The legacy of Martin Gutzwiller

Last November, the Faculty of Science of the University of Fribourg awarded the doctor honoris causa to Martin Gutzwiller, with a threefold motivation: His outstanding contributions to theoretical physics, his active interest for science in general and his relations to Fribourg. Reason enough for emphasizing the eminent role Gutzwiller played during the last half century, especially in the two still very active research areas of quantum chaos and correlated electrons, as described in some detail below. Special thanks to Michael Berry for his profound analysis of Gutzwiller's pioneering work in "quantum chaology".

Martin Gutzwiller was born 1925 in Basel. His father was an internationally known professor of law, from 1921 to 1926 at the University of Fribourg, from 1926 to 1936 at the University of Heidelberg and then, after having escaped with his family from Germany because of the harassment by the nazis, again in Fribourg from 1937 to 1956. Martin passed his first school years in Heidelberg. Back to Switzerland, he received his further education in Trogen and at the Collège Saint Michel in Fribourg, where he passed the final two years of gymnasium. In 1944 he started studying physics at the University of Fribourg, but then he enrolled at the ETH in Zürich, where he received the diploma in 1949. His diploma work on the magnetic moment of nucleons with vector-meson coupling, supervised by Wolfgang Pauli, undoubtedly had a strong impact on his view of physics. 45 years later, in a letter to Physics Today (August 1994), he admits having received "a marvelous education in early field theory", but at the same time having been frustrated because the problem posed by Pauli could not be handled in a satisfactory way. Thus he pleads for coming back to "down-to-earth physics", instead of "chasing an elusive goal on the basis of abstract models".

After having received his diploma, Martin Gutzwiller worked during one year as an engineer in microwave transmission at Brown Boveri in Baden. In 1951 he moved to the US, where he spent most of the time since. At the University of Kansas he made his Ph. D. studies under the guidance of Max Dresden, on "Quantum Theory of Fields in Curved Space". From 1953 to 1960 he worked on geophysics in a laboratory of Shell in Houston, Texas. A position at the IBM Zurich Research Laboratory, then still in Adliswil, brought him back to Switzerland for three years, but subsequently he settled definitely down in New York. He remained a researcher at IBM, from 1963 to 1970 at the Watson Laboratory and from 1970 to 1993 in Yorktown Heights. He was at the same time Adjunct Professor in Metallurgy at the Columbia University. After his retirement from IBM he became an Adjunct Professor at the Yale University.

Martin Gutzwiller has published about 40 papers, most of them alone. He received prestigious prizes, such as the Dannie Heinemann prize of the American Physical Society (1993) or the Max-Planck Medal of the German Physical Society (2003). His international recognition is also well documented by four issues of Foundations of Physics (2000/2001), published at the occasion of his 75th birthday. It is worth mentioning that his research activities were broader than quantum chaos and correlated electrons, they included such diverse topics as dislocations in solids, the quantum Toda lattice and the ephemerides of the moon.

Dionys Baeriswyl, Uni Fribourg

Martin Gutzwiller and his periodic orbits

Michael Berry, H H Wills Physics Laboratory, Tyndall Avenue, Bristol BS8 1TL, UK

In the 1970s, physicists were made aware, largely through the efforts of the late Joseph Ford, that classical hamiltonian mechanics was enjoying a quiet revolution. The traditional emphasis had been on exactly solvable models, with as many conserved quantities as degrees of freedom, in which the motion was integrable and predictable. Examples are the Kepler ellipses of planetary motion, and the simple pendulum: 'as regular as clockwork'. The new research, incorporating Russian analytical mechanics and computer simulations inspired by statistical mechanics, revealed that most (technically, 'almost all') dynamical systems behave very differently. There are few conserved quantities, and motion, in part or all of the phase space, is nonseparable and unpredictable, that is, unstable: initially neighbouring orbits diverge exponentially. This is classical chaos.

It was quickly realised that this classical behaviour must have implications for quantum physics, especially semiclassical physics, e.g. for the arrangement of high-lying energy levels and the morphology of eigenfunctions. The study of these implications became what is now called quantum chaos (though I prefer the term quantum chaology). This is an area of research in which Martin Gutzwiller made a seminal contribution, described in the following, which I have adapted from a speech honouring his 70th birthday. Since a substantial part of my own scientific life has been devoted to the development and application to Martin's ideas, I won't attempt to be detached.

Martin published the last of his series of four papers [1-4] on periodic orbits exactly forty years ago. I encountered them at that time, while Kate Mount and I were writing our review of semiclassical mechanics. That was prehistoric semiclassical mechanics: before catastrophe theory demystified caustics, before asymptotics beyond all orders lifted divergent series to new levels of precision, and above all before we knew about classical chaos.

Of Martin's series of papers, the most influential was the last one [4], containing the celebrated 'Gutzwiller trace formula'. That was a tricky calculation, based on the Van Vleck formula for the semiclassical propagator, giving the density of quantum states (actually the trace of the resolvent operator) as a sum over classical periodic orbits. In particular, Martin calculated the contribution from an individual unstable periodic orbit. Nowadays we can see this as one of the 'atomic concepts' of quantum chaology, but in those days chaos was not appreciated. But he emphasized the essential novelty of his calculation in a similar way: it applies even when the classical dynamics is nonseparable. I'm rather proud of what we wrote at the beginning of 1972, as the last sentence of our review:

"*Finally, the difficulties raised by Gutzwiller's (1971) theory of quantization, which is perhaps the most exciting recent development in semiclassical mechanics, should be studied deeply in order to provide insight into the properties of quantum states in those systems, previously almost intractable, where no separation of variables is possible.*"

The trace formula could be approximated by taking just one periodic orbit and its repetitions. This led to an approximate 'quantization formula' that gave good results when applied to the lowest states of an electron in a semiconductor, whose mass depended on direction. I am referring to the birth of Martin's treatment of the anisotropic Kepler problem [5].

For a few years, his calculation was widely misinterpreted (among the ignorant it is misinterpreted even today) as implying a relation between the individual energy levels and individual periodic orbits of chaotic systems. One might call this the 'De Broglie interpretation' of the trace formula: that there is a level at each energy for which the action of a periodic orbit is a multiple of Planck. This is nonsense: the simplest calculation shows that the number of levels is hopelessly overestimated – in a billiard, for example, there is an 'infra-red catastrophe', that is, the prediction of levels at arbitrarily low energies.

Martin's papers quickly inspired others. In 1974, Jacques Chazarain showed that the trace formula could be operated 'in reverse', so that a sum over energy levels generated a function whose singularities were the actions of periodic orbits. This was exact, not semiclassical, and led (often unacknowledged) to what later came to be called 'inverse quantum chaology' and 'quantum recurrence spectroscopy'. In 1975 Michael Tabor and I generalized some of the results in the first of Martin's semiclassical papers [1] to get the general trace formula for integrable systems, where the periodic orbits are not isolated but fill tori. In nuclear physics, similar formulas had been obtained by Strutinsky in the context of the shell model. Tabor and I used our result to show that the level statistics in integrable systems are Poissonian - more about that later. William Miller and André Voros resolved a puzzle about the application of the trace formula for a stable orbit: by properly quantizing transverse to the orbit, they restored the missing quantum numbers; then Martin's single-orbit quantization rule makes sense, as the 'thin-torus' limit of Bohr-Sommerfeld quantization.

Probably Martin didn't realize that his formula was so fashionable at that time that it induced a certain hysteria. Michael Tabor and I were quietly finishing the work I just described when we learned that William Miller wanted to visit us in Bristol, to talk about his new work on periodic orbits. We convinced ourselves that this must be the same as ours, and laboured day and night (up a ladder, actually, because Michael was helping me paint my new house) to get our paper written and submitted before he arrived. We were foolish to panic, because William's work was completely different.

An awkward feature of stable orbits, recognized clearly by Martin in those early days, was that focusing occurs along them, leading for certain repetition numbers and stability indices to divergences of the contributions he calculated, associated with bifurcations. That awkwardness was removed in 1985 by Alfredo Ozorio de Almeida and John Hannay, who applied ideas from catastrophe theory that had come into semiclassical mechanics in the 1970s. Their development of Martin's formula became popular much later, when the features they predicted could be detected numerically.

In the early 1970s, Ian Percival made us aware of the amazing developments in classical mechanics by Arnold and Sinai, before chaos became popular. Percival insisted that semiclassical mechanics must take account of chaos. Later, we learned more about chaos from Joseph Ford. Of course Martin had paved the way with his trace formula for unstable orbits.

A persistent question was whether the formula could generate asymptotically high levels for a chaotic system. My opinions fluctuated. In 1976 I thought it could not, arguing that long orbits - required to generate the high levels - were so unstable that the Van Vleck propagator would not be valid for them. Instead, I thought (using ideas developed by Balian and Bloch) that periodic orbits could at best describe spectra smoothed on scales that were large compared with the mean spacing – but still classically small, so that some detail beyond the Weyl rule was accessible, though still not individual levels. This question is still not settled definitively, but my pessimistic opinion was changed by two developments.

The first was energy level statistics. In the 1970s, following a suggestion from Balazs Gyorffy, I imported from nuclear physics the idea that random matrices could be relevant in the quantum mechanics of chaos. The first application of this suggestion was not to chaotic systems at all, but to integrable systems, where it was shown – as I just mentioned – that the levels are not distributed according to random-matrix theory. That work inspired Allan Kaufman and Steven McDonald to the first calculation of level spacings for a chaotic system: the stadium. Then I did the same for Sinai's billiard. In those days we were fixated on the spacings distribution. My way of deriving level repulsion was a generalization of Wigner's: through the codimension of degeneracies. This gave the same result as random-matrix theory for small spacings, and explained the differences between the different ensembles, but gave no clue as to why random-matrix theory worked for all spacings, and why it was connected with classical chaos.

Then came Oriol Bohigas and Marie-Joya Giannoni and Charles Schmit. What they did, in the early 1980s, was simple but very important. They repeated the calculations that Kaufman and McDonald and I had done, for the same systems and using the same numerical methods, but instead of focusing on the one statistic of the level spacing they appreciated that the random-matrix analogy is much broader: it predicts all the spectral statistics, in particular long-range ones. They calculated one of these: the spectral rigidity (equivalent to the number variance).

Their observation was enormously influential. In particular, it was central to my construction in 1985 of the beginnings of the semiclassical theory of spectral statistics from Martin's atoms: the periodic orbits. Another crucial ingredient in this was also a development of periodic-orbit theory: the inspired realization by John Hannay and Alfredo Ozorio de Almeida that the Gutzwiller contributions of long orbits obey a sum rule whose origin is classical and whose structure is universal - that is, independent of details. Pure mathematicians (Margulis, Parry, Pollicott) had found similar rules - more general in that they applied to dissipative as well as hamiltonian systems, but also more restricted in that Hannay and Ozorio's theory applied also to integrable systems (where Tabor and I had found their particular result in 1977 but failed to appreciate its general significance). Thus periodic orbits were able to reproduce key formulas from random-matrix theory, and random-matrix universality found a natural explanation as the inheritance by quantum mechanics of the classical universality of long orbits. There was more: the periodic orbit theory of spectral statistics showed clearly and simply why and how random-matrix theory must break down for correlations involving sufficiently many levels. There were misty mathematical aspects – now being clarified – of those arguments, but the formulas were not misty, and were the first step in convincing me that long orbits in Martin's trace formula were meaningful.

The second step sprang from the realization - increasingly urgent in the early 1980s - that the series of periodic orbits in the trace formula does not converge. The cause was realized by Martin in 1971 [4]:

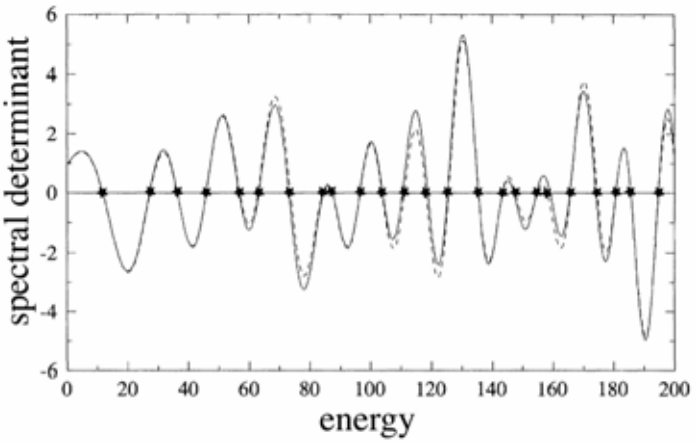
"*Even more serious is the fact that there is usually more than a countable number of orbits in a mechanical system, whereas the bound states of a Hamiltonian are countable.*"

The failure of the trace formula to converge was emphasized especially by André Voros, who pointed out that this defect is shared by the formally exact counterpart of the formula for billiards with constant negative curvature, namely the Selberg trace formula. And later Frank Steiner taught us that trace formulas can sometimes converge conditionally, in ways depending delicately on the topology of the orbits (expressed as Maslov phases). Eventually these concerns about convergence led naturally to the study of zeta functions. The idea there is to find a function where the energy levels are zeros, rather than steps or spikes as in the density of states. The grandparent of all these objects is Riemann's zeta function of number theory. I learned its possible relevance to quantum chaology from Oriol Bohigas, and also from Martin's semiclassical interpretation of the Faddeev-Pavlov scattering billiard, where Riemann's zeta function gives the phase shifts [6, 7]. It is amazing that Martin had already realized the connection with zeta functions in his 1971 paper. He wrote:

"*This response function is remarkably similar to the so-called zeta functions which mathematicians have invented in order to survey and classify the periodic orbits of abstract mechanical systems.*"

(He cited Smale). And in 1982 Martin explicitly wrote a semiclassical zeta function of the kind we consider today, and used it in conjunction with some tricks from statistical mechanics to sum the periodic orbits for the anisotropic Kepler system [7, 8].

A crucial ingredient turned out to be the Riemann-Siegel formula, that makes the sum over integers for the Riemann zeta function converge. I realized this in 1986, and later developed the idea with Jon Keating [9]; we were helped by André Voros's precise definitions of the regularized products in these zeta functions. The result was an adaptation of the trace formula to give a convergent sum over periodic orbits, soon employed to good effect by Keating and Martin Sieber [10] (see the figure). A related idea was the invention of cycle expansions by Predrag Cvitanovic and Bruno Eckhardt; in these, essential use is made of symbolic dynamics to speed the convergence of the sum over orbits. This application of coding to semiclassical mechanics was also originally Martin's idea: he used it in the 1970s and early 1980s to classify and then estimate the sum over the orbits, again for the anisotropic Kepler problem [7, 8].



Quantum spectral determinant (zeta function) for a particle confined between branches of a hyperbola, calculated exactly (dashed curve) and from a renormalized version [9,10] of Gutzwiller's sum over the unstable classical periodic orbits (full curve); the energy levels are the zeros, indicated by stars. Reproduced from [10], with permission.

The two applications of Martin's periodic-orbit ideas that I have just described, to spectral statistics and to zeta functions, were combined by Eugene Bogomolny and Jonathan Keating. This development, and more recent insights from Martin Sieber, Fritz Haake and Sebastian Müller, are taking the derivation of random-matrix formulas from quantum chaology to new levels of sophistication and refinement.

In the mid-1980s, Eric Heller discovered that for some chaotic systems the wavefunctions of individual states are scarred by individual short periodic orbits, in ways that depend on how unstable these are. From this came further extensions of Martin's ideas, to new sorts of spectral series

of periodic orbits, not involving traces, and for Wigner functions as well as wavefunctions.

In spite of all this progress, we are still unable to answer definitively and rigorously the central question Martin posed in 1971 [4]:

"*What is the relation between the periodic orbits in the classical system and the energy levels of the corresponding quantum system?*"

Of course the trace formula itself is one such relation, but I am sure that what Martin meant is: how can periodic orbits be used for *effective* calculations of *individual* levels. For the lowest levels there is no problem, but – and again I quote from Martin's 1971 paper -

"*the semiclassical approach to quantum mechanics is supposed to be better the larger the quantum number*"

and to reproduce the spectrum for high levels, using even the convergent versions of the trace formula that are now available, requires an exponentially large number of periodic orbits. This is a gross degree of redundancy unacceptable to anybody who appreciates the spectacular power of asymptotics elsewhere. Martin's old ideas continue to challenge us.

A few years ago, I refereed an application for research funding for a German-British collaboration. This required me to comment on the applicants' "timetable for research" and their "list of deliverables". I wrote "In science there are no deliverables; researches are not potatoes". Martin Gutzwiller ignored these toxic fashions. What makes him so attractive as a scientist is that he refuses to follow *any* fashion; instead, he generates ideas that *become* the fashion.

References

[1] Gutzwiller, M. C.,1967, The Phase Integral Approximation in Momentum Space and the Bound States of an Atom *J. Math. Phys*. **8**, 1979-2000
[2] Gutzwiller, M. C.,1969, The Phase Integral Approximation in Momentum Space and the Bound States of an Atom II *J. Math. Phys.* **10**, 1004-1020
[3] Gutzwiller, M. C.,1970, The Energy Spectrum According to Classical Mechanics *J. Math. Phys.* **11**, 1791-1806
[4] Gutzwiller, M. C.,1971, Periodic orbits and classical quantization conditions *J. Math. Phys.* **12**, 343-358
[5] Gutzwiller, M. C.,1973, The Anistropic Kepler Problem in Two Dimensions *J. Math. Phys.* **14**, 139-152
[6] Gutzwiller, M. C.,1983, Stochastic behavior in quantum scattering *Physica D* **7**, 341-355
[7] Gutzwiller, M. C.,1982, The Quantization of a Classically Ergodic System *Physica D* **5**, 183-207
[8] Gutzwiller, M. C.,1977, Bernoulli Sequences and Trajectories in the Anisotropic Kepler Problem *J. Math. Phys.* **18**, 806-823
[9] Berry, M. V. & Keating, J. P.,1992, A new approximation for zeta(1/2 +it) and quantum spectral determinants *Proc. Roy. Soc. Lond.* **A437**, 151-173
[10] Keating, J. P. & Sieber, M.,1994, Calculation of spectral determinants *Proc. Roy. Soc. Lond.* **A447**, 413-437

After graduating from Exeter and St Andrews, **Michael Berry** entered Bristol University, where he has been for considerably longer than he has not. He is a physicist, focusing on the physics of the mathematics…of the physics. Applications include the geometry of singularities (caustics on large scales, vortices on fine scales) in optics and other waves, the connection between classical and quantum physics, and the physical asymptotics of divergent series. He delights in finding the arcane in the mundane – abstract and subtle concepts in familiar or dramatic phenomena:

- Singularities of smooth gradient maps in rainbows and tsunamis;
- The Laplace operator in oriental magic mirrors;
- Elliptic integrals in the polarization pattern of the clear blue sky;
- Geometry of twists and turns in quantum indistinguishability;
- Matrix degeneracies in overhead-projector transparencies;
- Gauss sums in the light beyond a humble diffraction grating.

Martin Gutzwiller and his wave function

Dionys Baeriswyl, Département de physique, Université de Fribourg, 1700 Fribourg
Werner Weber, Fachbereich Physik, Universität Dortmund, DE-44221 Dortmund

Gutzwiller's work on correlated electrons is mostly concentrated in three papers, written in the time span 1962 to 1964 [1, 2, 3]. A short fourth paper was published a few years later [4]. In essence, Gutzwiller introduced a variational ansatz, where charge fluctuations are reduced as compared to Hartree-Fock theory, thus quantifying Van Vleck's qualitative idea of minimum polarity [5].

Historically, electronic correlations were first studied for the homogeneous electron gas, much less for electrons in narrow bands such as *d*-electrons in transition metals. A noticeable exception was Anderson's paper on the kinetic origin of antiferromagnetism in transition metal compounds, where a localized basis of Wannier functions was used [6]. In the same spirit, Gutzwiller wrote down the Hamiltonian

$$H = -t\sum_{\langle ij\rangle}(c^{\dagger}_{i\sigma}c_{j\sigma} + c^{\dagger}_{j\sigma}c_{i\sigma}) + U\sum_{i} n_{i\uparrow}n_{i\downarrow} \qquad (1)$$

where the first term describes electron hopping between the neighboring sites of a lattice ($c^{\dagger}_{i\sigma}$ and $c_{i\sigma}$ are, respectively, creation and annihilation operators for electrons at site i with spin σ) and the second term is the interaction, which acts only if two electrons meet on the same site ($n_{i\sigma} = c^{\dagger}_{i\sigma}c_{i\sigma}$). Quantum chemists had previously used a similar model for π-electrons in conjugated polymers, but they had included the long-range part of the Coulomb interaction. Curiously, shortly after Gutzwiller's first paper on the subject, two publications appeared where the same Hamiltonian (1) is treated, but without reference to Gutzwiller's work, one by Hubbard [7], the other by Kanamori [8]. One

has to conclude that the three papers [1, 7, 8] were written completely independently and that the Hamiltonien (1), now universally referred to as Hubbard model, was in the air, especially for investigating the problem of correlated electrons in transition metals.

In contrast to Gutzwiller, who did not care too much about the justification of the model, Hubbard estimated the different Coulomb matrix elements between localized *d* wave functions, and he also explained how in transition metals with partly filled 3*d* shells and a partly filled 4*s* shell the *s*-electrons can effectively screen the Coulomb interactions between *d*-electrons. The fact, pointed out by Gutzwiller [3], that the three authors, himself, Hubbard and Kanamori, obtained qualitatively different results, shows that, despite of its formal simplicity, the model was – and still is – very challenging.

Gutzwiller's main contributions to the field of correlated electrons are his ansatz for the ground state of the Hubbard model and his ingenious way of handling this wave function. He starts from the ground state $|\Psi_0\rangle$ of the hopping term, the filled Fermi sea. This would just yield the Hartree-Fock approximation, which treats neutral and "polar" configurations on the same footing. Thus he adds a projector term, now called correlator, that reduces charge fluctuations. His ansatz reads

$$|\Psi\rangle = \prod_i [1-(1-\eta)n_{i\uparrow}n_{i\downarrow}]\,|\Psi_0\rangle \qquad (2)$$

or, written in a different way,

$$|\Psi\rangle = e^{-g\hat{D}}\,|\Psi_0\rangle \qquad (3)$$

where $\hat{D} = \sum_i n_{i\uparrow}n_{i\downarrow}$ is the number of doubly occupied sites and g is related to Gutzwiller's parameter η by $\eta = e^{-g}$.

The problem of evaluating the ground state energy

$$E[\Psi] = \frac{\langle\Psi|\hat{H}|\Psi\rangle}{\langle\Psi|\Psi\rangle} \qquad (4)$$

for this trial state still represents a formidable task. Exact results were only obtained in one dimension [9, 10]. For other dimensions, Variational Monte Carlo (VMC), pioneered for the Gutzwiller ansatz by Horsch and Kaplan [11], has been widely used in recent years [12].

Gutzwiller himself proposed an approximate way of evaluating Eq. (4) [3]. His procedure, known as "Gutzwiller approximation", involves two steps [13]. In a first step, the expectation value is factorized with respect to spin. In a second step, the remaining expectation values are assumed to be configuration-independent. This leads to a purely combinatorial problem. In the limit of infinite dimensions, the Gutzwiller approximation represents the exact solution for the Gutzwiller ansatz, as shown by Metzner and Vollhardt [14, 10]. This interesting result marked the beginning of a new era in the theory of correlated electrons, that of the Dynamical Mean-Field Theory [15].

The result of the Gutzwiller approximation can be represented in terms of a renormalized hopping, $t \rightarrow \gamma t$. For $U \rightarrow \infty$, γ depends on the electron density n as $\gamma = (1 - n)/(1 - n/2)$. Therefore, when approaching half filling ($n \rightarrow 1$), the electron motion is completely suppressed, and the system is a Mott insulator. Brinkman and Rice noticed that within the Gutzwiller approximation the jamming of electrons (for $n = 1$) occurs at a large but finite value of U and is signaled by the vanishing of double occupancy [16]. They associated the critical point with the Mott metal-insulator transition. However, a closer scrutiny shows that this conclusion is an artifact of the Gutzwiller approximation. Indeed, for an exact treatment of the Gutzwiller ansatz (and finite lattice dimensions) double occupancy remains finite for all finite values of U. Moreover, the Gutzwiller ansatz itself is of limited validity for large values of U, as seen clearly by comparing it with the exact solution in one dimension.

Nevertheless, a Mott transition does occur for the Hubbard model, but in the sense of a topological transition from a phase with finite Drude weight for small values of U to one with vanishing Drude weight at large U, in agreement with Kohn's distinction between metals and insulators [17]. To show this in a variational framework [1], we have used a pair of trial ground states [18], the Gutzwiller wave function $|\Psi\rangle$ together with the "inverted" ansatz

$$|\Psi'\rangle = e^{-h\hat{T}}|\Psi_\infty\rangle \qquad (5)$$

where $\hat{T} = \sum_{\langle i,j\rangle}(c^\dagger_{i\sigma}c_{j\sigma} + c^\dagger_{j\sigma}c_{j\sigma})$ is the hopping operator, $|\Psi_\infty\rangle$ is the ground state for $U \rightarrow \infty$ and h is a variational parameter. One readily shows that $|\Psi\rangle$ has a finite Drude weight and lower energy for small U, while the Drude weight vanishes for $|\Psi'\rangle$, which is preferred for large U. A metal-insulator transition occurs for a value of U of the order of the band width, in good agreement with Quantum Monte Carlo results.

So far, we have assumed the Gutzwiller ansatz to be "adiabatically" linked to the filled Fermi sea $|\Psi_0\rangle$, which is the main reason for the metallic character of $|\Psi\rangle$. However, if we allow for a broken symmetry within $|\Psi_0\rangle$, we may find a competing ground state with qualitatively different properties. For instance, allowing for different magnetic moments on the two sublattices of a bi-partite lattice, one can obtain an antiferromagnetic insulator already below the Mott transition, i.e., before electrons are essentially localized. This is indeed found for the square lattice ($n = 1$), where the Mott transition is replaced by a smooth crossover from a band (or "Slater" [19]) insulator with small alternating magnetic moments at small U to a (Heisenberg) antiferromagnetic insulator with fully developed local moments at large U. Interestingly, this is not the case for the honeycomb lattice, where antiferromagnetism sets in essentially together with the Mott transition [20], although the detailed behavior close to the transition appears to be more complicated – and quite intriguing [21].

As a second example of a broken symmetry we mention bond alternation in conjugated polymers, or, more precisely, the fate of the Peierls instability in the presence of Coulomb interaction. Eric Jeckelmann, during his Ph.D. thesis,

1 From this point on, we will concentrate mostly on our own work, with apologies to other authors.

studied the one-dimensional Peierls-Hubbard model where the bond length dependence of the hopping amplitude *t* provides a coupling between the electrons and the lattice [22]. He used the Gutzwiller ansatz but added both the electronic gap and the lattice dimerization as variational parameters. The result for the dimerization Δ, as a function of *U* and for fixed electron-lattice couplings λ, is shown in Fig. 1. In contrast to Unrestricted Hartree-Fock, where the Peierls insulator is rapidly replaced by a spin-density wave (a Slater insulator), the dimerization is found to remain finite for all values of *U*. It even increases initially, as discovered long before this work [23], and exhibits a maximum for $U \approx 4t$, where a crossover to spin-Peierls behavior occurs. These variational results are in good agreement with subsequent calculations using the Density Matrix Renormalization Group.

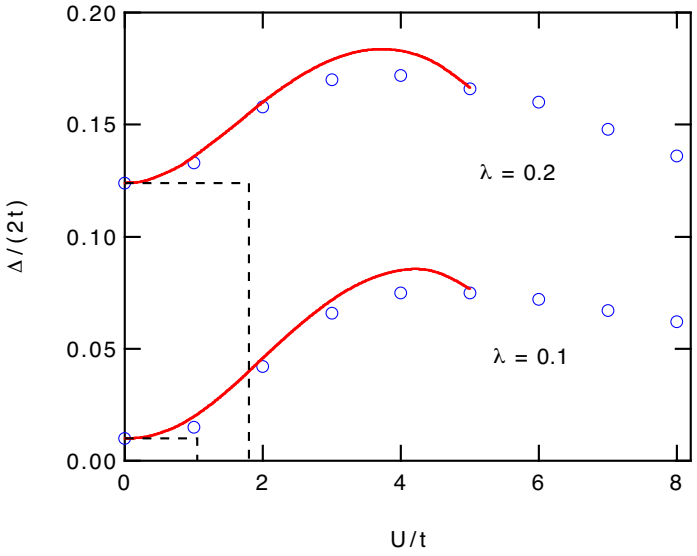


Figure 1: Dimerization in the Hubbard-Peierls model. Circles: VMC, full lines: analytical small U expansion, broken lines: Unrestricted Hartree-Fock.

As a third example we discuss results of the Ph. D. thesis of David Eichenberger [24], who studied the Hubbard model on a square lattice, using the modified Gutzwiller ansatz

$$|\Psi\rangle = e^{-h\hat{T}} e^{-g\hat{D}} |\Psi_0\rangle \qquad (6)$$

The additional factor $e^{-h\hat{T}}$ leads to a substantial improvement of the ground state energy and provides a kinetic exchange. We were particularly interested in the possibility of a superconducting ground state with *d*-wave symmetry, taken into account in the reference state $|\Psi_0\rangle$. Fig. 2 shows the VMC result for the superconducting order parameter for the Hubbard model on an 8×8 square lattice with both nearest (*t*) and next-nearest neighbor hoppings (*t'*) and a realistic Hubbard parameter $U = 8t$. Our results agree very well with other studies using completely different methods.

We turn now to the problem of itinerant ferromagnetism, which has been the main motivation for Gutzwiller (and for Hubbard and Kanamori as well) to study the Hamiltonian (1). The most simple trial state is the ground state of an effective single-particle model where the bands for up and down spins are shifted relative to each other. The "exchange splitting" is then determined by minimizing the total energy. This leads to the Stoner criterion, according to

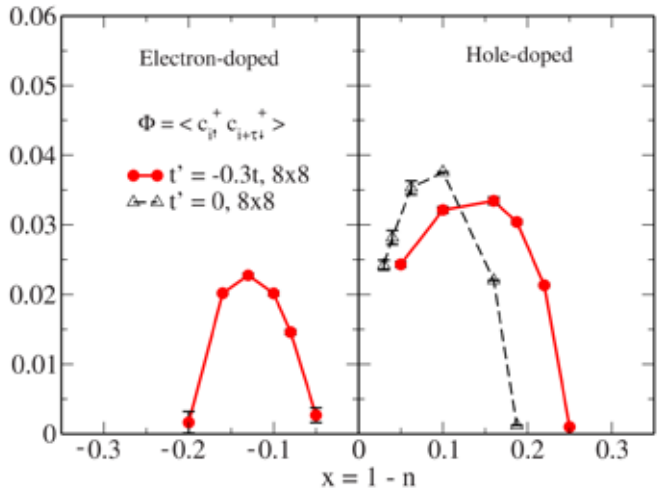


Figure 2: Superconducting order parameter as a function of doping for the Hubbard model on the square lattice.

which ferromagnetism occurs if $U\rho(\epsilon_F) > 1$, where $\rho(\epsilon_F)$ is the density of states per spin at the Fermi energy. Already in 1953 Van Vleck argued that the Stoner theory could not be the whole story, but that electronic correlations had to be taken into account. Gutzwiller's scheme is well suited for doing that. The results obtained in this way still leave space for ferromagnetism, but the stability region in parameter space is strongly reduced as compared to that of Stoner's theory [25]. In fact, the necessary *U* values are so large that one has to conclude that the single-orbital Hubbard model is not adequate for describing the ferromagnetism of transition metals.

There is another more fundamental reason why the single-band Hubbard model cannot be taken too seriously for describing transition metals. These materials are characterized by narrow partly filled 3*d*-bands located within a broad *s*-band and overlapping with even broader *p* bands, and therefore it is far from obvious how a one-band model should be able to describe their magnetic properties. This problem must have been clear to Gutzwiller, who used the smart title "Correlation of Electrons in a Narrow *s* Band" for one of his papers [3]. Notwithstanding this loophole, a realistic model should add uncorrelated electrons representing the *s*-band to the correlated electrons of the *d*-band. The Periodic Anderson Model is a first step in this direction, it admits two orbitals at each site, one of which is localized and correlated through an on-site interaction, the other is delocalized and uncorrelated. The two bands are hybridized. Using a generalized Gutzwiller ansatz together with a corresponding Gutzwiller approximation, one finds not only the usual renormalization of the correlated band by a factor γ, but also a renormalization of the hybridization by $\sqrt{\gamma}$ [26, 27].

The next step is to treat two or more correlated orbitals at a site. Here, Jörg Bünemann in his Ph.D. thesis has contributed a great deal to generalize the Gutzwiller formalism [28]. The generalization leads to an enormous expansion of the Gutzwiller wave function, as many additional correlators have to be introduced. The relevant local multi-electron configurations can be represented by the eigenstates of an atomic Hamiltonian, which reproduces the atomic multiplet spectrum of the partly filled 3*d* shell. This extension also

leads to a rapid increase of the number of variational parameters in the Gutzwiller wave function. If the number of different orbitals is N (N can be as large as 5 for an open d shell), the number of independent variational parameters can reach $2^{2N} - 2N - 1$, which may be of the order of 1000 [28]. The variational parameters represent the occupancies of all possible multiplet states. At the first instance, the atomic multiplet spectrum is governed by three Slater-Condon or Racah integrals, when spherical symmetry is assumed for the atoms. Yet, the site symmetry in a crystal is lower than spherical. Incorporation of the correct site symmetry results in many further modifications and extensions of the method.

The multi-band Gutzwiller method allows the investigation of 3d transition metals and compounds on a quantitative basis. An ab initio single-particle Hamiltonian can be constructed using Density-Functional Theory (DFT). The simplest way to incorporate DFT results is to extract a tight-binding model by fitting the hopping amplitudes to the DFT bands, but more elaborate methods are available, such as down-folding the DFT bands to a reduced Wannier basis [29]. We have carried out various studies on magnetic 3d elements and on compounds of 3d elements. One paper dealt with the Fermi surface of ferromagnetic Ni. DFT predicts a hole ellipsoid around the X point of the Brillouin zone, which is missing in the data. The multi-band Gutzwiller method was based on a one-particle Hamiltonian derived from paramagnetic DFT bands for Ni including wide 4s and 4p bands.
Using typical interaction parameters for Ni, our calculations reproduced the observed Fermi surface topology [30]. Another paper dealt with the magnetic anisotropy in ferromagnetic Ni [31]. Here again, pure DFT results did not yield the correct answers, while the Gutzwiller method gave very good agreement with experiment. In all cases, the renormalization parameters γ have been found to be of the order of 0.7, indicating moderately strong correlation effects.

Finally we mention the issue of metallic anti-ferromagnetism in iron pnictides, a new class of high-temperature superconductors. Our calculations were based on down-folded DFT bands. The results indicate also in this case moderately strong correlations. The atomic magnetic moments were found to agree well with experiment, in contrast to the DFT results and also to model calculations [32].

The examples mentioned above demonstrate that Gutzwiller's simple ansatz evolved into a powerful tool for dealing with correlated electron systems. The method has recently also been applied successfully to cold bosonic atoms in an optical lattice. At the age of 50, Gutzwiller's wave function in its extensions remains competitive for describing correlated states of matter.

References

[1] M. C. Gutzwiller, Phys. Rev. Lett. **10**, 169 (1963).
[2] M. C. Gutzwiller, Phys. Rev. B **134**, A923 (1964).
[3] M. C. Gutzwiller, Phys. Rev. B **137**, A1726 (1965).
[4] K. A. Chao and M. C. Gutzwiller, J. Appl. Phys. **42**, 1420 (1971).
[5] J. H. van Vleck, Rev. Mod. Phys. **25**, 220 (1953).
[6] P. W. Anderson, Phys. Rev. **115**, 2 (1959).
[7] J. Hubbard, Proc. Roy. Soc. **A276**, 238 (1963).
[8] J. Kanamori, Prog. Theor. Phys. **30**, 275 (1963).
[9] W. Metzner and D. Vollhardt, Phys. Rev. Lett. **59**, 121 (1987); F. Gebhard and D. Vollhardt, Phys. Rev. Lett. **59**, 1472 (1987).
[10] For a review see F. Gebhard, The Mott Metal-Insulator Transition: Models and Methods, Springer 1997.
[11] P. Horsch and T. A. Kaplan, J. Phys. C **16**, L1203 (1983).
[12] For a recent review of the method for the fully projected Gutzwiller wave function ($g \to \infty$) see B. Edegger, V. N. Muthukumar and C. Gros, Adv. Phys. **56**, 927 (2007).
[13] For a clear presentation see P. Fulde, Electron Correlations in Molecules and Solids, Springer Series in Solid-State Sciences **100** (1990).
[14] W. Metzner and D. Vollhardt, Phys. Rev. Lett. **62**, 324 (1989).
[15] For an early review see A. Georges, G. Kotliar, W. Krauth and M. J. Rozenberg, Rev. Mod. Phys. **68**, 13 (1996).
[16] W. Brinkman and T. M. Rice, Phys. Rev. B **2**, 4302 (1970).
[17] W. Kohn, Phys. Rev. **133**, A171 (1964).
[18] L. M. Martelo, M. Dzierzawa and D. Baeriswyl, Z. Phys. B **103**, 335 (1997).
[19] J. C. Slater, Phys. Rev. **82**, 538 (1951).
[20] M. Dzierzawa, D. Baeriswyl and L. M. Martelo, Helv. Phys. Acta **70**, 124 (1997); for a review see D. Baeriswyl, Found. Phys. **30**, 2033 (2000).
[21] Z. Y. Meng, T. C. Lang, S. Wessel, F. F. Assaad and A. Muramatsu, Nature **464**, 847 (2010).
[22] E. Jeckelmann, Ph D. thesis, University of Fribourg (1995); E. Jeckelmann and D. Baeriswyl, Synth. Met. **65**, 211 (1994).
[23] P. Horsch, Phys. Rev. B **24**, 7351 (1981); D. Baeriswyl and K. Maki, Phys. Rev. B **31**, 6633 (1985).
[24] D. Eichenberger, Ph. D. thesis, University of Fribourg (2008); D. Baeriswyl, D. Eichenberger and M. Menteshashvili, New J. Phys. **11**, 075010 (2009).
[25] P. Fazekas, Electron Correlation and Magnetism, World Scientific 1999.
[26] T. M. Rice and K. Ueda, Phys. Rev. Lett. **55**, 995 (1985).
[27] C. M. Varma, W. Weber and L. J. Randall, Phys. Rev. B **33**, 1015 (1986).
[28] J. Bünemann, Ph. D. thesis, University of Dortmund (1998); J. Bünemann, W. Weber and F. Gebhard, Phys. Rev. B **57**, 6896 (1998).
[29] For a recent review see O. K. Andersen and L. Boeri, Ann. Phys. (Berlin) **523**, 8 (2011).
[30] J. Bünemann *et al.*, Europhys. Lett. **61**, 667 (2003).
[31] J. Bünemann, F. Gebhard, T. Ohm, S. Weiser and W. Weber, Phys. Rev. Lett. **101**, 236404 (2008).
[32] T. Schickling *et al.*, Phys. Rev. Lett. **108**, 036406 (2012).

Werner Weber received his PhD from the TU Munich in 1972. He worked first at a variety of research institutions, at the MPI for Solid State Research in Stuttgart, at the Research Center in Karlsruhe (now K.I.T.), at Bell Laboratories, Murray Hill. He then became a faculty member at the TU Dortmund, where he retired in 2010. His research area is theoretical solid state physics, with main emphasis on materials science theory. He assumed many duties in university self-administration, even presently. In the spirit of Martin Gutzwiller, he recently changed his field of interest to activities in climate research, including applications.