

## 6 SCIENTIFIC HIGHLIGHT OF THE MONTH

---

### Reflections on the Life and Science of Balazs L. Gyorffy (1938-2012)

#### “Life without U”

G. Malcolm Stocks (*ORNL, USA*), Walter M. Temmerman (*Daresbury Laboratory, UK*), Julie B. Staunton (*Warwick University, UK*), James F. Annett (*University of Bristol, UK*), Ingrid Mertig (*Martin Luther University and MPIfM, Halle, Germany*), Peter Weinberger (*Formerly, Technical University Vienna, Austria*), and Paul J. Durham (*Daresbury Laboratory, UK*)

#### Introduction

The December issue of the Psi-k Newsletter carried the sad news of the death on October 25, 2012 of Professor Balazs L. Gyorffy, together with a reprint of a formal obituary that was written by Professor Robert Evans, FRS. As part of a broader tribute to Professor Gyorffy, this issue carries a compilation of contributions from some of Balazs’ collaborators, friends and colleagues from within Psi-k and outside, reflecting on their experiences of working with him. Balazs’ enthusiasm for science and life was irrepressible and a source of pleasure for those that shared in his scientific genius and knew him as a loyal and considerate friend. From the beginning, Balazs focused on what we now call “first principles” electronic approaches and eschewed the introduction of adjustable parameters whenever possible, often humorously positing that in condensed matter physics there is only one parameter - the electronic charge and that is known pretty well! At the center of Balazs’ attention was the “electron glue” (possibly his coinage) <sup>1</sup> and how the interactions between the  $10^{24}$  electrons that comprise it give rise to the richness of materials properties and functionalities.

In his long and highly productive career, Balazs made seminal contributions to many areas of condensed matter and materials physics - from the fundamentals of electronic structure theory, multiple scattering theory, alloy theory, superconductivity, magnetism, relativistic electron theory, strongly correlated electron theory, symmetry and symmetry breaking in alloy and magnetic phase transformations, to the subtle manifestations and consequences of Berry curvature in materials physics - a subject on which he published a number of papers in the years after his “official” retirement. Throughout his career, Balazs worked closely with experimentalists,

---

<sup>1</sup>While the etymology of this evocative term cannot for certain be established it is one that Balazs used early and much loved.

often pioneering the theoretical developments necessary for the theorist to “calculate what is actually measured” without the need of intervening models and unnecessary approximations. While obtaining the most direct contact possible with experiment was a cardinal principle, simply getting agreement with experiment was never sufficient - one had to understand how this agreement arose in terms of the underlying electronic structure from which one can carry the insights and intuition gained to more complex situations and new phenomena.

Although Balazs’ scientific life was centered in Bristol, his influence on the progression of condensed matter and materials theory was international and inclusive. During his long career at Bristol, Balazs mentored many students and postdocs that since have gone on to illustrious careers of their own. Indeed many of these are now professors and senior researchers at major universities and laboratories in the UK, continental Europe and North America. In addition Balazs was a valued collaborator and advisor to innumerable scientists and research groups around the world. His ability to see the big picture, to make connections across apparently disparate fields of physics, and his deep insights into electronic structure theory and materials phenomena were an endless source of inspiration to many.

Beginning in the mid-1970’s, Balazs took up the challenge of maintaining UK leadership in the development of first principles electronic techniques with his involvement (along with Volker Heine and others) in founding and sponsoring the Collaborative Computational Project-9 (CCP9) - a role that would be extended to the whole of Europe through his efforts in helping shape the Psi-k network. With this in mind it is therefore appropriate that the Psi-k newsletter has agreed to carry a series of articles of remembrance by a few of the many colleagues that had the privilege and pleasure of working with him. The spirit of these is not to chronicle the full scope of Balazs’ contributions to science but to highlight some of the areas of greatest impact and provide insights into what it was like to be with him during these scientific adventures.

**Malcolm Stocks: “If you have the opportunity, it is a good idea to work with the best”**

I believe that I first met Balazs in late 1968 at the University of Sheffield when I was assigned to assist him in supervising an undergraduate Physics “problem” class. What is perhaps most remarkable about this is that I am no longer completely sure of these circumstances; remarkable because it is now so hard to imagine any interaction with Balazs without it being forever imprinted on one’s memory. My second point of interaction was centered in Oak Ridge and would lay the foundation for much of my scientific career and greatly influence that of Balazs. The catalyst for this was Sam Faulkner who also met Balazs at Sheffield. Sam had been awarded a Fulbright Fellowship and was on leave from Oak Ridge National Laboratory (ORNL) in the USA. On returning to Oak Ridge, Sam invited Balazs to act as a consultant to the Theory Group in the Metals and Ceramics Division. This 1969 visit began a lifelong relationship with Oak Ridge. It is likely during this visit that Balazs first became interested in the electronic structure theory of disordered systems and multiple scattering theory - according to Sam “out of politeness” for being invited.

By the late 1960’s it was becoming increasingly clear that the “coherent potential approximation”

(CPA) held a special place in the theory of disordered systems in that it was the first self-consistent effective medium theory of the effects of disorder on the electronic structure. In addition the CPA was shown to sit at the top of a hierarchy of such theories that included the virtual crystal approximation (VCA) and averaged t-matrix approximation (ATA). Unlike the ansätze of the VCA and ATA, the CPA provided a way to self-consistently determine the “best” effective medium whose properties would accurately represent the configurationally averaged properties of the real disordered alloy. In a nutshell, CPA enforces the condition that replacement of the effective or coherent potential by true electron-ion potential at a site (in modern parlance the Kohn-Sham potential at that site) produce no additional scattering when averaged over all possible occupancies of that site. Not surprisingly the “coherent potential” turns out to be a complex (literally) energy dependent quantity that has to be found iteratively.

Sam Faulkner, who had been a student of Jan Korringa at Ohio State University, was very aware of the power of the CPA. Indeed, his thesis had been on disordered systems theory and it was Jan Korringa who first proposed the ATA. In addition, it was Sam Faulkner (together with Harold Davis and Hugh Joy) who, after coming to Oak Ridge in the early 1960’s, had developed the first Korringa-Kohn-Rostoker (KKR) electronic structure code - a code made possible by the power of the then leadership CDC and IBM computers at Oak Ridge. It was into this environment that I came as a postdoc and Balazs came as a visitor. During his first visit to Oak Ridge, Balazs wrote a paper on a generalization of the CPA to liquid metals with short-range order. I, on the other hand, was working on implementing the CPA within the context of generalized tight binding models to systems such as copper-nickel and silver-palladium. In addition I had also been reading the papers of Paul Soven who had proposed a method by which one could implement the CPA within a KKR-based “band structure” formalism. Try as I might, I could not see a way in which Soven’s ideas could be converted into a practical computational approach. All that changed during a visit of Balazs to Oak Ridge in 1971 when he left me with a set of notes that he would subsequently publish in *Physical Review B* 5, 2382 (1972). These notes were a model of clarity, insight, and compactness that I found quite wonderful. The notes laid out a formalism in which the path to implementation of the CPA within the language of KKR was clear. It was this set of notes, together with a little bit of thinking, that persuaded me to move to Bristol to work with Balazs on what became KKR-CPA.

The essential insight of Balazs’ formulation was to write the equations of multiple scattering theory in terms of what is now known as the scattering path operator. This formalism then allowed the KKR-CPA equations to be written down in a compact form and furthermore provided a method for calculating the scattering path operator in terms of the inverse of the KKR matrix which turned out to only depend on the t-matrix corresponding to the “coherent potential” at a site and the KKR structure constants that describe propagation between the sites and which in turn depend only on the lattice structure.

Despite the clarity of exposition and the clear pathway to implementation, actually developing the KKR-CPA was extremely difficult, not least because the computer power available at the time was woefully inadequate. Fortunately, we were soon to be joined in our endeavor by Walter Temmerman who was to take up the task of writing a code that used k-space integration to obtain the scattering path matrix while Sandro Guiliano and Roberto Ruggeri, who were visiting Bristol from the University of Messina in Sicily investigated obtaining them in real

space. It is interesting that Sandro refused to fly and so ended up driving the length of Italy and across the rest of Europe to Bristol, dragging Roberto along with him. From these small beginnings but with the endless optimism that ‘it would all work out’ that collaborating with Balazs engendered (sometimes in spite of considerable evidence to the contrary) the basis of the KKR-CPA methods and codes that we know today were slowly put together. To say that conversations with Balazs about how things were progressing could be animated is to point only to the shadow - charged with espresso, puffing his pipe, armed with a piece of chalk and access to the enormous blackboard that was in my office, “discussions” with Balazs were events to be savored.

For me, the scientific directions that were initiated in Bristol during the early 1970’s set the stage for my career and allowed me to lead the privileged life of a research scientist - for the most part at Oak Ridge National Laboratory. In this I was not alone! To follow for a moment but one thread, charge self-consistency (SCF) was added to the basic KKR-CPA in collaboration with Hermann Winter in the early 1980’s, in part while we were both spending a year as Walter’s guests in Daresbury - Hermann was from the then Kernforschungszentrum Karlsruhe. The theory and implementation of KKR-CPA within DFT was the thesis topic of Duane Johnson while a student of Frank Pinski at Cincinnati. The implementation of the relativistic (Rel) KKR-CPA based on the Dirac equation was first taken up by Julie Staunton as graduate student with Balazs and would set the stage for Paul Strange and Hubert Ebert who followed on as Balazs’ postdocs. The early 1980’s saw development of the concentration functional approach, which made it possible to predict short-range ordering and order-disorder transformation temperatures entirely from first principles and to identify the features of the electron glue responsible for the specific clustering or ordering tendencies in particular alloy systems. These ideas were first implemented by John Wadsworth, another of Balazs graduate students, and were subsequently much further developed by Julie, Frank and Duane. In short, to work with Balazs was to be constantly assailed by new ideas and possibilities. So, it should be no surprise that so many of those mentioned have gone on to be distinguished scientists in their own right. Following additional threads would serve to multiply this many-fold.

There are many fables about Balazs that, over the years, have spread through the legions of his friends and collaborators. Sometimes Balazs elevated the “bit part” of the absent minded Professor to an Academy award winning performance - perhaps some of his wife Carole’s acting and playwright theatrical training had rubbed off on him, but more likely it was intrinsic. For example, I am fairly sure that the number of ways that one can put a transparency on a overhead projector the “wrong way round” is finite - but not to Balazs. Sadly, modern technology and PowerPoint have largely removed the opportunity for young scientists to explore the possibilities.

Above all, Balazs was a kind and loyal friend who would go to great lengths to make sure that his colleagues were taken care of when visiting Bristol. For example, when my wife Barbara and young son Ian first arrived in Bristol, Balazs and Carole not only welcomed us but made sure that we could “inherit” the flat that they were vacating as they moved to their new home in Cotham. Sometimes, however, Balazs’ kindnesses would also add to his mythology! During our time in Bristol I had to make a trip to the USA leaving my family behind. At some point Balazs, concerned for how Barbara and Ian were getting along in my absence, knocked on the door of the flat and was duly invited in. Out of politeness Balazs put the pipe that he had

been smoking on his arrival into the pocket of his overcoat. After some conversation, Barbara noticed that smoke was emanating from Balazs' pocket of which she promptly informed him. Unfazed, Balazs simply turned his pocket inside out emptying the burning embers onto the carpet, with quite predictable results - an encounter that remains forever burned on Barbara's memory. Balazs, we shall miss you.

### **Walter Temmerman: “My recollections of working with Balazs”**

Balazs influenced my life profoundly. As a young Ph.D. student in theoretical physics in Prof. Ziman's group at the University of Bristol it was the custom to find one's own thesis adviser from the senior staff. In my days this involved Michael Berry, Bob Evans and Balazs Gyorffy. The project of Balazs Gyorffy, in collaboration with G. Malcolm Stocks, entailed writing a computer programme to solve the KKR-CPA equations for disordered alloys, making use of Ole Andersen's tricks of linearization approximation in band theory. What attracted me to this project was that it was very specific and its success rate could be measured. Also I liked the style in which Balazs and Malcolm were performing physics. A lasting memory of a discussion with Balazs and Malcolm is Balazs happily puffing his pipe, sitting on a pile of computer outputs which Malcolm stored underneath the blackboard.

Life with Balazs was never boring. My Ph.D. was funded by the British Council and after this I was fortunate enough to become Balazs' post-doc on a Science Research Council grant to study the k-dependent band structure of Cu-Ni alloys [Phys. Rev. Lett. 41, 339 (1978)]. But in my first year of post-doc, Balazs was gone on a sabbatical at Stony Brook. He had done nothing with respect to my appointment and his farewell message to me was to go to Senate House and present myself. That was to guarantee my inclusion on the university pay roll. As incredible as this was, it has worked.

Balazs was for life. As the first chairman of the newly created UK's CCP9 (Computational Collaborative Project on “Computational Studies of the Electronic Structure of Solids”) in 1980, together with Volker Heine, they employed me as its scientific secretary, placed at Daresbury Laboratory. So, it seemed, I followed my thesis adviser in whatever I did. Balazs was also instrumental in my marriage to Dzigka Szotek, his post-doc, whom he sent from Bristol to Daresbury to get acquainted with the KKR-CPA code. This was the beginning of a very fruitful collaboration and a beautiful life. A few years later, the period of high temperature superconductivity (HTS) arrived. I jumped on the 'bandwagon' and focussed on exploring the materials specific aspects of the parent compounds of high  $T_c$  superconductors (HTCS), but in due course joined forces with Balazs. His idea was to solve the Kohn-Sham Bogolubov-de Gennes equations, with a suitably parametrized pairing interaction. Following an earlier study of Nb, involving the first-principles KKR electronic structure and a phenomenological attractive pairing interaction [Phys. Rev. B48, 1202 (1993)], for high temperature superconductors Balazs suggested to combine the so-called eight-band model Hamiltonian, derived from the first-principles electronic structure of  $\text{YBa}_2\text{Cu}_3\text{O}_7$  (YBCO) by Ole Andersen, with a phenomenological electron-electron attractive interaction operating between different sites and/or orbitals of the model with a strength defined by a constant K [Phys. Rev. Lett. 76, 307 (1996)]. The eight-band model proved to provide

a good quantitative description of the first-principles local density approximation (LDA) band structure of the superconducting cuprates in the normal state within 2 eV of the Fermi energy  $\epsilon_F$ . In this 'tight-binding model', orbitals located on non-generic structural elements separating the  $\text{CuO}_2$  bilayers, such as the chain in  $\text{YBa}_2\text{Cu}_3\text{O}_7$ , were deleted. As a consequence, it was strictly speaking a two-dimensional (2D) model. Balazs wanted to focus on establishing where the Cooper force, binding electrons in these materials into pairs, was operating. He suggested to parametrize an electron-electron interaction in terms of the orbitals of the model for the electronic structure of the normal state [Phys. Rev. B58, 1025 (1998)]. Thus one could choose the attraction to occur between two electrons e. g. one at site  $\mathbf{R}$  in the orbital labelled by  $L$  and the other at site  $\mathbf{R}'$  and in orbital  $L'$ , and describe it by the coupling constant  $K_{RL;R'L'}$ , giving rise to the pairing potential binding the electrons and holes in the appropriate, tight-binding, BdG equations, which would then be solved self-consistently to determine the quasi-particle spectrum and hence the superconducting gap in the ground state. The value of the coupling constant was so chosen that the predicted superconducting transition temperature  $T_c$  would agree with the experimentally observed one, namely  $T_c=92\text{K}$  for YBCO. Among many pairing scenarios the favourite one turned out to be a d-wave pairing, where the members of the Cooper pair resided on the nearest-neighbour Cu atoms in  $d_{x^2-y^2}$  orbitals. The calculated gap anisotropy for this d-wave intralayer nearest-neighbour scenario agreed very well with the ARPES experiment of Schabel et al. [Phys. Rev. B 57, 2796 (1997)] for the sample with  $T_c = 92$  K. Similarly, our calculated specific heat compared very well with the measurements [Phys. Rev. Lett. 73, 2744 (1994)] which gave us confidence that our BdG equations could be regarded as capturing the essential physics of the superconducting state. For the low temperature penetration depth our calculations at optimal doping was compared to measurements of A. Carrington et al. [Phys. Rev. B59, R14173 (1999)], revealing paramount importance of the chain in YBCO for zero temperature penetration depth. We have observed a linear dependence of the low temperature penetration depth at all studied doping levels [Phys. Rev B62, 3997 (2000)]. We have also shown that changing the chemical potentials,  $\mu$ , in the eight-band model, for the favourite d-wave pairing, gave a good quantitative account of the observed rise and fall of  $T_c$  with the carrier concentration  $\delta_n$ , namely doping [Phys. Rev. B58, 522 (1998)]. Moreover, we have obtained very encouraging results for the superconducting gap as a function of doping [Physica C 353, 23-28 (2001)], despite the fact that our approach has been strictly speaking a weak coupling BCS-like theory.

Our studies of the electronic structure of high  $T_c$ 's have brought us to thinking about the importance of electron correlations in these materials. As suggested by Perdew and Zunger, one way of improving on the LDA description of electron correlations was to introduce the so-called self-interaction correction (SIC) to LDA, which we implemented for solids within our version of LMTO-ASA (SIC-LMTO-ASA) code in the beginning of nineties, and over the years applied to a variety of systems. But Balazs has invented his own "brand" of the self-interaction correction (SIC), the so-called local SIC (LSIC), formulated within the multiple scattering theory, which we have implemented within a KKR-CPA code [Phys. Rev. B71, 205109 (2005)]. Unlike in the SIC implementation within the LMTO-ASA method, where localized states have been described in terms of the exponentially decaying Wannier functions, in the LSIC-KKR-CPA, the localized states have been associated with sharp resonances. Using an 'alloy analogy', we have applied

this local SIC approach to studying the famous  $\alpha-\gamma$  phase transition in Ce, and have been able to conclude that the transition is driven by entropy and not the internal energy. Also, we have shown that at high temperatures our first principles LSIC-KKR-CPA approach; where only the thermal fluctuations play a dominant role, has been comparable to the LDA+U+DMFT method. This local SIC contribution typified one of the many issues Balazs has always drawn our attention to. Namely, is it a local effect or does one need to consider the whole crystal lattice? He has been thinking about generalizing this first-principles effective one-electron static approach to a dynamical theory, using the non-local CPA averaging, giving rise to a dynamical mean field-like theory, but without U. Balazs has always referred to such a parameter-free many-body theory as “Life without U”, and this has become synonymous with him. As we have already for a while been living in the world without HIM, “Life without U” appears to have acquired an additional complexity.

### **Julie Staunton: “Balazs”**

Those of us lucky enough to have worked with Balazs appreciated his fascination and profound insight for Physics. As condensed matter and materials physicists we know that the essential question for our research concerns the complexity arising from the  $10^{24}$  electrons in a material all interacting with each other and the heavier, slower nuclei as well as external fields. Balazs emphasised the subtleties and beauty of this complex glue and took his characteristically uncompromising approach in describing it. One should start from ‘first principles’ so that the results can be compared directly with increasingly sophisticated experimental measurements - a standpoint which means that there is no hiding place if the theory does not come up to scratch but enormous satisfaction when it does. This philosophy led him to be such a dominant figure internationally in driving the development of computational electronic structure to which the Psi-k Network owes him so much.

The description of the condensed matter physics of materials gets a little easier if one assumes that the nuclei position themselves on a perfect regular lattice and that thermal effects do not need to be addressed. Balazs impressed on us that Nature is not like this - all materials are disordered in some way - there are lattice defects, the nuclei vibrate about their average positions, the electrons behave differently at different temperatures etc. Balazs pioneered ways to treat the effects of disorder - producing the SCF-KKR-CPA method, as discussed by Malcolm and Walter above, for a quantitative description of disordered alloys and so on. The SCF-KKR-CPA, together with its cousin, the SCF-LMTO-CPA, remains one of the few first principles method for describing electrons in a disordered crystal which can be combined with DFT. With other colleagues I greatly enjoyed working with Balazs to use these ideas on magnetic materials and we devised a theory of metallic magnetism in which these SCF-KKR-CPA techniques deal with thermally induced local moment magnetic fluctuations [J.Phys. F 15,1337, (1984); PRL 69, 371,(1992)]. The resulting disordered local moment (DLM) picture was the first fully first-principles approach to the problem of the temperature dependence of magnetism in metals. In Balazs’ words, “at no stage does it map the many-electron problem onto an effective Heisenberg model, and yet it deals, qualitatively, with both the ground state and the demise of magnetic long-range order at the Curie temperature in a material-specific, parameter-free manner”. En-

route to developing this theory Balazs proposed a version of a constrained density-functional theory for configurations of non-collinear local moments, an approach now also used in ab-initio spin-dynamics calculations. He used a particularly elegant phrase - “temporarily broken ergodicity” - to describe the time scale separation between the relatively slowly varying local moment orientations and the other faster electronic degrees of freedom. One early success for the theory, which he was quick to realise should emerge from it, was the prediction of a wave-vector and energy-dependent local exchange splitting in the electronic structure of the paramagnetic state of ferromagnetic metals, later observed in PES and IPES experiments on bcc iron.

Balazs is well-known as one of the pioneers in the use of relativistic quantum mechanics to describe electrons in solids. He played a significant role in establishing the theory of magneto-crystalline anisotropy and analysing relativistic effects on spin-dependent transport, photoemission and magnetic X-ray scattering. As one small example, I recall the fun in revisiting with him the RKKY interaction, expressed of course with multiple scattering theory language, where we found the magnetic anisotropy that comes when the jellium, in which the magnetic impurities are embedded, is treated with relativistic quantum mechanics [J.Phys. C 21, 1595, (1988)].

Balazs was exceptionally talented in interpreting the results of often detailed computational results and then producing an elegant, beautiful understanding of an effect. For example a number of us had carried out some calculations of the compositional ordering in NiPt alloys using the first-principles concentration wave theory that Balazs had developed earlier with Malcolm Stocks. We found the L1<sub>0</sub> ordering that is observed experimentally. For an isoelectronic transition metal alloy with its almost filled d-bands this was at first a bit of puzzle but Balazs showed how to interpret the electronic mechanism underpinning the size effect produced by the off-diagonal disorder in this alloy. It described electronically why “big” and “small” atoms tend to order into simple structures [PRL, 66, 766, (1991)].

Balazs was a fantastic lateral thinker with an encyclopedic physics knowledge - his ability to make connections and set a new context for apparently disparate topics in theoretical physics is one of the many reasons why physics and his co-workers will miss him so much. Many scientific meetings will be the poorer without his pertinent and thought-provoking points. His dynamism and enthusiasm made him such an inspirational character in Physics and such fun to work with. He showed what it is to be a proper, fully signed up Physicist. Even though Balazs was my Physics father (he supervised my PhD work), as he was to many others, it was because he was a ‘Force of Nature’ that I had assumed that he would always be around to offer advice and inspire with new ideas. Many of us are massively grateful to his support especially in the early stages of our careers. For my part he played the pivotal role in giving me the confidence to go for jobs, promotions etc. In one instance I am sure he used a technique learnt and adapted from his swimming coaches to build up my confidence. He always made sure that his PhD students broadened and deepened their physics education - e. g. in my case introducing me to Gauge Field Theories and pointing out the connection between the Higgs particle and condensed matter concepts. He was also very receptive and encouraging to ideas from young physicists even if kindly having to point out holes and hitches in them.

Over the last 10 years or so much work in condensed matter physics has been directed at materials whose electrons are particularly difficult to describe accurately owing to their strong correlations



but which have intriguing effects. A useful and productive approach such as LDA+DMFT has been to graft a simpler model of some of the electronic glue attributes onto a more complete, computationally heavier one based on DFT. This model has at least one parameter, a  $U$ . Over recent years, as Walter has commented, Balazs had been discussing with a number of us ways to address this physics from 'first principles' and to remove the need for this and other parameters, making his physicist's joke that we should go for 'Life without  $U$ '. Unfortunately that phrase has new poignancy which gets it into the title of this article and which we all are trying to come to terms with. Balazs - thank you for everything.

### **James Annett: “Balazs Gyorffy and Superconductivity”**

Balazs made many contributions to the theory of superconductivity, from his early work on estimating electron-phonon coupling to theories of Cooper pair tunnelling and superconducting qubits for quantum computations. Here I just want to highlight some of the themes he was still actively working on in the most recent five to ten years. In particular some of this work had a clear link to ab initio electronic structure, notably in numerical solutions to the Bogoliubov de Gennes equations. While his other work such as on qubits drew on ideas from quantum optics, which went back to his original work on the laser with Willis Lamb.

Balazs took a very active interest in the possibility of spin triplet superconductivity in the material  $\text{Sr}_2\text{RuO}_4$ . He had first suggested that some nearly ferromagnetic metals could become triplet superconductors in a classic paper from 1977 [I. Foukes and B Gyorffy, *Phys. Rev. B* 15 1395-1398 (1977)]. Together with Karol Wysokinski and Grzegorz Litak (Lublin) we developed a simple phenomenological model based on the known bandstructure [Annett et al., *Phys. Rev. B* 66, 134514 (2002)]. The approach was very similar to his eight band work on high temperature superconductivity, described above by Walter Temmerman. Balazs was very interested in the additional possibilities caused by the existence of spin-1 Cooper pairs, and he was always looking for a possible “smoking gun” experiment which he could measure the Cooper pair spin directly. This was the motivation for his final project, together with Martin Gradhand, on Berry curvatures and Berry phases in spin-triplet superconductors and his hope was to find a unique spin transport effect which would be a signature of triplet pairing. While this was not completed at the time of his death, we were also able to confirm a prediction he had made together with Hardy Gross and Klaus Capelle [K. Capelle et al, *Phys. Rev. B* 58, 473-489 (1998)] for the existence of circular dichroism in spin triplet superconductors [K.I. Wysokinski et al, *Phys. Rev. Lett.* 108, 077004 (2012)]. Again there is a connection to the ideas of Berry curvature for the Bogoliubov quasiparticles, which he was following up at the time of his death.

Another system where spin triplet pairing can occur is in multilayers of ferromagnets and ordinary singlet superconductors. Again Balazs's interest in this went back to his earlier work, for example his work on ab initio spin-transport and spin-current torques in ferromagnetic multilayers [A. Vernes, B. Gyoeffy and P. Weinberger, *Phys. Rev. B* 76, (2007)]. Together with experimentlists Mark Blamire and Jason Robinson at Cambridge, Lesley Cohen at Imperial and Victor Petrashov at RHUL Balazs was very interested in developing the theory of spin-transport

in such multilayers, and again looking for a unique transport property which would prove conclusively the existence of spin triplet Cooper pairs. Daniel Fritsch was working together with Balazs and myself on this problem at the time of Balazs's death, and the work is still in progress. He was also exploring with Balazs Ujfalussy an idea to implement the Bogolubov de Gennes equations directly within an ab initio KKR codes.

Finally Balazs was always also looking for applications in superconducting systems of his favourite theories of CPA, non-local CPA (NLCPA) and the disordered local moment (DLM) method. Some years ago we implemented the CPA for disordered superconductors [A.M. Martin et al., Phys. Rev. B 60 7523-7535 (1999)], showing that it is the correct mean-field approach for treating disorder superconducting alloys, just as it is in the normal state. This was later extended to the non-local CPA [R. Moradian et al., Phys. Rev. Lett. 89, 287002 (2002)], extending the normal state work NLCPA done with Julie Staunton and Derwyn Rowlands to the superconducting case. One of Balazs's last PhD students, Garry Batt, then further extended this approach to the problem of 'Fermi arcs' in high temperature superconductivity, combining NLCPA and the DLM to consider a d-wave superconductor with phase fluctuations of the order parameter on neighbouring atoms. This fitted into Balazs's long standing interest in what he called the "pre-formed pair" scenario, by which the anomalous properties of underdoped cuprate superconductors was to be understood as the result of phase fluctuations of the superconducting order parameter [J. Quintanilla et al., J. Phys. Condens. Matter 14 6591-6600 (2002)].

These are only a fraction of the many papers which Balazs contributed to on the theme of superconductivity over his long and productive career. I apologize to the many collaborators, students and colleagues whose work with Balazs I have been unable to mention. Balazs made so many profound contributions and his energy and permanent enthusiasm will be sadly missed very much by all who knew him.

### **Ingrid Mertig: "To Balazs"**

A whole community of scientists is indebted to Balazs Györfy for the tools they are using daily in their studies of metals and alloys. In addition, Balazs had a very strong and charismatic personality, an inextinguishable scientific curiosity, and a very broad knowledge in theoretical physics. He definitely stood out as a scientist of fascinating insight and knowledge, with an impressive record of pioneering contributions in theoretical solid-state physics.

My first contact with Balazs was a virtual one via "electron-phonon interaction". I was a PhD student at TU Dresden and calculated electron-phonon coupling constants for Lanthanides and Actinides based on the Gaspari-Györfy theory a method that he developed in 1972 to describe superconductivity in metals.

In real life, I met Balazs at the International symposium on electronic structure of solids in Gaussig (East Germany). He came to Gaussig with his enthusiasm and his charisma and presented his work on the KKR-CPA method for disordered alloys. Everybody was infected by the ideas and all members of the Dresden electronic structure team wanted to do KKR-CPA, meaning that all of us would have liked to collaborate with Balazs.

Since 1990, we frequently met in scientific meetings and have been members in the same European networks, particularly in Psi-k. At one of these meetings he tried to explain to me the Berry phase concept. We ended up with a “twisted belt” in a Bristolian pub. This was the beginning of our collaboration on relativistic effects in semi-classical transport theory based on the Boltzmann equation. Balazs started to visit my group regularly. Having Balazs as a guest for extended stays had a very strong and positive impact for the Martin Luther University and for the Max Planck Institute of Microstructure Physics in Halle.

For me the collaboration was like a “late postdoc” with Balazs. During exciting discussions he opened the door for us to the understanding of the role of Berry curvature in solid-state theory and we developed a method to calculate the Berry curvature within the KKR scheme. We shared the common interest in a relativistic Boltzmann equation and we have been working hard on this subject. This work is not yet finished and we promise to proceed. But we will miss Balazs’s brilliant mind.

### **Peter Weinberger: “From phase shifts to time-dependent theories”**

Balazs Gyorffy entered my life for the first time in 1975, when I wrote a letter to the editor on his paper in the Journal of Physics on the electron-phonon interaction making use of phase shifts. The calculation of the latter was how our common experiences started. After the letter to the editor, I got a very friendly collaboration offer from Balazs. Unfortunately I was still busy with my own version of fully relativistic KKR programme, an enterprise for which I was accused to be completely demented. I finally arrived in Bristol exactly on his 40th birthday. Now, anybody who knew about Balazs’ commitments to ‘Wiener Schnitzel’, in particular of the rather large type, would have guessed that ‘Schnitzels’ were his dearest birthday wish. So there we were, since Carole gave up on this project. Finally we toasted bread together, grinded it in a coffee mill, since bread crumbs - most likely an unknown exotic ingredient at that time in England - were needed, prepared the Schnitzels and fried them in two pans. Balazs was happy! Phase shifts and Schnitzels started our friendship some 35 years ago.

Well, and then came the age of CPA. With the help of the Oak Ridge programme we finally got a relativistic version thereof running. I have to say that in the early eighties Balazs was probably one of the very few around who was convinced that a relativistic approach might turn out to be important. What followed were more visits to Bristol and quite a few summers Balazs, sometimes accompanied by Carole, spent in Vienna.

When after the first success of the TB-LMTO method I posed to Laszlo Szunyogh and Balazs Ujfalussy, in Vienna at the time, the question of why can’t we do a similar thing in KKR and a new age in the KKR community started, triggering off quite a few common publications with Balazs, in particular, when a spin-polarized relativistic version thereof started to run. The Screened KKR method became standard since then - essentially thanks to the enthusiasm of Laszlo Szunyogh and Balazs Ujfalussy.

Although within a Greens function approach also electric and optical transport properties became computable on an ab-initio basis, it was Balazs who was a bit sceptical whenever we had current- or magnetic-field induced phenomena in mind. After about a two summer long dis-

cussion, working with Andras Vernes, we finally got it, the ultimate set of equations, namely a time-dependent Dirac equation in the presence of an external electro-magnetic field. Balazs was enthusiastic and insisted to send the paper to PRL, where it had a delay time of about a year, being finally only published as a rapid communication in PRB. This paper I still consider to be our greatest common success, since it is oriented towards the future, to time-dependent magnetic phenomena.

I am pretty sure Balazs loved to spend summers in Vienna. And he had very good reasons:

- (1) There were all the Hungarian guys, Laszlo Szunogh, Balazs Ujfalussy, Laszlo Udvardi and a couple of bright PHD students from Budapest. They ‘conversed’ in Hungarian all day long.
- (2) He got a separate swimming lane in the ‘Arbeiterschwimmverein’, in a 50 m pool, reserved only for him!
- (3) He enjoyed tremendously to go down to the Naschmarkt for lunch, an open market nearby, in particular to a very small place serving giant Wiener Schnitzel (and a second one on the house, if the first one was not big enough), and
- (4) We, he and I, got on very well as far as physics, politics and cultural engagements were concerned. It was an ideal matching of wave lengths.

From phase shifts to time-dependent theories: it was indeed a long way I had the privilege to accompany Balazs, it was for nearly half of his life-time.

### **Paul Durham: “Memories of Balazs”**

#### *His influence:*

For those of us like Walter, Dzidka and I who were lucky enough to work and have daily contact with him when we were young, Balazs’s influence was indelible. In those early days in Bristol while we were learning to be researchers we became imprinted with his way of thinking about physics and were all the better for it. Talking with Balazs was a terrific way to understand how physics all fits together. Moreover, you learned how your own work fitted into what everyone else was doing at the time all over the world. Balazs made you feel in the swim of physics. It goes without saying that he had loads of ideas, but the striking thing about him was the generosity with which he shared them with you. A chat with Balazs could give you enough material for a year’s research and Balazs’s interest in your own ideas gave you a tremendous surge of confidence - you knew you were on to something worthwhile. But most of all, it was such fun to be with him - he was a wonderfully attractive man in every way, and we are so glad to have known him.

#### *The “Uncertainty” Principle:*

Balazs spoke and, especially, wrote very good English. If you wrote a paper with him, it was always a good idea for you to do the easy bit - describing what you actually did - and to get him to write the introduction and conclusion, where he could deploy his powers of expression to the full on what he did best - explaining what the work meant. No doubt these powers derived from his very wide reading and he could talk marvellously about European and American literature. I once mentioned that I had just read Joseph Roth’s novel - The Radetzky March - and Balazs

immediately launched into a fascinating disquisition on the book as a chronicle of the late Austro-Hungarian Empire. He had some foibles though. I never heard him talking about the uncertainty principle without him pronouncing it “uncertainty” - but then he made this version sound so right, somehow, that I sometimes use it myself.

*Car story:*

Most conversations with Balazs were very absorbing. A couple of years ago he was visiting Daresbury and I took him to lunch in my new car, of which I was very proud. We talked about physics during lunch, continued on the drive back to the Lab and then on into my office, covering my blackboard, as usual with Balazs. After a few minutes our security guys phoned to say that I had left my car not only unlocked and with the door wide open, but also with the keys in the ignition and the engine running. I guess that talking physics with Balazs was a full-brain activity.

*Andrzej's story:*

Andrzej Pindor came from Poland to Bristol in the late 1970's and early 1980's and worked with Balazs and Walter mostly on alloys, KKR-CPA and so on. Their discussions, conducted in perfect English voiced in (loud) central European accents, were celebrated in Bristol. Now in Canada, Andrzej writes:

“I certainly have a lot of fond memories of Balazs and our heated and often loud political discussions. It was so telling of Balazs that our quite different political views and the mentioned heated discussions did not affect not only our professional but also our personal relations. One case of such discussions sticks in my mind - we were having one of these discussions in a pub. The pub was closing and we moved to the street in front of the pub (I remember that Sam Faulkner was there too). It must have been well after 11 pm and at certain stage a window in one of the buildings opened and someone shouted [in a Bristol accent]: Be quiet! Go back where you came from and leave us in peace! Balazs, always quick on his feet, shouted back: Hey, I live here! (or something to this effect). This, however, cooled us down and we went our own ways postponing the discussion to a next time.”.