibility κ is strongly reduced. Normal-liquid ^{3}He has therefore been called an *almost-localized* Fermi liquid.

4 From the Gutzwiller approximation to infinite dimensions

My 1984 Review of Modern Physics article [30] explained Gutzwiller's variational approach to the Hubbard model, the Gutzwiller approximation, and the Brinkman-Rice transition and thereby drew attention to the usefulness of this non-perturbative investigation scheme for correlated fermions. Nevertheless there remained questions about the nature of the Gutzwiller approximation, whose results are simple and mean-field-like. In fact, the latter feature is one of the reasons why the results of the Gutzwiller approximation, which originally had been derived for lattice fermions, are applicable even to liquid ^{3}He [30, 36]. The question was, therefore, whether the Gutzwiller approximation could also be derived by other, more conventional methods of quantum many-body theory in some limit. During 1983-84 I discussed this question with several colleagues, in particular with Andrei Ruckenstein at Bell Laboratories, Murray Hill, in 1983. At that time, Andrei tried to understand whether it was possible to generalize the Brinkman-Rice transition to correlated electronic systems in the presence of disorder [37]. This eventually led him and Gabi Kotliar to formulate a functional integral representation of the Hubbard and Anderson models in terms of auxiliary bosons, whose simplest saddle-point approximation (*slave-boson mean-field theory*) reproduces exactly the results of the Gutzwiller approximation [38]. Thus they had shown that the results of the Gutzwiller approximation could also be obtained without the use of the Gutzwiller variational wave function. We will return to this mean-field theory in Section 4.1.1.

4.1 Calculation of expectation values with the Gutzwiller wave function

As mentioned earlier, mean-field theories can be constructed in different ways. In particular, the Gutzwiller approximation, which was originally based on the quasi-classical counting of electronic configurations on a real-space lattice [13, 28], had been re-derived as a saddle-point approximation for electrons expressed in terms of auxiliary bosons [38]. At the same time, the

question of whether the Gutzwiller approximation could also be derived in a controlled way by calculating expectation values with the Gutzwiller wave function using conventional many-body perturbation theory was still open. In 1986, I suggested to Walter Metzner, then a diploma student of physics at the Technical University of Munich, to calculate the ground-state energy of the one-dimensional Hubbard model with the Gutzwiller wave function by means of many-body perturbation theory. It turned out that expectation values of the momentum distribution and the double occupation can be expressed as power series in the small parameter g^2-1, where g is the correlation parameter in the Gutzwiller wave function (5a).[5] The coefficients of the expansions are determined by diagrams which are identical in form to those of a conventional Φ^4 theory. However, lines in a diagram do not correspond to one-particle Green functions of the non-interacting system, $G^0_{ij,\sigma}(t)$, but to one-particle density matrices, $g^0_{ij,\sigma} = \langle \hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma}\rangle_0$. Walter showed that it was possible to determine these coefficients to all orders in $d = 1$. This facilitated the exact analytic calculation of the momentum distribution and the double occupation, and thereby of the ground state energy of the Hubbard chain, in terms of the Gutzwiller wave function [40, 41].

In particular, for $n = 1$ and $U \gg t$ the ground state energy obtained with the Gutzwiller wave function in $d = 1$ has the form [40, 41]

$$E_G = -\left(\frac{4}{\pi}\right)^2 \frac{t^2}{U}\,\frac{1}{\ln \overline{U}}, \tag{19}$$

where $\overline{U} = U/(8|\varepsilon_0|)$, with $\varepsilon_0 < 0$ as the energy of the non-interacting particles. Hence the exact result, $E \sim -t^2/U$, obtained from second-order perturbation theory is found to be multiplied by a factor which is non-analytic in U. This explained why the ground state energy E_G for the Hubbard model is not very accurate, as noted earlier on the basis of numerical investigations of one-dimensional rings [42].

Does the result (19) automatically imply that $|\Psi_G\rangle$ is a poor wave function in the strong-coupling limit? The answer is quite subtle: while it is true that $|\Psi_G\rangle$ is not a very good wave function for the *Hubbard model* at $U \gg t$, it is nevertheless an excellent wavefunction in $d = 1$ for the t-J *model*, the effective model for large U, where doubly occupied sites have been projected out; for a more detailed discussion see Section 2.1 of Ref. [43]. This is demonstrated by the results for the spin-spin correlation function C^{SS}_j, with $j \equiv |\boldsymbol{R}_j|$. Florian Gebhard, also a diploma student at the Technical University of Munich at that time, to whom I had suggested to calculate correlation functions for the Hubbard model in terms of the Gutzwiller wave function using the technique developed in Refs. [40, 41], was able to analytically evaluate four different correlation functions in $d = 1$ [44, 45]. The result for the spin-spin correlation function explicitly showed that in the strong coupling limit ($U = \infty$) the Gutzwiller wave function describes spin correlations in the nearest-neighbor, isotropic Heisenberg chain extremely well. For $n = 1$ and $U = \infty$ we obtained [44, 45]

$$C^{SS}_{j>0} = (-1)^j\,\frac{Si(\pi j)}{\pi j} \;\overset{j\to\infty}{\sim}\; \frac{(-1)^j}{2j} \tag{20}$$

[5] For a more detailed account see Section 2.3 of Ref. [39].

where $Si(x)$ is the sine-integral. The asymptotic behavior implies a logarithmic divergence at momentum $2k_F$, signaling antiferromagnetic fluctuations. Comparison with the exact analytic result for the spin correlation function of the Heisenberg model for $j = 1, 2$ and for large j, where [46, 47] $C_j^{SS} \sim (-1)^j j^{-1} (\ln j)^{1/2}$, shows that the Gutzwiller wave function without doubly occupied sites ($U = \infty$) yields excellent results in $d = 1$ [44, 45]. The same is true for hole-hole correlations in the limit $n \lesssim 1$ and $U = \infty$. Shortly afterwards Haldane [48] and Shastry [49] independently proved that the Gutzwiller wave function for $U = \infty$ is the *exact* solution of the spin-1/2 antiferromagnetic Heisenberg chain for an exchange interaction J_{ij} which decreases as[6] $J_{ij} \sim 1/|i - j|^2$. Thus the Gutzwiller wave function corresponds [48] to the one-dimensional version of Anderson's resonating valence bond (RVB) state [26].

4.1.1 Simplifications in the limit $d \to \infty$

Our results [40, 41, 44, 45] had demonstrated that in $d = 1$ it was possible to calculate expectation values in terms of the Gutzwiller wave function analytically for all interaction strengths. However, our attempts to generalize this to dimensions $d > 1$ failed. To gain insight into the density dependence of the coefficients of the power series in $g^2 - 1$ in dimensions $d > 1$ Walter Metzner computed the sums over the internal momenta of the diagrams of many-body perturbation theory by Monte-Carlo integration. The results for the lowest-order contribution to the correlation energy for $d = 1$ up to $d = 15$ led to a surprise. Namely, the plot of the results for the second-order diagram as a function of d (Fig. 2) showed that for large d the value of this diagram converged to a simple result which could also be obtained if one assumed that the momenta carried by the lines of a diagram are *independent*, i.e., that there is no momentum conservation at a vertex. When summed over all diagrams this approximation gave exactly the results of the Gutzwiller approximation [40,41]. Thus we had re-derived the Gutzwiller approximation within conventional many-body perturbation theory! In view of the random generation of momenta in a typical Monte-Carlo integration over momenta we concluded that the assumed independence of momenta at a vertex is correct in the limit of infinite spatial dimensions ($d \to \infty$). The results of the Gutzwiller approximation thus correspond to the evaluation of expectation values in terms of the Gutzwiller wave function in the limit of infinite dimensions. This provided a straightforward explanation of the mean-field character of the Gutzwiller approximation.
The drastic simplifications of diagrammatic calculations in the limit $d \to \infty$ allow one to calculate expectation values of the kinetic energy and the Hubbard interaction in terms of Gutzwiller-type wave functions exactly [50,51]. However, these calculations become quite difficult or even untractable when it comes to calculating with Gutzwiller-correlated wave functions of the more general form

$$|\Psi_G\rangle = g^{\hat{D}} \, |\Psi_0\rangle \tag{21}$$

where $|\Psi_0\rangle$ is no longer the ground state of the Fermi gas, but a more complicated one-particle starting wave function. This has to do with the fact that, in spite of the simplifications arising

[6] This distance dependence of the exchange coupling leads to a partial frustration of the spin orientation whereby the antiferromagnetic correlations are weaker than in the original Heisenberg model.

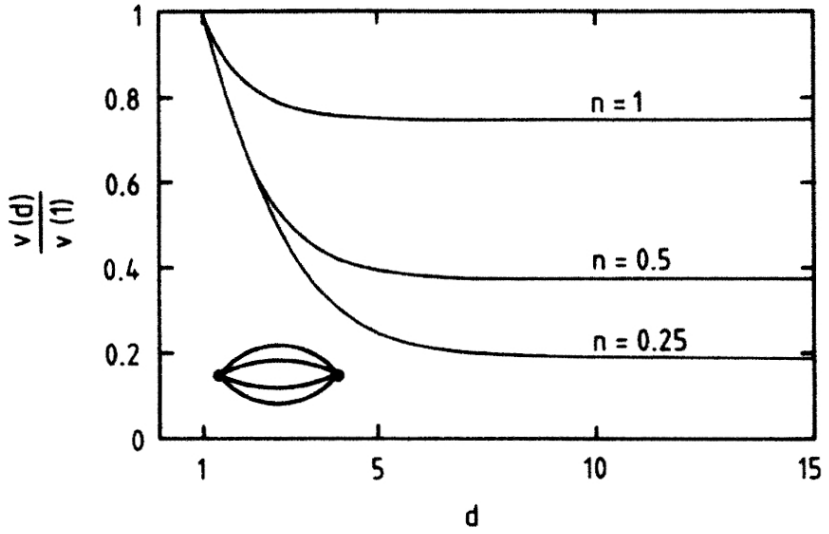

Fig. 2: *Value of the second-order diagram for the ground state energy of the Hubbard model (see insert) as calculated with the Gutzwiller wave function for spatial dimensions $d = 1, \ldots, 15$, and normalized by the value for $d = 1$, $v(1) = (2/3)(n/2)^3$, where n is the particle density. In the limit of high dimensions the normalized values $v(d)/v(1)$ approach the constant $3n/4$. As discussed in the text the same result is obtained within a diagrammatic approximation that yields the results of the Gutzwiller approximation; from Ref. [41].*

from the diagrammatic collapse in $d = \infty$, the remaining diagrams have to be calculated in terms of $|\Psi_0\rangle$. Florian Gebhard [52] showed that this problem can be overcome when $|\Psi_0\rangle$ in (21) is written in the form

$$|\Psi_0\rangle = g^{-\sum\limits_{i\sigma} \mu_{i\sigma} \hat{n}_{i\sigma}} \; |\tilde{\Psi}_0\rangle \tag{22}$$

where $|\tilde{\Psi}_0\rangle$ is again an arbitrary, normalized one-particle wave function and the local chemical potentials $\mu_{i\sigma}$ are explicit functions of g and the local densities $\tilde{n}_{i\sigma} = \langle\tilde{\Psi}_0|\hat{n}_{i\sigma}|\tilde{\Psi}_0\rangle$. The operator in (22) corresponds to a gauge-transformation by which the local chemical potentials can be chosen such that all Hartree bubbles disappear in $d = \infty$. With this re-interpretation all diagrammatic calculations remain identical to the earlier ones, but vertices are given a new value and lines correspond to

$$\tilde{g}^0_{ij,\sigma} = g^0_{ij,\sigma}\,(1 - \delta_{ij}), \tag{23}$$

where now $\tilde{g}^0_{ii,\sigma} \equiv 0$, and hence $\Sigma_{ii,\sigma} \equiv 0$. Consequently, in $d = \infty$ results are obtained without the calculation of a single diagram. So what remains in $d = \infty$ at all? First of all one finds that the "law of mass action", (14), is valid even locally and for arbitrary states $|\tilde{\Psi}_0\rangle$ (even for states with long-range order). Secondly, the expectation value of the Hubbard-Hamiltonian in terms of (21), (22) assumes the following general form for arbitrary $|\tilde{\Psi}_0\rangle$:

$$\langle\hat{H}\rangle = -t \sum_{\langle \boldsymbol{R}_i, \boldsymbol{R}_j\rangle} \sum_{\sigma} \sqrt{q_{i\sigma}}\,\sqrt{q_{j\sigma}}\; g^0_{ij,\sigma} + U \sum_i \bar{d}_i, \tag{24}$$

where $\langle \boldsymbol{R}_i, \boldsymbol{R}_j\rangle$ denotes nearest-neighbor sites, $\bar{d}_i = \langle\hat{D}_i\rangle$, and $q_{i\sigma}$ is given by q_σ in (15) with n_σ replaced by $\tilde{n}_{i\sigma}$. In the translationally invariant case $|\Psi_0\rangle \equiv |\mathrm{FG}\rangle$ the two wave-functions $|\Psi_0\rangle$ and $|\tilde{\Psi}_0\rangle$ are the same up to a trivial factor, and $q_{i\sigma} \equiv q_i$, whereby (15) is re-derived.

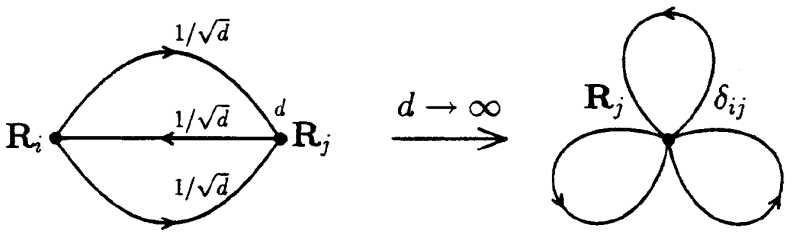

Fig. 3: *Contribution to the irreducible self-energy for the Hubbard model in second-order perturbation theory in U and its collapse in the limit $d \to \infty$.*

Interestingly, the result (24) is identical to the saddle-point solution of the slave-boson mean-field theory for the Hubbard model [38] mentioned at the beginning of Section 4. In fact, one finds that in $d = \infty$ the general set of Gutzwiller-correlated wave functions (21) with (22) reproduce the full set of static saddle-point equations of the slave-boson approach. This provides a direct connection between two seemingly different approaches, the slave-boson mean-field theory and the diagrammatic calculation of expectation values in terms of the Gutzwiller wave function in the limit $d = \infty$. It also shows that the slave-boson approach obeys the variational principle and is valid for an arbitrary starting wave function $|\tilde{\Psi}_0\rangle$; for a brief review see Ref. [53].

Calculations with the Gutzwiller wave function in $d = \infty$ are thus possible without the calculation of a single diagram. Later Gebhard and collaborators generalized this approach to multi-band Hubbard models. This led them to the formulation of a *Gutzwiller density-functional theory* which can be used to calculate, for example, the dispersion of quasi-particle excitations in the Fermi liquid state of transition metals and other materials [54, 55].

4.2 Lattice fermions in infinite spatial dimensions

By studying the Hubbard model with the Gutzwiller wave function Walter Metzner and I had found that in the limit $d \to \infty$ diagrammatic calculations greatly simplify. Apparently, this limit was not only useful for the investigation of spin models, but also in the case of lattice fermions. To better understand this point, we analyzed the diagrams involved in the calculation of expectation values with the Gutzwiller wave function in more detail. As mentioned earlier, the form of the diagrams is identical to that of the usual Feynman diagrams in many-body perturbation theory, but lines correspond to one-particle density matrices, $g^0_{ij,\sigma} = \langle \hat{c}^\dagger_{i\sigma} \hat{c}_{j\sigma} \rangle_0$. We showed that in the limit $d \to \infty$ diagrams collapse in position space [50, 51], such that only local contributions remain (Fig. 3). In other words, momentum conservation at a vertex of a skeleton diagram becomes irrelevant in the limit $d \to \infty$, implying that the momenta carried by the lines of a graph are indeed independent. In particular, the diagrams contributing to the proper self-energy are purely diagonal in $d = \infty$.

4.2.1 Diagrammatic collapse in $d = \infty$

The reason behind the diagrammatic collapse can be understood as follows. The one-particle density matrix may be interpreted as the amplitude for transitions between site $\boldsymbol{R}_i$ and $\boldsymbol{R}_j$. The square of its absolute value is therefore proportional to the *probability* for a particle to hop from $\boldsymbol{R}_j$ to a site $\boldsymbol{R}_i$. In the case of nearest-neighbor sites $\boldsymbol{R}_i$, $\boldsymbol{R}_j$ on a lattice with coordination number Z, this implies $|g^0_{ij,\sigma}|^2 \sim \mathcal{O}(1/Z)$. For nearest-neighbor sites $\boldsymbol{R}_i$, $\boldsymbol{R}_j$ on a hypercubic lattice (where $Z = 2d$), one therefore finds for large d

$$g^0_{ij,\sigma} \sim \mathcal{O}\left(\frac{1}{\sqrt{d}}\right). \tag{25}$$

For general i, j one finds [56, 51]

$$g^0_{ij,\sigma} \sim \mathcal{O}\Big(1/d^{\|\boldsymbol{R}_i - \boldsymbol{R}_j\|/2}\Big), \tag{26}$$

where $\| \boldsymbol{R} \| = \sum_{n=1}^{d} |R_n|$ is the length of $\boldsymbol{R}$ in the Manhattan metric.
It is important to bear in mind that, although $g^0_{ij,\sigma} \sim 1/\sqrt{d}$ vanishes for $d \to \infty$, the particles are not localized but are still mobile. Indeed, even in the limit $d \to \infty$ the off-diagonal elements of $g^0_{ij,\sigma}$ contribute, since a particle may hop to d nearest neighbors with reduced amplitude $t^*/\sqrt{d}$. For non-interacting electrons at $T = 0$ the expectation value of the kinetic energy is given by

$$E^0_{\rm kin} = -t \sum_{\langle \boldsymbol{R}_i, \boldsymbol{R}_j \rangle} \sum_{\sigma} g^0_{ij,\sigma} \, . \tag{27}$$

On a hypercubic lattice the sum over the nearest neighbors (NN) leads to a factor $\mathcal{O}(d)$. In view of the $1/\sqrt{d}$ dependence of $g^0_{ij,\sigma}$ it is therefore necessary to scale the NN-hopping amplitude t

$$t \to \frac{t^*}{\sqrt{d}}, \; t^* = \text{const.}, \tag{28}$$

since only then the kinetic energy remains finite for $d \to \infty$. The same result is obtained in a momentum-space formulation.[7]
A rescaling of the microscopic parameters of the Hubbard model with d is only required in the kinetic energy. Namely, since the interaction term is purely local, it is independent of the spatial dimension. Altogether this implies that only the Hubbard Hamiltonian with a rescaled kinetic energy

$$\hat{H} = -\frac{t^*}{\sqrt{d}} \sum_{\langle \boldsymbol{R}_i, \boldsymbol{R}_j \rangle} \sum_{\sigma} \hat{c}^\dagger_{i\sigma} \hat{c}_{j\sigma} + U \sum_{\boldsymbol{R}_i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} \tag{29}$$

has a non-trivial $d \to \infty$ limit where both terms, the kinetic energy and the interaction, are of the same order of magnitude in d.

[7] This can be seen by calculating the density of states (DOS) of non-interacting particles. For nearest-neighbor hopping on a d-dimensional hypercubic lattice $\varepsilon_{\boldsymbol{k}}$ has the form $\varepsilon_{\boldsymbol{k}} = -2t \sum_{i=1}^{d} \cos k_i$ (here and in the following we set Planck's constant $\hbar$, Boltzmann's constant k_B, and the lattice spacing equal to unity). The DOS corresponding to $\varepsilon_{\boldsymbol{k}}$ is given by $N_d(\omega) = \sum_{\boldsymbol{k}} \delta(\omega - \varepsilon_{\boldsymbol{k}})$, which is the probability density for finding the value $\omega = \varepsilon_{\boldsymbol{k}}$ for a random choice of $\boldsymbol{k} = (k_1, \ldots, k_d)$. If the momenta k_i are chosen randomly, $\varepsilon_{\boldsymbol{k}}$ is the sum of d independent (random) numbers $-2t \cos k_i$. The central limit theorem then implies that in the limit $d \to \infty$ the DOS is given by a Gaussian, i.e., $N_d(\omega) \stackrel{d\to\infty}{\longrightarrow} \frac{1}{2t\sqrt{\pi d}} \exp\Big[-\Big(\frac{\omega}{2t\sqrt{d}}\Big)^2\Big]$. Only if t is scaled with d as in (28) does one obtain a non-trivial DOS $N_\infty(\omega)$ in $d = \infty$ [57, 50] and thus a finite kinetic energy.

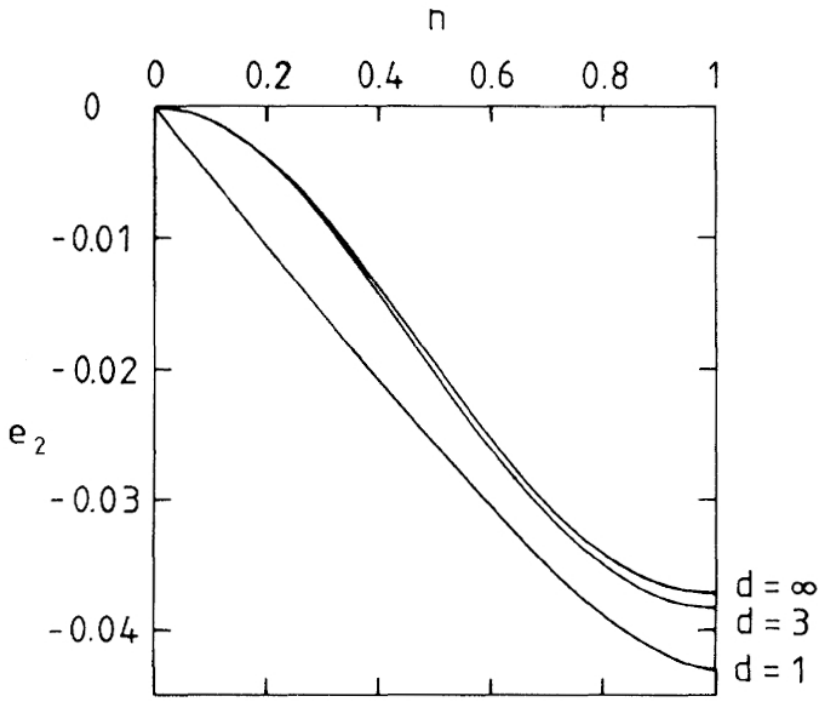

Fig. 4: *Correlation energy $E_c^{(2)} = (2U^2/|\varepsilon_0|)e_2$ of the Hubbard model calculated in second-order Goldstone perturbation theory in U vs. density n for dimensions $d = 1, 3, \infty$. Here ε_0 is the kinetic energy for $U = 0$ and $n = 1$; from Ref. [50].*

4.2.2 Simplifications of quantum many-body perturbation theory in the limit $d \to \infty$

Walter and I now wanted to understand to what extent the simplifications that occur in diagrammatic calculations with the Gutzwiller wave function in $d = \infty$ carry over to general many-body calculations for the Hubbard model. For this purpose, we evaluated the second-order diagram in Goldstone perturbation theory [58] that determines the correlation energy at weak coupling [50]. Due to the diagrammatic collapse in $d = \infty$, calculations were again found to be much simpler.[8] Namely, the nine-dimensional integral in $d = 3$ over the three internal momenta reduces to a single integral in $d = \infty$, implying that in $d = \infty$ the calculation is simpler than in any other dimension. More importantly, the numerical value obtained in $d = \infty$ turned out to be very close to that in the physical dimension $d = 3$ and therefore provides an easily tractable, quantitatively reliable approximation (see Fig. 4).

These results clearly showed that microscopic calculations for correlated lattice fermions in $d = \infty$ dimensions were useful and very promising. Further insights were made quickly: Müller-Hartmann [59] showed that in infinite dimensions only on-site interactions remain dynamical,

[8] The one-particle Green function (propagator) $G^0_{ij,\sigma}(\omega)$ of the non-interacting system obeys the same $1/\sqrt{d}$ dependence as the one-particle density matrix $g^0_{ij,\sigma}$ (see (25)). This follows directly from $g^0_{ij,\sigma} = \lim_{t\to 0^-} G^0_{ij,\sigma}(t)$ and the fact that the scaling properties do not depend on the time evolution and the quantum mechanical representation. The Fourier transform of $G^0_{ij,\sigma}(\omega)$ also preserves this property. For this reason the same results as those obtained in the calculation with the Gutzwiller wave function hold: all connected one-particle irreducible diagrams collapse in position space, i.e., they are purely diagonal in $d = \infty$.

that the proper self-energy becomes momentum-independent

$$\Sigma_\sigma(\boldsymbol{k},\omega) \overset{d\to\infty}{\equiv} \Sigma_\sigma(\omega) \tag{30a}$$

and hence is purely local in position space

$$\Sigma_{ij,\sigma}(\omega) \overset{d\to\infty}{=} \Sigma_{ii,\sigma}(\omega)\delta_{ij}\,, \tag{30b}$$

as in the case of diagrams calculated with the Gutzwiller wave function [50, 51], and therefore typical Fermi liquid features are preserved (Sec. 4.2.5) [60]. Schweitzer and Czycholl [61] demonstrated that calculations for the periodic Anderson model also become much simpler in high dimensions.[9] In particular, Brandt and Mielsch [65] derived the exact solution of the Falicov-Kimball model for infinite dimensions by mapping the lattice problem onto a solvable atomic problem in a generalized, time-dependent external field.[10] They also noted that such a mapping is, in principle, also possible for the Hubbard model.

Due to the property (30), the most important obstacle for actual diagrammatic calculations in finite dimensions $d \geq 1$ – namely, the integration over intermediate momenta – is greatly simplified in $d = \infty$. Nevertheless, the limit $d \to \infty$ does not affect the *dynamics* of the system. Hence, in spite of the simplifications in position (or momentum) space, the problem retains its full dynamics in $d = \infty$.

4.2.3 Interactions beyond the on-site interaction

In the case of more general interactions than the Hubbard interaction, e.g., nearest neighbor interactions such as

$$\hat{H}_{nn} = \sum_{\langle \boldsymbol{R}_i,\boldsymbol{R}_j\rangle} \sum_{\sigma\sigma'} V_{\sigma\sigma'}\hat{n}_{i\sigma}\hat{n}_{j\sigma'} \tag{31}$$

the interaction constant has to be scaled, too, in the limit $d \to \infty$. In the case of (31), which has the form of a classical interaction, the "classical" scaling

$$V_{\sigma\sigma'} \to \frac{V^*_{\sigma\sigma'}}{Z} \tag{32}$$

is required. Of course, the propagator still has the dependence (26). Due to (32), all contributions, except for the Hartree-term, are found to vanish in $d = \infty$ [59]. Hence, nonlocal interactions only contribute through their Hartree approximation, which is purely static. This gives the Hubbard interaction a unique role: of all interactions for fermionic lattice models only the Hubbard interaction remains dynamical in the limit $d \to \infty$ [59].

[9] For a more detailed discussion of the simplifications occurring in the investigation of Hubbard-type lattice models or the t-J model [62, 63] in high dimensions see Ref. [64].

[10] Alternatively, it can be shown that in the limit $Z \to \infty$ the dynamics of the Falicov-Kimball model reduces to that of a *non*-interacting, tight-binding model on a Bethe lattice with coordination number $Z = 3$, which can thus be solved exactly [66].

4.2.4 One-particle propagator

Due to the $\boldsymbol{k}$-independence of the irreducible self-energy, (30a), the one-particle propagator of an interacting lattice fermion system is given by

$$G_{\boldsymbol{k},\sigma}(\omega) = \frac{1}{\omega - \varepsilon_{\boldsymbol{k}} + \mu - \Sigma_\sigma(\omega)}\,. \tag{33}$$

Most importantly, the $\boldsymbol{k}$ dependence of $G_{\boldsymbol{k}}(\omega)$ comes entirely from the energy dispersion $\varepsilon_{\boldsymbol{k}}$ of the *non*-interacting particles. This means that in a homogeneous system described by the propagator

$$G_{ij,\sigma}(\omega) = \frac{1}{L}\sum_{\boldsymbol{k}} G_{\boldsymbol{k},\sigma}(\omega)\, e^{i\boldsymbol{k}\cdot(\boldsymbol{R}_i - \boldsymbol{R}_j)}\,, \tag{34}$$

its local part, $G_{ii,\sigma}$, is given by

$$G_{ii,\sigma}(\omega) = \frac{1}{L}\sum_{\boldsymbol{k}} G_{\boldsymbol{k},\sigma}(\omega) = \int\limits_{-\infty}^{\infty} d\varepsilon\, \frac{N_0(\varepsilon)}{\omega - \varepsilon + \mu - \Sigma_\sigma(\omega)}\,, \tag{35}$$

where $N_0(\varepsilon)$ is the density of states of the non-interacting system. In the paramagnetic phase we can suppress site and spin indices and write $G_{ii,\sigma}(\omega) \equiv G(\omega)$. The spectral function of the interacting system (often referred to as the DOS as in the non-interacting case) is then given by

$$A(\omega) = -\frac{1}{\pi}\,\mathrm{Im}\, G(\omega + i0^+)\,. \tag{36}$$

4.2.5 Consequences of the $\boldsymbol{k}$-independence of the self-energy: Fermi liquid behavior

We now discuss some further consequences of the $\boldsymbol{k}$-independence of the self-energy in the paramagnetic phase as derived by Müller-Hartmann [60]. At $T = 0$, the one-particle propagator (33) takes the form (again we suppress the spin index)

$$G_{\boldsymbol{k}}(\omega) = \frac{1}{\omega - \varepsilon_{\boldsymbol{k}} + E_F - \Sigma(\omega)}\,. \tag{37}$$

In general, even when $\Sigma(\omega)$ is $\boldsymbol{k}$-dependent, the Fermi surface is defined by the $\omega = 0$ limit of the denominator of (37) as

$$\varepsilon_{\boldsymbol{k}} + \Sigma_{\boldsymbol{k}}(0) = E_F. \tag{38a}$$

According to Luttinger and Ward [67], the volume within the Fermi surface is not changed by interactions, provided the latter can be treated in perturbation theory. This is expressed by

$$n = \sum_{\boldsymbol{k}\sigma} \Theta\Big(E_F - \varepsilon_{\boldsymbol{k}} - \Sigma_{\boldsymbol{k}}(0)\Big), \tag{38b}$$

where n is the particle density and $\Theta(x)$ is the step function. The $\boldsymbol{k}$-dependence of $\Sigma_{\boldsymbol{k}}(0)$ in (38a) implies that, in spite of (38b), the shape of the Fermi surface of the interacting system will be quite different from that of the non-interacting system (except for the rotationally invariant

case $\varepsilon_{\boldsymbol{k}} = f(|\boldsymbol{k}|)$. By contrast, for lattice fermion models in $d = \infty$, where $\Sigma_{\boldsymbol{k}}(\omega) \equiv \Sigma(\omega)$, the Fermi surface itself (and hence the volume enclosed) is not changed by interactions. The Fermi energy is simply shifted uniformly from its non-interacting value E_F^0, i.e., $E_F = E_F^0 + \Sigma(0)$, to keep n in (38b) constant. Thus the $\omega = 0$ value of the local propagator, $G(0)$, and hence of the spectral function, $A(0) = -\frac{1}{\pi}\,\mathrm{Im}\,G(i0^+)$, is not changed by interactions. This behavior is well-known from the single-impurity Anderson model [4]. Renormalizations of $N(0)$ can only come from a $\boldsymbol{k}$-dependence of Σ, i.e., if $\partial\Sigma/\partial\boldsymbol{k} \neq 0$.
For $\omega \to 0$ the self-energy has the property

$$\mathrm{Im}\,\Sigma(\omega) \propto \omega^2, \tag{38c}$$

which implies Fermi liquid behavior. The effective mass of the quasiparticles

$$\frac{m^*}{m} = 1 - \left.\frac{d\Sigma}{d\omega}\right|_{\omega=0} = 1 + \frac{1}{\pi}\int_{-\infty}^{\infty} d\omega\, \frac{\mathrm{Im}\Sigma(\omega + i0^-)}{\omega^2} \;\geq\; 1 \tag{38d}$$

is seen to be enhanced. In particular, the momentum distribution

$$n_{\boldsymbol{k}} = \frac{1}{\pi}\int_{-\infty}^{0} d\omega\, \mathrm{Im}\,G_{\boldsymbol{k}}(\omega) \tag{39}$$

has a discontinuity at the Fermi surface, given by $n_{k_F^-} - n_{k_F^+} = (m^*/m)^{-1}$, where $k_F^{\pm} = k_F \pm 0^+$.

5 Dynamical mean-field theory for correlated lattice fermions

The diagrammatic simplifications of many-body perturbation theory in infinite spatial dimensions provide the basis for the construction of a comprehensive mean-field theory for lattice fermions that is diagrammatically controlled and whose free energy has no unphysical singularities. The construction is based on the scaled Hamiltonian (29). Since the self-energy is momentum independent but retains its frequency dependence, i.e., describes the full many-body dynamics of the interacting system,[11] the resulting theory is mean-field-like *and* dynamical and hence represents a *dynamical mean-field theory* (DMFT) for lattice fermions which is able to describe genuine correlation effects.

5.1 Derivation of the self-consistent DMFT equations

The DMFT equations can be derived in different ways. They all employ the fact that in $d = \infty$ lattice fermion models with a local interaction reduce to an effective many-body problem whose dynamics corresponds to that of correlated fermions on a single site embedded in a bath provided by the other fermions. This is illustrated in Fig. 5.
The single-site action and the DMFT equations were first derived by Václav Janiš [68] within a generalization of the self-consistent coherent potential approximation (CPA)[12] to lattice fermion

[11] This is in contrast to Hartree-Fock theory where the self-energy is merely a static potential.

[12] The CPA is a well-known mean-field theory for non-interacting, disordered systems. It becomes exact in the limit $d, Z \to \infty$ [69].

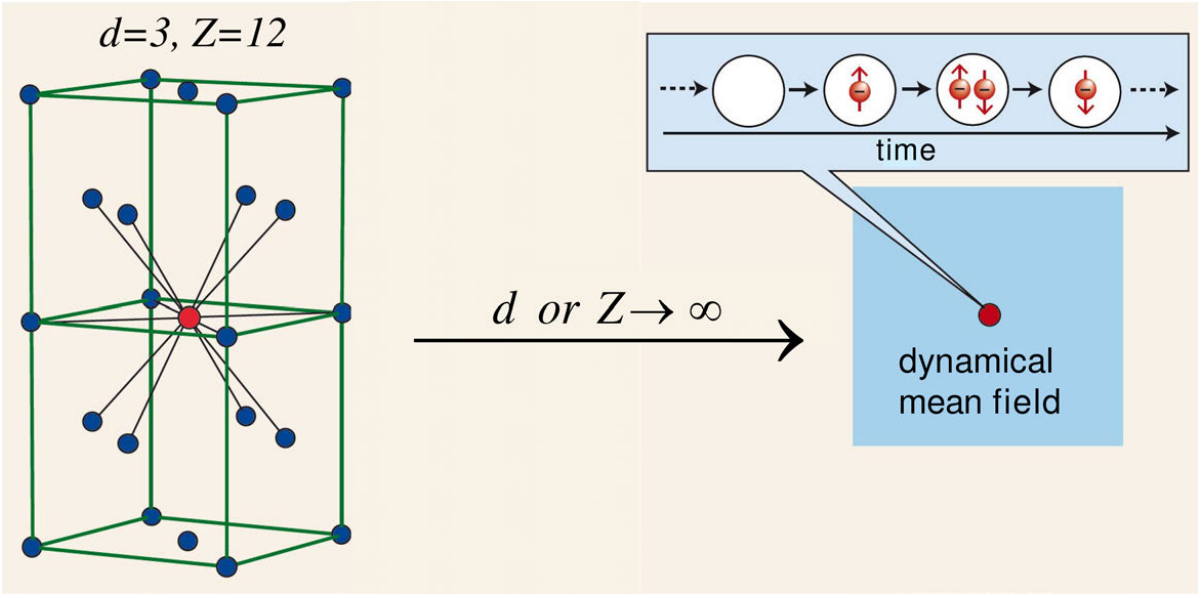

Fig. 5: *In the limit $Z \to \infty$ the Hubbard model effectively reduces to a dynamical single-site problem, which may be viewed as a lattice site embedded in a dynamical mean field. Electrons may hop from the mean field onto this site and back, and interact on the site as in the original Hubbard model (see Fig. 1). The local propagator $G(\omega)$, i.e., the return amplitude, and the dynamical self-energy $\Sigma(\omega)$ of the surrounding mean field play the main role in this limit. The quantum dynamics of the interacting electrons is still described exactly.*

models with local interaction and local self-energy, such as the Falicov-Kimball and Hubbard model in the limit $d = \infty$; for details see Refs. [68, 70, 18]. Shortly after that Václav joined me, then at the RWTH Aachen University, on an Alexander-von-Humboldt fellowship. Before we could start to solve the self-consistency equations [70], I received a preprint from Antoine Georges and Gabi Kotliar [71] in which they had formulated the DMFT by mapping the lattice problem onto a self-consistent single-impurity Anderson model. This mapping was also employed by Mark Jarrell [72].

Although the DMFT equations derived within the CPA approach and the single-impurity approach are identical, the latter was immediately adopted by the community since it is connected with the well-studied theory of quantum impurities and Kondo problems [4], for whose solution efficient numerical codes such as the quantum Monte-Carlo (QMC) method [73] had been developed and were readily available. For this reason the single-impurity based derivation of the DMFT immediately became the standard approach. For a detailed discussion see the review by Georges, Kotliar, Krauth, and Rozenberg [74]; for an introductory presentation see the article by Gabi Kotliar and myself [75].

The DMFT equations are given by

(A) the *local propagator* $G_\sigma(i\omega_n)$, which is expressed as a functional integral

$$G_\sigma(i\omega_n) = -\frac{1}{\mathcal{Z}} \int \prod_\sigma Dc^*_\sigma Dc_\sigma \; [c_\sigma(i\omega_n) c^*_\sigma(i\omega_n)] \; e^{-S_{\rm loc}} \tag{40}$$

with the partition function

$$\mathcal{Z} = \int \prod_{\sigma} Dc_{\sigma}^{*} Dc_{\sigma}\, e^{-S_{\rm loc}} \tag{41}$$

and the local action

$$S_{\rm loc} = -\int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \sum_{\sigma} c_{\sigma}^{*}(\tau_1)\mathcal{G}_{\sigma}^{-1}(\tau_1 - \tau_2)c_{\sigma}(\tau_2) + U\int_0^\beta d\tau\, c_{\uparrow}^{*}(\tau)c_{\uparrow}(\tau)c_{\downarrow}^{*}(\tau)c_{\downarrow}(\tau). \tag{42}$$

Here $\mathcal{G}_\sigma$ is the effective local propagator (also called *bath Green function*, or *Weiss mean field*)[13] which is defined by a Dyson-type equation

$$\mathcal{G}_\sigma(i\omega_n) = \Big([G_\sigma(i\omega_n)]^{-1} + \Sigma_\sigma(i\omega_n)\Big)^{-1}. \tag{43}$$

Furthermore, by identifying the Hilbert transform of the *lattice Green function*

$$G_{\boldsymbol{k}\,\sigma}(i\omega_n) = \frac{1}{i\omega_n - \varepsilon_{\boldsymbol{k}} + \mu - \Sigma_\sigma(i\omega_n)} \tag{44}$$

with the local propagator (40) one obtains
(B) the *self-consistency condition*

$$G_\sigma(i\omega_n) = \frac{1}{L}\sum_{\boldsymbol{k}} G_{\boldsymbol{k}\,\sigma}(i\omega_n) \;=\; \int_{-\infty}^{\infty} d\varepsilon\, \frac{N(\varepsilon)}{i\omega_n - \varepsilon + \mu - \Sigma_\sigma(i\omega_n)} \tag{45}$$

$$= \; G_\sigma^0(i\omega_n - \Sigma_\sigma(i\omega_n))\,. \tag{46}$$

In (45) the ionic lattice on which the electrons live is seen to enter only through the DOS of the non-interacting electrons. Eq. (46) illustrates the mean-field character of the DMFT-equations particularly clearly: the local Green function of the interacting system is given by the *non-interacting* Green function G_σ^0 with a renormalized energy $i\omega_n - \Sigma_\sigma(i\omega_n)$, which corresponds to the energy $i\omega_n$ measured relative to the energy of the surrounding dynamical fermionic bath, i.e., the energy of the mean field $\Sigma_\sigma(i\omega_n)$.
The self-consistent DMFT equations can be solved iteratively: starting with an initial value for the self-energy $\Sigma_\sigma(i\omega_n)$ one obtains the local propagator $G_\sigma(i\omega_n)$ from (45) and thereby the bath Green function $\mathcal{G}_\sigma(i\omega_n)$ from (43). This determines the local action (42) that is needed to compute a new value for the local propagator $G_\sigma(i\omega_n)$ from (40) and, by employing the old self-energy, a new bath Green function $\mathcal{G}_\sigma$, and so on. In spite of the fact that the solution can be obtained self-consistently, there remains a complicated many-body problem which is generally not exactly solvable. A generalization of the DMFT equations for the Hubbard model in the presence of local disorder was derived in Ref. [76].
It should be stressed that although the DMFT corresponds to an effectively local problem, the propagator $G_{\boldsymbol{k}}(\omega)$ is a momentum-dependent quantity. Namely, it depends on the momentum through the dispersion $\varepsilon_{\boldsymbol{k}}$ of the non-interacting electrons. However, there is no additional momentum-dependence through the self-energy, since it is strictly local within the DMFT.

[13] In principle, the local functions $\mathcal{G}_\sigma(i\omega_n)$ and $\Sigma_\sigma(i\omega_n)$ can both be viewed as a "dynamical mean field" acting on particles on a site, since they all appear in the bilinear term of the local action (42).

5.1.1 Solution of the self-consistent DMFT equations

The dynamics of the Hubbard model remains complicated even in the limit $d = \infty$ due to the purely local nature of the interaction. Hence an exact, analytic evaluation of the self-consistent set of equations for the local propagator G_σ or the effective propagator $\mathcal{G}_\sigma(i\omega_n)$ is not possible. A valuable semi-analytic approximation is provided by the *iterated perturbation theory* (IPT) [71,77]. Exact evaluations become feasible when there is no coupling between the frequencies. This is the case, for example, in the Falicov-Kimball model [65, 78].
Solutions of the self-consistent DMFT equations require extensive numerical methods, in particular quantum Monte Carlo simulations [72, 79, 80, 74, 81], the numerical renormalization group [82–84], exact diagonalization [85–87], and other techniques.
It quickly turned out that the DMFT is a powerful tool for the investigation of electronic systems with strong correlations [88, 74]. It provides a non-perturbative and thermodynamically consistent approximation scheme for finite-dimensional systems that is particularly valuable for the study of intermediate-coupling problems where perturbative techniques fail; for detailed discussions see Refs. [89, 75, 90, 91, 43].

5.2 The LDA+DMFT approach to correlated materials

The Hubbard model is able to explain important general features of correlated electrons, but it cannot describe the physics of real materials in any detail. Namely, realistic approaches must take into account the explicit electronic and lattice structure of the systems.
For a long time the electronic properties of solids were investigated by two essentially separate communities, one using model Hamiltonians in conjunction with many-body techniques, the other employing density functional theory (DFT) [92, 93]. DFT and its local-density approximation (LDA) are *ab initio* approaches that do not require empirical parameters as input. They proved to be highly successful techniques for the calculation of the electronic structure of real materials [94]. Still, it was soon recognized that DFT/LDA is severely restricted in its ability to describe strongly correlated materials such as f-electron systems and Mott insulators. For such systems the model Hamiltonian approach is more powerful since there exist systematic theoretical techniques to investigate the many-electron problem with increasing accuracy. Nevertheless, the uncertainty in the choice of the model parameters and the technical complexity of the correlation problem itself prevent the model Hamiltonian approach from being flexible enough to study real materials. The two approaches are therefore largely complementary. In view of the individual power of DFT/LDA and the model Hamiltonian approach, respectively, a combination of these techniques for *ab initio* investigations of real materials is clearly desirable. One of the first successful attempts in this direction was the LDA+U method [95, 96], which combines LDA with a Hartree-like, static mean-field approximation for a multi-band Anderson lattice model. This method turned out to be a very useful tool in the study of long-range ordered, insulating states of transition metals and rare-earth compounds. However, the *paramagnetic* metallic phase of correlated electron systems clearly requires a treatment which includes dynamical effects, i.e., the frequency dependence of the self-energy.

Here the so-called LDA+DMFT approach, whose foundations were laid in the papers by Anisimov, Poteryaev, Korotin, Anokhin, and Kotliar [97] as well as Lichtenstein and Katsnelson [98], has led to an enormous progress in our understanding of correlated electron materials [97–106, 75]. LDA+DMFT is a computational scheme that merges electronic band structure calculations in the local density approximation (LDA) or generalized-gradient approximations (GGA) with many-body physics originating from the local Hubbard interaction and Hund's rule coupling terms, and then solves the corresponding correlation problem by DMFT. Sometimes this combined approach is also referred to as DFT+DMFT.
As in the case of the Hubbard model the many-body model constructed within the LDA+DMFT scheme consists of two parts: a kinetic energy which describes the specific band structure of the uncorrelated electrons, and the local interactions between the electrons in the same orbital as well as in different orbitals. It is then necessary to take into account a double counting of the interaction, since the LDA already includes some of the static contributions of the electronic interaction; for details, see Refs. [101–106]). This complicated many-particle problem with its numerous energy bands and local interactions is then solved within DMFT, usually by the application of quantum Monte-Carlo (QMC) techniques. By construction, LDA+DMFT includes the correct quasiparticle physics and the corresponding energetics. It also reproduces the LDA results in the limit of weak Coulomb interaction U. More importantly, LDA+DMFT correctly describes the correlation induced dynamics near a Mott-Hubbard metal-insulator transition and beyond. Thus, LDA+DMFT and related, material-specific dynamical mean-field approaches that are presently being developed [107–109] are, in principle, able to account for the physics at all values of the Coulomb interaction and doping.

6 Summary and outlook

By now the DMFT has developed into a powerful method for the investigation of electronic systems with strong correlations. It provides a comprehensive, non-perturbative and thermodynamically consistent approximation scheme for the investigation of finite-dimensional systems (in particular for dimension $d = 3$), and is particularly useful for the study of problems where perturbative approaches fail. For this reason, the DMFT has now become the standard mean-field theory for fermionic correlation problems. The generalization of this approach and its applications is currently a subject of active research. Here non-local generalizations of the DMFT play an important role [90, 81]. They make it possible to study and explain even short range correlation effects which occur on the scale of several lattice constants. Furthermore, investigations of inhomogeneous bulk systems and of internal and external inhomogeneities, such as surfaces and interfaces [110–116], lead to an improved understanding of correlation effects in thin films and multi-layered nanostructures. This is particularly desirable in view of the novel functionalities of these structures and their possible applications in electronic devices.
The investigation of correlation phenomena in the field of cold atoms in optical lattices is another intriguing field of current research. Within a short time it led to the development of a versatile instrument for the simulation and investigation of quantum mechanical many-particle

systems [117–121]. While for electrons in solids the Hubbard model with its purely local interaction is a rather strong assumption, it can describe cold atoms in optical lattices very accurately since the interaction between the atoms is indeed extremely short ranged. Here the DMFT has once again proved to be extremely useful. Experiments with cold atoms in optical lattices can even assess the quality of the results of the DMFT. The results obtained in this way show that the DMFT indeed leads to reliable results even for finite dimensional systems [120].
The study of correlated electrons out of equilibrium within non-equilibrium DMFT [122–128] has become yet another fascinating new research area. Non-equilibrium DMFT will be able to explain, and even predict, the results of time-resolved experiments; for an upcoming review, see Ref. [129].
The combination of the DMFT with methods for the computation of electronic band structures (LDA+DMFT) has led to a conceptually new theoretical framework for the realistic study of correlated materials. In 10 to 15 years from now, DMFT-based approaches can be expected to be as successful and standardized as the presently available density-functional methods. The development of a comprehensive theoretical approach which allows for a quantitative understanding and prediction of correlation effects in materials, ranging from complex inorganic materials all the way to biological systems, is one of the great challenges for modern theoretical physics. For details I refer to the scientific program of the Research Unit FOR 1346 *Dynamical Mean-Field Approach with Predictive Power for Strongly Correlated Materials* [130] which is being funded by the Deutsche Forschungsgemeinschaft since 2010. The Research Unit FOR 1346 initiated the series of Autumn Schools on correlated materials which are held at the Forschungszentrum Jülich since 2011. The lecture notes of these Autumn Schools provide an excellent introduction into this very active field of research [131–134].

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References

[1] N.F. Mott, Rev. Mod. Phys. **40**, 677 (1968)

[2] N.F. Mott, *Metal-Insulator Transitions* (Taylor and Francis, London, 2nd ed., 1990)

[3] M. Imada, A. Fujimori, and Y. Tokura, Rev. Mod. Phys. **70**, 1039 (1998)

[4] A.C. Hewson, *The Kondo Problem to Heavy Fermions* (Cambridge University Press, 1997)

[5] N. Grewe and F. Steglich, in *Handbook on the Physics and Chemistry of Rare Earths*, Vol. 14, ed. by K.A. Gschneidner, L. Eyring (North Holland, Amsterdam, 1991), p. 343

[6] K. Baberschke, M. Donath, and W. Nolting (eds.): *Band-Ferromagnetism*, Lecture Notes in Physics, Vol. 580, (Springer, Heidelberg, 2001)

[7] J.R. Schrieffer (ed.): *Handbook of High-Temperature Superconductivity* (Springer, Berlin, 2007)

[8] E. Dagotto: *Nanoscale Phase Separation and Collossal Magnetoresistance* (Springer, Berlin, 2002)

[9] H. v. Löhneysen, A. Rosch, M. Vojta, and P. Wölfle, Rev. Mod. Phys. **79**, 1015 (2007)

[10] Y. Tokura, Physics Today, July 2003, p. 50.

[11] J.H. de Boer and E.J.W. Verwey, Proc. Phys. Soc. **49, No. 4S**, 59 (1937)

[12] N.F. Mott and R. Peierls, Proc. Phys. Soc. A **49**, 72 (1937)

[13] M.C. Gutzwiller, Phys. Rev. Lett. **10**, 159 (1963)

[14] J. Hubbard, Proc. Roy. Soc. London A **276**, 238 (1963)

[15] J. Kanamori, Prog. Theor. Phys. **30**, 275 (1963)

[16] E. Lieb and F.Y. Wu, Phys. Rev. Lett. **20**, 1445 (1968)

[17] P. Fulde: *Electron Correlations in Molecules and Solids* (Springer, Berlin, 1995)

[18] D. Vollhardt, p. 339 in *Lectures on the Physics of Strongly Correlated Systems XIV*, AIP Conference Proceedings vol. 1297, ed. by A. Avella and F. Mancini (American Institute of Physics, Melville, 2010); `http://arxiv.org/abs/1004.5069v3`

[19] R.J. Baxter: *Exactly Solved Models in Statistical Mechanics* (Academic Press, London, 1982)

[20] E. Feenberg: *Theory of Quantum Fluids* (Academic, New York, 1969)

[21] R.P. Feynman: *Statistical Physics* (Benjamin, Reading, 1972)

[22] V.R. Pandharipande and R.B. Wiringa, Rev. Mod. Phys. **51**, 821 (1979)

[23] R.B. Laughlin, Phys. Rev. Lett. **50**, 1395 (1983)

[24] C.M. Varma and Y. Yafet, Phys. Rev. B **13**, 2950 (1976)

[25] O. Gunnarsson and K. Schönhammer, Phys. Rev. B **28**, 4315 (1983)

[26] P.W. Anderson, P.A. Lee, M. Randeria, T.M. Rice, N. Trivedi, and F.C. Zhang, J. Phys.: Condens. Matter **16**, R755 (2004)

[27] J. Bardeen, L.N. Cooper and J.R. Schrieffer, Phys. Rev. **108**, 1175 (1957)

[28] M.C. Gutzwiller, Phys. Rev. **137**, A1726 (1965)

[29] T. Ogawa, K. Kanda, and T. Matsubara, Prog. Theor. Phys. **53**, 614 (1975)

[30] D. Vollhardt, Rev. Mod. Phys. **56**, 99 (1984)

[31] P.G.J. van Dongen and D. Vollhardt, Phys. Rev. B **40**, 7252 (1989)

[32] W.F. Brinkman and T.M. Rice, Phys. Rev. B **2**, 4302 (1970)

[33] T.M. Rice and W.F. Brinkman, in *Alloys, Magnets, and Superconductors*, ed. by R.E. Mills, E. Ascher, and R. Jaffee (McGraw-Hill, New York, 1971), p. 593

[34] K. Levin and O.T. Valls, Phys. Rep. **98**, 1 (1983)

[35] P.W. Anderson and W.F. Brinkman, in *The Physics of Liquid and Solid Helium*, Part II, ed. by K.H. Bennemann and J.B. Ketterson (Wiley, New York, 1978), p. 177

[36] D. Vollhardt, P. Wölfle, and P.W. Anderson, Phys. Rev. B **35**, 6703 (1987)

[37] For a personal account by Andrei Ruckenstein of the developments leading to the formulation of the Kotliar-Ruckenstein slave-boson mean-field theory see: `http://www.aspenphys.org/aboutus/history/presidentialessays/ruckenstein.html`

[38] G. Kotliar and A.E. Ruckenstein, Phys. Rev. Lett. **57**, 1362 (1986)

[39] D. Vollhardt, Ann. Phys. (Berlin), **524**, 1 (2012) [Einstein Lecture] `http://dx.doi.org/10.1002/andp.201100250`

[40] W. Metzner and D. Vollhardt, Phys. Rev. Lett. **59**, 121 (1987)

[41] W. Metzner and D. Vollhardt, Phys. Rev. B **37**, 7382 (1988)

[42] T.A. Kaplan, P. Horsch and P. Fulde, Phys. Rev. Lett. **49**, 889 (1982)

[43] D. Vollhardt, p. 31 in *Proceedings of the International School of Physics Enrico Fermi, Course CXXI*, ed. by R.A. Broglia and J.R. Schrieffer (North-Holland, Amsterdam, 1994); http://www.physik.uni-augsburg.de/theo3/Research/research_varenna.vollha.de.shtml

[44] F. Gebhard and D. Vollhardt, Phys. Rev. Lett. **59**, 1472 (1987)

[45] F. Gebhard and D. Vollhardt, Phys. Rev. B **38**, 6911 (1988)

[46] R.R.P. Singh, M.E. Fisher, and R. Shankar, Phys. Rev. B **39**, 2562 (1989)

[47] T. Giamarchi and H.J. Schulz, Phys. Rev. B **39**, 4620 (1989)

[48] F.D.M. Haldane, Phys. Rev. Lett. **60**, 635 (1988)

[49] B.S. Shastry, Phys. Rev. Lett. **60**, 639 (1988)

[50] W. Metzner and D. Vollhardt, Phys. Rev. Lett. **62**, 324 (1989)

[51] W. Metzner, Z. Phys. B **77**, 253 (1989)

[52] F. Gebhard, Phys. Rev. B **41**, 9452 (1990)

[53] D. Vollhardt, P.G.J. van Dongen, F. Gebhard, and W. Metzner, Mod. Phys. Lett. B **4**, 499 (1990)

[54] J. Bünemann, F. Gebhard, and W. Weber, Found. of Physics **30**, 2011 (2000)

[55] J. Bünemann, Chapt. 5 in [132]

[56] P.G.J. van Dongen, F. Gebhard, and D. Vollhardt, Z. Phys. **76**, 199 (1989)

[57] U. Wolff, Nucl. Phys. B **225**, 391 (1983)

[58] W. Metzner and D. Vollhardt, Phys. Rev. B **39**, 4462 (1989)

[59] E. Müller-Hartmann, Z. Phys. B **74**, 507 (1989)

[60] E. Müller-Hartmann, Z. Phys. B **76**, 211 (1989)

[61] H. Schweitzer and G. Czycholl, Solid State Comm. **69**, 171 (1989)

[62] W. Metzner, P. Schmit, and D. Vollhardt, Phys. Rev. B **45**, 2237 (1992)

[63] R. Strack and D. Vollhardt, Phys. Rev. B **46**, 13852 (1992)

[64] D. Vollhardt, p. 57 in *Correlated Electron Systems*, ed. by V.J. Emery (World Scientific, Singapore, 1993); http://www.physik.uni-augsburg.de/theo3/Research/research_jerusalem.vollha.en.shtml

[65] U. Brandt and C. Mielsch, Z. Phys. B **75**, 365 (1989)

[66] P.G.J. van Dongen and D. Vollhardt, Phys. Rev. Lett. **65**, 1663 (1990)

[67] J.M. Luttinger and J.C. Ward, Phys. Rev. **118**, 1417 (1960)

[68] V. Janiš, Z. Phys. B **83**, 227 (1991)

[69] R. Vlaming and D. Vollhardt, Phys. Rev. B, **45**, 4637 (1992)

[70] V. Janiš and D. Vollhardt, Int. J. Mod. Phys. B **6**, 731 (1992)

[71] A. Georges and G. Kotliar, Phys. Rev. B **45**, 6479 (1992)

[72] M. Jarrell, Phys. Rev. Lett. **69**, 168 (1992)

[73] J.E. Hirsch and R.M. Fye, Phys. Rev. Lett. **56**, 2521 (1986)

[74] A. Georges, G. Kotliar, W. Krauth, and M.J. Rozenberg, Rev. Mod. Phys. **68**, 13 (1996)

[75] G. Kotliar and D. Vollhardt, Physics Today, March 2004, p. 53

[76] V. Janiš and D. Vollhardt, Phys. Rev. B **46**, 15712 (1992)

[77] X.Y. Zhang, M.J. Rozenberg, and G. Kotliar, Phys. Rev. Lett. **70**, 1666 (1993)

[78] J.K. Freericks and V. Zlatić, Rev. Mod. Phys. **75**, 1333 (2003)

[79] M.J. Rozenberg, X.Y. Zhang, and G. Kotliar, Phys. Rev. Lett. **69**, 1236 (1992)

[80] A. Georges and W. Krauth, Phys. Rev. Lett. **69**, 1240 (1992)

[81] E. Gull, A.J. Millis, A.I. Lichtenstein, A.N. Rubtsov, M. Troyer, P. Werner, Rev. Mod. Phys. **83**, 349 (2011)

[82] R. Bulla, Phys. Rev. Lett. **83**, 136 (1999)

[83] W. Hofstetter, Phys. Rev. Lett. **85**, 1508 (2000)

[84] R. Bulla, T.A. Costi, and T. Pruschke, Rev. Mod. Phys. **80**, 395 (2008)

[85] M. Caffarel and W. Krauth, Phys. Rev. Lett. **72**, 1545 (1994)

[86] Q. Si, M.J. Rozenberg, G. Kotliar, and A.E. Ruckenstein, Phys. Rev. Lett. **72**, 2761 (1994)

[87] M.J. Rozenberg, G. Moeller, and G. Kotliar, Mod. Phys. Lett. B **8**, 535 (1994)

[88] T. Pruschke, M. Jarrell, and J.K. Freericks, Adv. Phys. **44**, 187 (1995)

[89] A. Georges, in *Lectures on the Physics of highly correlated electron systems VIII*, ed. by A. Avella and F. Mancini, AIP Conference Proceedings, Vol. 715 (American Institute of Physics, Melville, 2004), p. 3

[90] T. Maier, M. Jarrell, T. Pruschke, and M.H. Hettler, Rev. Mod. Phys. **77**, 1027 (2005)

[91] K. Byczuk, W. Hofstetter, and D. Vollhardt, in *Fifty Years of Anderson Localization*, ed. by E. Abrahams (World Scientific, Singapore, 2010), p. 473; reprinted in Int. J. Mod. Phys. B **24**, 1727 (2010)

[92] P. Hohenberg and W. Kohn, Phys. Rev. B **136**, 864 (1964)

[93] W. Kohn and L.J. Sham, Phys. Rev. **140**, A1133 (1965)

[94] R.O. Jones and O. Gunnarsson, Rev. Mod. Phys. **61**, 689 (1989)

[95] V.I. Anisimov, J. Zaanen, and O.K. Andersen, Phys. Rev. B **44**, 943 (1991)

[96] V.I. Anisimov, F. Aryasetiawan, and A.I. Lichtenstein, J. Phys.: Condens. Matter **9**, 767 (1997)

[97] V.I. Anisimov, A.I. Poteryaev, M.A. Korotin, A.O. Anokhin, and G. Kotliar, J. Phys.: Condens. Matter **9**, 7359 (1997)

[98] A.I. Lichtenstein and M.I. Katsnelson, Phys. Rev. B **57**, 6884 (1998)

[99] I.A. Nekrasov, K. Held, N. Blümer, A.I. Poteryaev, V.I. Anisimov, and D. Vollhardt, Eur. Phys. J. B **18**, 55 (2000)

[100] K. Held, I.A. Nekrasov, N. Blümer, V.I. Anisimov, and D. Vollhardt, Int. J. Mod. Phys. B **15**, 2611 (2001)

[101] A.I. Lichtenstein, M.I. Katsnelson, and G. Kotliar, p. 428 in *Electron Correlations and Materials Properties*, ed. by A. Gonis, N. Kioussis, and M. Ciftan (Plenum, NY, 2002)

[102] K. Held, I.A. Nekrasov, G. Keller, V. Eyert, N. Blümer, A.K. McMahan, R.T. Scalettar, T. Pruschke, V.I. Anisimov, and D. Vollhardt, Psi-k Newsletter **56**, 65 (2003); reprinted in Phys. Status Solidi B **243**, 2599 (2006)

[103] G. Kotliar, S.Y. Savrasov, K. Haule, V.S. Oudovenko, O. Parcollet, C.A. Marianetti, Rev. Mod. Phys. **78**, 865 (2006)

[104] K. Held, Adv. Phys. **56**, 829 (2007)

[105] M.I. Katsnelson, V.Yu. Irkhin, L. Chioncel, A.I. Lichtenstein, and R.A. de Groot, Rev. Mod. Phys. **80**, 315 (2008)

[106] J. Kuneš, I. Leonov, M. Kollar, K. Byczuk, V.I. Anisimov, and D. Vollhardt, Eur. Phys. J. Special Topics **180**, 5 (2010)

[107] S. Biermann, F. Aryasetiawan, and A. Georges, Phys. Rev. Lett. **90**, 086402 (2003)

[108] J. Minár, L. Chioncel, A. Perlov, H. Ebert, M.I. Katsnelson, and A.I. Lichtenstein, Phys. Rev. B **72**, 45125 (2005)

[109] C. Taranto, S. Andergassen, J. Bauer, K. Held, A. Katanin, W. Metzner, G. Rohringer, and A. Toschi, Phys. Rev. Lett. **112**, 196402 (2014)

[110] M. Potthoff and W. Nolting, Phys. Rev. B **59**, 2549 (1999)

[111] J.K. Freericks: *Transport in multilayered nanostructures: The dynamical mean-field approach* (Imperial College Press, London, 2006)

[112] M. Takizawa, H. Wadati, K. Tanaka, M. Hashimoto, T. Yoshida, A. Fujimori, A. Chikamtsu, H. Kumigashira, M. Oshima, K. Shibuya, T. Mihara, T. Ohnishi, M. Lippmaa, M. Kawasaki, H. Koinuma, S. Okamoto, and A.J. Millis, Phys. Rev. Lett. **97**, 057601 (2006)

[113] L. Chen and J.K. Freericks, Phys. Rev. B **75**, 1251141 (2007)

[114] R.W. Helmes, T.A. Costi, and A. Rosch, Phys. Rev. Lett. **100**, 056403 (2008)

[115] L. Chioncel, I. Leonov, H. Allmaier, F. Beiuseanu, E. Arrigoni, T. Jurcut, and W. Pötz, Phys. Rev. B **83**, 035307 (2011)

[116] F. Lechermann, L. Boehnke, and D. Grieger, Phys. Rev. B **87**, 241101(R) (2013)

[117] D. Jaksch, C. Bruder, J.I. Cirac, C.W. Gardiner, and P. Zoller, Phys. Rev. Lett. **81**, 3108 (1998)

[118] M. Greiner, O. Mandel, T. Esslinger, T.W. Hänsch, and I. Bloch, Nature **415**, 39 (2002)

[119] A. Rapp, G. Zarand, C. Honerkamp, W. Hofstetter, Phys. Rev. Lett. **98**, 160405 (2007)

[120] U. Schneider, L. Hackermüller, S. Will, T. Best, I. Bloch, T.A. Costi, R.W. Helmes, D. Rasch, and A. Rosch, Science **322**, 1520 (2008)

[121] I. Bloch, J. Dalibard, and W. Zwerger, Rev. Mod. Phys. **80**, 885 (2008)

[122] V. Turkowski and J.K. Freericks, Phys. Rev. B **71**, 085104 (2005)

[123] J.K. Freericks, Phys. Rev. B **77**, 075109 (2008)

[124] N. Tsuji, T. Oka, and H. Aoki, Phys. Rev. B **78**, 235124 (2008)

[125] M. Eckstein, and M. Kollar, Phys. Rev. B **78**, 205119 (2008)

[126] J.K. Freericks, H.R. Krishnamurthy, and T. Pruschke,
Phys. Rev. Lett. **102**, 136401 (2009)

[127] M. Eckstein, M. Kollar, and P. Werner, Phys. Rev. Lett. **103**, 056403 (2009)

[128] M. Eckstein and P. Werner, Phys. Rev. B **82**, 115115 (2010)

[129] H. Aoki, N. Tsuji, M. Eckstein, M. Kollar, T. Oka, and P. Werner,
Rev. Mod. Phys. **86**, 779 (2014)

[130] See the homepage of the DFG Research Unit FOR 1346 *Dynamical Mean-Field Approach with Predictive Power for Strongly Correlated Materials:*
`http://www.physik.uni-augsburg.de/for1346/`

[131] E. Pavarini, E. Koch, D. Vollhardt, and A.I. Lichtenstein (eds.):
The LDA+DMFT approach to strongly correlated materials
Reihe Modeling and Simulation, Vol. 1 (Forschungszentrum Jülich, 2011)
`http://www.cond-mat.de/events/correl11`

[132] E. Pavarini, E. Koch, F. Anders, and M. Jarrell (eds.):
Correlated Electrons: From Models to Materials
Reihe Modeling and Simulation, Vol. 2 (Forschungszentrum Jülich, 2012)
`http://www.cond-mat.de/events/correl12`

[133] E. Pavarini, E. Koch, and U. Schollwöck (eds.):
Emergent Phenomena in Correlated Matter
Reihe Modeling and Simulation, Vol. 3 (Forschungszentrum Jülich, 2013)
`http://www.cond-mat.de/events/correl13`

[134] E. Pavarini, E. Koch, D. Vollhardt, and A.I. Lichtenstein (eds.):
DMFT at 25: Infinite Dimensions
Reihe Modeling and Simulation, Vol. 4 (Forschungszentrum Jülich, 2014)
`http://www.cond-mat.de/events/correl14`