HCM Newsletter

Ψ_k Network

AB INITIO (FROM ELECTRONIC STRUCTURE) CALCULATION OF COMPLEX PROCESSES IN MATERIALS

Number 6 December 1994

Proposal: ERB4050PL930589
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Editorial

In this Newsletter, apart from abstracts, in the section **News from the Network** you can find information on the issues discussed at the last Network's Management Board meeting. Reports on collaborative visits and workshops are in the section **News from the Working Groups**, and just after that there is an announcement of *a research assistant position* at the University of Antwerp. In the section **Highlight of the Month**, placed at the very end of the Newsletter, there is an article by Balazs L. Gyorffy (the spokesman for the *V.a* Working Group) and P. Miller on *"Bogolubov de Gennes Equations"*. This article is meant to give you more details about one of the main scientific activities of this Working Group.

Regarding the scientific collaborations, we would appreciate very much if you acknowledged the HCM Network's support in, and notified us about, every publication that had resulted from the collaboration within the Network. Also, we would like to stress the need for acknowledgement of the Network in all your publications that have resulted owing to the computer codes that you picked up at any one of the '*hands-on computer code*' workshops that were organised by the Network in the past year. This is of paramount importance, since at the end of every callendar year we have to submit a report to Brussels on the Network's activities and accomplishments. Additionally, we would like you to inform us of any new computer code or technique that has resulted from the collaborations within the Network. All this counts for Brussels.
With respect to acknowledging the Network's support in your publications could you please use e.g. the following:

This paper resulted from a collaboration within, and was partially funded by, the Human Capital and Mobility Network on "Ab initio (from electronic structure) calculation of complex processes in materials" (Contract: ERBCHRXCT930369).

Moreover, for the record, please send us *the title, authors, and journal's name* of all your publications, that resulted from the Network's collaboration, where you specifically acknowledged the Network.
Regarding the computer codes, that have resulted from the collaboration within the Network, please let us know: *what the code does and which nodes, persons, participated in its development.*

The following e-mail addresses are repeated for your convenience, and are the easiest way to contact us.

	function
psik-coord@daresbury.ac.uk	**messages to the coordinator**
psik-management@daresbury.ac.uk	**messages to the NMB**
psik-network@daresbury.ac.uk	**messages to the whole Network**

The claims forms for your expenses concerning any Network's activity that you have participated in should be sent to us at the address below.

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News from the Network

The Network's Management Board met in Paris on the 4th of November.
The most important issue discussed was **The Network's International Conference**, which will take place in *Schwabisch Gmund* (near Stuttgart) on *September 18-21, 1996*. Professor O.K. Andersen is the chairman of the Organising Commitee. It is planned that the Conference will have at least 300 participants and will represent all the scientific activities of our Network. It will be a conference open to everybody, however the members of our Network will be able to obtain some financial support. The decision concerning the policy of subsidising the members of the Network will be taken at the next meetings of the NMB. Please do reserve the dates in your diary for this special conference. The first circular of the Conference will be sent out in March next year.

There were some important decisions taken concerning the increase of the size of the Network by all the *unfunded* nodes from EU countries, however, only within the existing funds. We have the approval of Brussels for that, but some formal administrative steps need to be followed in order that the nodes in question would be able to get financial support for their possible collaborative visits and other activities within the Network. All those, yet *unfunded* nodes, will soon hear from us concerning their detailed addresses and representatives. So, the size of the Network will increase to over seventy nodes. We hope, that this will generate many more collaborations and scientific publications.

Concerning the summary of this year's activity of the Network, there have been nine workshops organised, representing main activities of most of the Working Groups. So, the training aspect of our Network met its demands very successfully. However, only 16 collaborative visits have taken place. And this is the area where we need to strengthsen our activity and increase the output. We have generated very few common publications on any scale, and especially in comparison with other networks like ours.

REPORT ON THE BERLIN WORKSHOP ON

"Ab-initio Molecular-Dynamics Calculations of Structural, Elastic, and Vibrational Properties of Polyatomic Systems"

The workshop "Ab-initio Molecular-Dynamics Calculations of Structural, Elastic, and Vibrational Properties of Polyatomic Systems" was held from October 3 to 7, 1994 in Berlin. The lectures took place in the Harnack House and the computer exercises in the Fritz-Haber Institute of the Max Planck Gesellschaft. Lecturers included V. Heine, J. Hafner, J. L. Martins, M. Scheffler, O. Pankrotov, E. Pehlke and several members of M. Scheffler's group. There were fourteen european participants from the EC, EFTA and Eastern Europe, and five overseas participants from the US, Canada, Brazil and Australia.

The participants followed in the morning a series of lectures on the methods of electronic structure calculation and their applications. The afternoons were dedicated to practical exercises using the program *fhi94md* developed by M. Scheffler's group. Proposed exercises included the generation of pseudopotentials, simulation of the phase transition in Si and the vibration of N_2.

(J. L. Martins)

Report on the course: Hands-on the TB-LMTO-ASA computer program
Max-Planck-Institut FKF, Stuttgart
October 24-28, 1994

The participants in the course came from Germany (7), France (2), Denmark (1), Greece (1), Hungary (1), Rumania (1), Sweden (1), and Switzerland (1). More than half belonged to the network.

The aim of the course was, that the participants should be able to (*i*) performe self-consistent LDA calculations using the TB-LMTO-ASA programs, (*ii*) judge whether the results are correct, and (*iii*) understand the results in terms of orbital decomposed band structures, atom and orbital projected density of states, charge densities, and Fermi surfaces.

To achieve this goal, each participant was given the published crystallographic data for one non trivial compound for which he/she had to perform a complete calculation.

The complete calculation was divided into five steps. Each of these steps consisted of an explanation of how it had to be performed (with some LMTO background information) followed by simultaneous execution of the step by all participants at the computers (each had a terminal and a user id at the local computer). After the step had be completed, there was a question and answer session for all, and finally all calculations were checked on the screen in order that all participants could learn from the 15 examples.

In addition to this, there were three tutorial lectures about the LMTO method and a lecture about the organization and structure of the LMTO code. Finally, the application of a more advanced and powerfull graphical package was demonstrated (the GNUPLOT was used for displaying the results in the course).

According to a questionnaire distributed at the end of the course, most of the participants were very satisfied with the course. Several of the participants were missing / had expected more LMTO theory. This course was, however, not intended as an LMTO theory course but a **Hands-on the TB-LMTO-ASA computer program** course.

(Ove Jepsen)

Report on a collaborative visit to Vienna within Ψ_k Network

S. Blügel (IFF, KFA-Jülich), J. Redinger (TU-Wien)
and R. Podloucky (U-Wien)

Wien, May 23rd–June 20th, 1994

The purpose of my visit to Vienna was threefold:

(1) I attended the HCM-electronic structure workshop: "Magnetic Surfaces, Interfaces and Multilayers" of the working group magnetism from May 29th–May 31st, organized by Peter Dederichs and Peter Weinberger.

(2) After this conference I stayed for about three weeks in the group of Peter Weinberger (Inst. für Techn. Elektrochemie, Techn. Universität Wien) with the purpose to establish a collaboration with Josef Redinger and Raimund Podloucky (Inst. für Phys. Chemie, Universtät Wien). It was our first task to extend my previous FLAPW calculations on the magnetism of 4d and 5d monolayers on Ag(100) to (111) oriented substrates. Meanwhile these calculations have been finished and a paper is in preparation. With Peter Weinberger we discussed the impact of the spin-orbit interaction on the magnetism of 4d and 5d metal films and calculations in this direction have been started. I had stimulating discussion with I. Turek (Academy of Sciences of the Czech Republic, Brno), V. Drchal (Academy of Sciences of the Czech Republic, Praha) and J. Kudrnovský (Academy of Sciences of the Czech Republic, Praha), visiting Peter Weinberger's group at the same time. All are working on the same subject of ultra-thin magnetic films. Some future projects have been discussed.

(3) I stayed also one week with Raimund Podloucky. We started there some calculations concerning the magnetism of small clusters. We discussed also the possibility to combine our effort in bringing the different FLAPW technologies together and develop in the future the programs together.

I also took the opportunity to visit Peter Blaha, Peter Mohn and Prof. K.-H. Schwarz with whom I had interesting discussions on the GGA and martensitic transformations.
Part of this stay was financed by Peter Weinberger's grant (Austrian Bundesministerium für Wissenschaft und Forschung, Projekt ZL.49.731/2–24/91), Raimund Podloucky and the HCM-network, working group magnetism.

(Stefan Blügel)

Report on visit by V. Heine to Berlin
2-5 October 1994

The purpose was to give two lectures in the Network Summer School on "*Ab initio Molecular Dynamics*", and to participate in discussion particularly on the research projects of individual participants.
The lectures were on

- Introduction to Pseudopotentials
- The Role and Design of Computer Experiments

Total cost: 417.00 pounds.

(V. Heine)

Report on visit by V. Heine to Gaustal, Norway
27 August-1 September 1994

As well as contributing to the scientific discussions, I attended the European Research Conference (ERC) on *Electronic Structure of Solids* as chairman of the Network for two purposes:

- To discuss with participants, the ESF attending official and past/present ERC chairmen the issue of not having an ERC in 1996 in order to avoid clashing with the open Network Conference. This was agreed.
- To talk, distribute a leaflet and answer questions about the Network, and how people generally may receive the information and participate in the work of the Network.

Total cost: 141.25 pounds.

(V. Heine)

Report on the collaborative visit
C. Demangeat (node of François Gautier, IPCMS, Strasbourg)
to P.H. Dederichs, R. Zeller, S. Blügel, (IFF, Jülich)
2-5, November, 1994.

Two points were particularly discussed.

1). Application of the fast KKR-CPA scheme developed by A.F. Tatarchenko and N.I. Kulikov (Troitsk, Russia) for the spin-polarized description of the non-stoichiometric $Pt_{3-x}Cr_{1+x}$ alloy.

It was mentioned that two points make these calculations realistic at medium range Workstations. The first one is the tetrahedron integration scheme for the evaluation of the CPA T-matrix of scattering. This let us to obtain high precision results with the small number of k-points in the Brillouin zone (500 - 1000). The second is the use of the noniterative procedure for finding the solution of the CPA equation which decrease computation time as needed for KKR calculations of ordered compounds. (A.F. Tatarchenko, N.I. Kulikov, PRB, 50, 8266, (94))

2). Application of the fast TB-KKR method developed by R. Zeller to the "experimental" Fe/Cr interfaces. (See, for example, C. Turtur and G. Bayreuther, PRL 72, 1557 (94), S. Miethaner and G. Bayreuther, Communication at ICMFS/MRS, Düsseldorf, September, 1994, A. Vega, L.C. Balbas, A. Chouairi, C. Demangeat and H. Dreyssé, PRB 49, 12797 (94), A. Vega, H. Dreyssé, C. Demangeat, A. Chouairi, and L.C. Balbas, J.Appl.Phys. 76(10) 15 November 1994.) A bilateral cooperation (PROCOPE) between Bayreuther's group (Regensburg) and Strasbourg's group try to investigate the local magnetic distribution of the "experimental" Fe/Cr interface. Due to absence of any periodicity in these systems only tight-binding scheme in the real space is able to give some insight into this problem. The very fast TB-KKR scheme developed by R. Zeller will be therefore a very useful tool for a more precise description of the local magnetic polarization at interfaces and particularly at the Fe/Cr interfaces.

(C. Demangeat)

Report on visit by Armin Burkhardt (MPI-Stuttgart) to Daresbury Laboratory (UK), 13-15 November 1994

I gave a seminar to members of the Theory and Computational Science Division on 'Scientific Workgroup Computing on Workstation Clusters'.

The abstract of the talk is included below:

Electronic structure calculations are the main activity in the Andersen group for theoretical physics at the MPI fuer Festkoerperforschung. During the last years the group moved its computational workload completely from a remote CRAY mainframe to a local cluster of 10 IBM-RS/6000 workstations connected to a FDDI ring. Besides the usual interactive services several batch processing systems were tested (CernNQS, NQS/Exec, IBM LoadLeveler). The group's experiences with these systems are summarized and the groups future strategy with respect to distributed and parallel computing are the main topic of the talk.

Moreover, I had lengthy discussions on distributed scientific workgroup computing with members of the Theory and Computational Science Division. Specifically NFS to DFS migration, ATM networking, distributed batch systems and visualisation for clustered workstations were discussed.

(A. Burkhardt)

Report of G. Bihlmayer and R. Podloucky (Univ. Vienna) on the visits at the University of L'Aquila (17-21 Oct. 1994) and the University of Cagliari (21-26 Oct. 1994)

The visit was made to deepen the already existing cooperation with A. Continenza (Univ. L'Aquila), S. Massidda (Univ. Cagliari) and their groups. These groups as well as our group in Vienna are experts in the FLAPW algorithms and computer application for bulk systems as well as surfaces. In L'Aquila we particularly discussed the development of forces for the FLAPW method, which was already started last year. At present, A. Continenza and her group are testing the force formulation a la Yu, Singh and Krakauer (PRB B43,p6411,1991) in the bulk version of our FLAPW codes. According to this test Yu's force formula works reasonable as long as only the results for total forces are compared to Yu et al.'s data. For some test cases, the different components (i.e. Hellman-Feynman term, core contribution, IBS term) as published by Yu et al. are totally different. Anyway, Continenza's calculated forces agree with the corresponding first derivatives of total energies. At present, the force subroutines are optimized (also be rewriting some of the equations) and such accelerated versions for Crays as well as local stations (e.g. IBM RS6000) should soon be available.

Another joint study consists in the calculation of correct band gaps, which -as it is well known- are wrong in general for standard electronic structure calculations within DFT because standard DFT treats only the ground state. We followed the idea of band gap corrections within a Generalized DFT by L. Fritsche (Physica B172,p7,1991) which is very easy to implement in the codes and also very fast to calculate. However, the results are only partially satisfying: whereas the gaps for one-element solids (such as Si, Ge) come out in very good agreement with experiment, the calculated gaps for semiconducting compounds (such as GaAs, ZnSe) are in rather bad agreement with experiment. For large-gap systems (such as NaCl) the agreement again is very good. We hope -in cooperation with L. Fritsche, J. Noffke and their groups in Clausthal- to clarify the gap problem.

With S. Massidda we decided to implement the forces according to Soler and Williams (PRB B40,p1560,1989) in the bulk FLAPW code because this formulation for the forces looks more compact and numerically reliable. This development will be done together with an adaption of the non-inversion symmetry code for local stations. Then we would have FLAPW bulk codes which work for any symmetry without restriction. All the force formulations can be rather directly built into the surface slab code which works for general symmetries already, on Crays as well as on local stations.

We thank our Italian colleagues for their hospitality and are looking forward to a deeper cooperation thanks to the HCM network. In our discussions we also addressed various methods to improve the calculation of the band-gap of semiconductors. Since no specific method seems to cover the whole range of semiconductors it is necessary to know the ranges of applicability of each method. For example, the so called 'gap-correction' used in our group for Ti-based and group IV semiconductors is severely wrong for III-V or II-VI type semiconductors. In these cases, the method used by Prof. Massidda seems to be more useful, but also more complex and time consuming.

In two seminary lectures in L'Aquila and Cagliari titled 'Martensitic Transformations of NiTi and PdTi' Mag. Bihlmayer tried to show, how the codes can be used to study problems of technological importance.

To coordinate further improvements of the codes and to make the exchange of code versions more easy, we installed accounts for Dr. Continenza and Prof. Massidda on our workstation in Vienna. Nevertheless, even the best computer-network is no substitute for personal talks and direct exchange of the experiences made with the codes. So we hope to see our Italian partners in Vienna and/or Italy next year to keep up personal contacts, to keep the flow of information running and to join our forces for mutual benefit.

(R. Podloucky)

Research Assistantship in Theoretical Condensed Matter Physics

University of Antwerp (RUCA), Belgium

Applications are invited for a position as research assistant with the group (TSM) of P.E. Van Camp and V.E. Van Doren to do research on density functional methods in polymers and biopolymers. The appointment is expected to start on October 1, 1995 and will be for a period of two years. However, the research done may lead to a Ph.D. degree in which case an extension necessary to obtain the degree will be provided. The annual salary will be 560.000 BEF (about $17,500, which amounts to $12,500 after taxes). The applicant should be a citizen of an EU country.

Topics of Theoretical Research at the TSM-group:

1. Research on new nonlocal density functionals capable of generating more realistic band structures as those obtained from local functionals and at the same time of reproducing the ground state and structural properties.
2. Application of local and nonlocal functionals in ab initio calculations of the total ground state energy of new materials from which the structural, electronic and optical properties can be derived. These materials include:

a. polymers and biopolymers such as polycytosine and polypyrol

b. the recently synthesized ternary nitrides which range from semicon- ductors to metals. Almost no measurements nor any calculations have been carried out as yet

c. binary III-V, II-VI, etc. semiconductor compounds

Collaborations of the TSM-group:

Scientific collaborations are already running between the TSM-group and:

a. Professor J.L. Martins, INESC, Lisbon, Portugal

b. Professor Paolo Cavaliere, Professor Nunzio Lipari, C.N.R.S.M., Brindisi, Italy

c. Professor Janos Ladik, University of Erlangen-Nrnberg, Erlangen, Germany

d. Dr. Galen Straub, Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM, U.S.A.

Candidates should send a curriculum vitae to:

P.E. Van Camp or V.E. Van Doren
Department of Physics, University of Antwerp (RUCA)
Groenenborgerlaan 171, B-2020 Antwerpen, Belgium

Interference, resonances, and bound states at the Pd(001) and Rh(001) surfaces

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Abstract

We have calculated the $\mathbf{k}_{||}$-, symmetry-, and layer-resolved density of states (DOS) at $\mathbf{k}_{||} = \mathbf{0}$ for Pd and Rh (001) surfaces. For the xy and $x^2 - y^2$ subbands, which do not hybridize with any other low-lying orbitals, the resulting DOS closely resembles that of a 1D-semiinfinite chain of non-degenerate tight-binding atomic orbitals perturbed by a repulsive potential at the terminal site. It displays interference induced oscillations and bound states or resonances of particular simplicity.

Phys. Rev. B (in press Oct 15, 1994)
Latex-file can be obtained from: vero@audrey.mpi-stuttgart.mpg.de

Overlayer and interface resonances and bound states at Pd/Ag(001) and Ag/Pd(001) surfaces

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Abstract

We have calculated the $\mathbf{k}_{||}$-, symmetry-, and layer-resolved density of states (DOS) at $\mathbf{k}_{||} = \mathbf{0}$ for complete pseudomorphic monolayers of Pd on Ag(001) and Ag on Pd(001). For the xy and $x^2 - y^2$ subbands, which do not hybridize with any other low-lying orbitals, the resulting DOS agrees quantitatively with that of a 1D-semiinfinite chain perturbed only at the overlayer, i.e. terminal, site and at the interface, i.e. penultimate, site. The Pd overlayer presents a repulsive potential to the silver. This results in a surface (overlayer) state strongly bound above each subband, in pushing an existing surface ($x^2 - y^2$) state on pure Ag(001) further above the band and in converting an existing resonance (xy) into an interface bound state. The Ag overlayer on the other hand presents an attractive potential to the Pd, resulting in a bound state below each subband and greatly weakened interface resonances at the subband tops.

(accepted Surf. Sci. (in press))
Latex-file can be obtained from: vero@audrey.mpi-stuttgart.mpg.de

Order N Methods in Self-Consistent Density Functional Calculations

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Abstract

We discuss the potential impact of N-scaling algorithms on self-consistent density functional calculations. N-scaling algorithms can increase numerical efficiency in two qualitatively different ways: First, by eliminating the $O(N^3)$ scaling of numerical diagonalizations or orthogonalizations, and second, through the transferability of localized electronic structure information between chemically related, but globally different systems. We argue that the second aspect is potentially of significant practical importance to self-consistent density functional calculations. We describe how the transferability of electronic structure information can be exploited and give numerical examples.

(Accepted for publication in Phys. Rev. B)
Postscript/LATEX versions can be obtained from: dd8f@mad1.fkp.physik.th-darmstadt.de

Electronic Structure of 4d Impurities in Rb: an LSDA+U Density-Functional Study

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Abstract

The electronic structure of the 4d substitutional impurities in Rb is studied by means of self-consistent density-functional calculations. Exchange and correlation corrections for localized orbitals, as they are included in the mean-field solution of the Anderson's model, are superimposed to the spin-dependent potential of the traditional local-spin-density approximation. We find ionic-like configurations and a quite important spin-polarization of the extended sp states. For Nb and Ru impurities we obtain two stable configurations in each case and their energetic stability is studied by means of constrained density-functional calculations. Our results are compared with the results of other calculations and with the available experimental data.

(accepted in J.Phys.: Condens. Matter)
Latex manuscript can be obtained from: nstefan@atlas.uoa.ariadne-t.gr

Quasi-particle band structure of NiO: The Mott-Hubbard picture regained

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Abstract

We demonstrate that the Hubbard correlation among Ni $3d$ electrons is able to reproduce the insulating character of NiO, the correct value of the gap, the orbital character of the valence band edge and the presence of satellite structures. We have determined the quasi-particle spectra starting from the complex single particle band structure of NiO and including the on-site Hubbard repulsion according to a recently developed three-body scattering theory which allows to treat highly correlated and highly hybridized systems. The calculated quasi-particle band structure is in excellent agreement with photoemission data.

(accepted to Phys. Rev. Lett.)
Revtex manuscript can be obtained from: manghi@imoax1.unimo.it

Fe-Induced Magnetization of Pd: The Role of Modified Pd Surface States

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Abstract

The magnetic properties of Fe-Pd multilayers are strongly affected by the high magnetic polarization of Pd. The origin of the magnetization of Pd in contact with Fe is examined. We found that a surface Pd(100) photoemission structure persists upon preparation of 1 and 2 monolayers Fe. Comparison with an *ab initio* calculation identifies this structure as a state distributed equally between the Fe and the adjacent Pd layer. Spin analysis of the photoelectrons shows that this state is magnetic, and the calculation reveals that it contributes to the large Pd moment at the interface of $0.32\mu_{\mathrm{B}}$.

(published in PRL)
Latex-file available from: s.bluegel@kfa-juelich.de

Electronic structure of buried α-$FeSi_2$ and β-$FeSi_2$: Soft-x-ray-emission and -absorption studies compared to bandstructure calculations

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Abstract

The electronic structure of buried α-$FeSi_2$ and β-$FeSi_2$ layers produced by ion-beam-synthesis has been studied. Using fluorescence spectroscopies, we were able to investigate the silicide layers, which are buried below a 600 Ångström Si cap layer, *in situ*. The occupied local Fe *d* density of states was determined by Fe L_3 soft-x-ray emission spectra, excited both with high-energy electrons and monochromatized synchrotron radiation. Using soft-x-ray absorption spectra recorded in the fluorescence-yield mode at the same Fe L_3 edge, the unoccupied Fe *d* density of states was determined. The formation of a bandgap of 0.8 ± 0.2 eV in the electronic states of *d*-symmetry at the Fe atoms of β-$FeSi_2$ could be observed in the experiments. We present *ab–initio* bandstructure calculations for α-$FeSi_2$ and β-$FeSi_2$ and compare the results to the spectroscopic data. The influence of a core hole on the soft x-ray absorption spectrum is studied by calculating the electronic structure of a substitutional impurity in the form of a core–$2p_{3/2}$ ionized Fe atom using a supercell calculation.

(accepted in Phys. Rev. B)
Latex-file available from: s.bluegel@kfa-juelich.de

Two–Dimensional Spin–Polarized States of Ag on Fe(100)

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Abstract

We present an experimental and theoretical investigation of the spin–dependent electronic structure of a Ag monolayer on Fe(100). By spin– and angle–resolved photoemission we identify several spin polarized states of two–dimensional character and determine their band dispersion. The experimental results are compared with *ab initio* band structure calculations. Three kinds of spin-polarized 2D states could be identified along the $\bar{\Gamma} - \bar{X}$ high–symmetry direction of the surface Brillouin zone: (i) 3d–derived Fe surface states which are only weakly modified by the Ag overlayer; (ii) Fe surface states with a substantial sp–character which, upon adsorption of a Ag overlayer, hybridize with the Ag atoms and form interface states; (iii) Ag–induced spin–polarized interface states which are shared by both of the constituents of the interface atoms and do not have any counterpart at the clean Fe surface.

(submitted to Phys. Rev. B)
Latex-file available from: s.bluegel@kfa-juelich.de

Magnetism of 4d and 5d Transition Metal Adlayers on Ag(001): Dependence on the Adlayer Thickness

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Abstract

We present results of ab–initio calculations for the electronic structure and the magnetic moments of 4d (Ru, Rh, Pd) and 5d transition metal bilayers (Ir, Pt) on the Ag(001) substrate. The bilayers of Rh, Pd, Ir, and Pt show ferromagnetism, but compared to the monolayers the moments are strongly reduced to less than $0.35\mu_B$. This indicates that the magnetism in the 4d and 5d metal films depends critically on the film thickness. These results put a severe upper limit on the experimental imperfections permitted to verify 4d and 5d magnetism.

(submitted to Phys. Rev. B, Rapid Comm.)
Latex-file available from: s.bluegel@kfa-juelich.de

Electronic properties of random magnetic surfaces

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Abstract

We have developed a self-consistent spin-polarized Green's function technique within the local spin-density formalism which is suitable for an efficient and reliable description of the electronic and magnetic properties of random transition metal surfaces. The all-electron linear muffin-tin orbital method in the tight-binding representation is used to describe the electronic states, while the semi-infinite nature of the system is incorporated within the surface Green's function approach. The potentials are treated within the atomic sphere approximation including both the monopole and the dipole components of the charge density. The effect of disorder is treated within the coherent potential approximation. Applications to random FeCo overlayers on a non-random fcc Cu(001) substrate are shown.

(appeared in Prog. Surf. Sci. **46**, 159, 1994)

Itinerant magnetism of disordered Fe-Co and Ni-Cu alloys in two and three dimensions

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Abstract

The electronic structure and band magnetism of disordered $Fe_{100-x}Co_x$ and $Ni_{100-x}Cu_x$ bulk alloys and of corresponding disordered overlayers on an fcc Cu(001) substrate were studied by means of the first-principles tight-binding linear muffin-tin orbital coherent potential approximation method. For the Fe-Co system, we found that the composition dependence of the averaged and the local Fe magnetic moments is strongly affected by the dimensionality of the system while the local Co moments remain nearly constant. In the bulk bcc alloys, a non-monotonous behavior of the averaged magnetization occurs due to the transition from weak to strong ferromagnetism. The averaged magnetization of the random overlayers depends linearly on the composition while the local Fe and Co moments are constant since the strong ferromagnetism is stabilized by the substrate throughout the whole composition range. For the Ni-Cu system, a transition from ferromagnetism to paramagnetism is found both in the bulk fcc alloys and in the overlayers. The ferromagnetism of the overlayers is reduced in comparison to the bulk systems of the same composition. The concentration trends of local densities of states, local numbers of electrons, and work functions are discussed.

(appeared in Phys. Rev. B **49**, 3352 ,1994)

Magnetism-induced ordering in two and three dimensions

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Abstract

A first principles theory of alloy ordering in two and three dimensions in the presence of ferromagnetism is described. Using the generalized perturbation method, the order-disorder transition from the bcc $Fe_{50}Co_{50}$ random alloy into the ordered CsCl structure FeCo alloy and its ordering temperature are found to agree reasonably well with available experimental data. A similar ordering tendency for the formation of the ordered c(2x2) phase of the $Fe_{50}Co_{50}$ surface alloy on fcc Cu(001) is investigated.

(to appear in Phys. Rev. B **50**, 1994)
Preprint available from jk@eecws7.tuwien.ac.at

Relativistic electronic structure of random alloys and their surfaces by linear band-structure methods

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Abstract

An efficient Green's function method is developed to calculate electronic and ground state properties of random alloys containing heavy elements and their surfaces. Based on the local density approximation, the all-electron fully-relativistic linear muffin-tin orbital method in the tight-binding representation is used to describe disorder within the coherent potential approximation and the semi-infinite geometry of surfaces. As a first application the electronic and ground state properties of a random fcc-$Cu_{75}Au_{25}$ alloy and its (001) surface are evaluated.

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Magnetic coupling of interfaces: a surface Green's function approach

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Abstract

An ab-initio theory of interface-interface interactions in metallic magnetic multilayers is discussed based on a surface Green's function formalism which reflects the underlying two-dimensional translational symmetry. Due to the short range character of the interlayer interactions in the tight-binding linear muffin-tin orbital method, the problem can be conveniently formulated in real space. In particular, a model consisting of two magnetic Co(001) slabs of varying thickness in a non-magnetic fcc Cu spacer is considered, for which a pronounced suppression of the long period oscillations was found with increasing thickness of the magnetic slabs.

(Phys. Rev. B – Rapid Communication: accepted)
Preprint available from jk@eecws7.tuwien.ac.at

Ferromagnetism of imperfect ultrathin Ru and Rh films on a Ag(001) substrate

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Abstract

We show by means of ab-initio electronic structure calculations that recently predicted ferromagnetism of perfect Ru and Rh monolayers on a Ag(001) substrate is highly sensitive to non-integer coverage by additional Ru or Rh atoms and overlayer-substrate interdiffusion. Both types of structural imperfections strongly reduce the local magnetic moments and lead, in some cases, to a complete extinction of the ferromagnetic state.

(submitted to Phys. Rev. Lett.)
Preprint available from turek@ipm.cz

Two- and three-dimensional aspects of surface state confinement

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Abstract

The confinement of surface state electrons on Cu(111) by nanoscale structures is modelled in this paper by a cylindrical sheath potential on the surface. The confined states can leak through the potential barrier and are also scattered into bulk states, and the contributions of these processes to the lifetime are discussed. Scattering into bulk states provides the most important energy broadening mechanism in this calculation, but contrary to experiment the broadening vanishes as the energy approaches the bottom of the surface state band. The limitations of a two-dimensional treatment of the scattering of surface states by surface potentials are discussed. In a two-dimensional approximation, the sheath model potential can reproduce very well the local density of states at the centre of a ring of discrete s-wave scatterers.

(submitted to Phys. Rev. B)
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The embedding method for confined quantum systems

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Abstract

We discuss the application of the embedding method to the problem of finding the eigenstates of confined quantum systems. Embedding is a general way of tackling boundary condition problems, giving a true variational principle, and we apply it to the confinement problem by embedding within an isotropic medium with a very large potential. Corrections for incomplete confinement are described. The method is tested on examples recently studied by Brownstein [Phys. Rev. Lett. **71**, 1427 (1993)], namely an electron in two dimensions confined within the quadrant of a circle, and a H atom off centre in a spherical cavity.

(submitted to Phys. Rev. B)
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Crystal Potential and Total Energy Calculations within the muffin–tin approach in Semi-Infinite Solids

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Abstract

In the present paper we consider the problem of solving the Poisson equation to obtain the Coulomb part of the crystal potential at the surface of semi–infinite or at the interface between two semi–infinite solids. The problem arises due to the breakdown of the translational invariancy for the direction perpendicular to the surface (interface). The new Green's function technique has been developed to search the solution of the semi–infinite problem and exact expressions have been obtained. In the framework of the muffin–tin geometry of crystal potentials the consequent expressions for the potentials and Coulomb part of the total energy are compared with the well known results in the bulk limit and a complete coincidence is found in this case.

(submitted to Phys. rev. B)
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Electron-Phonon Coupling and D-wave Superconductivity in the Cuprates

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Abstract

We derive an effective single-band Hubbard type Hamiltonian for CuO_2 planes in the cuprate high T_c superconductors. The Hamiltonian includes both electron-electron repulsion and electron-phonon coupling to oxygen vibrational modes. The effective Hamiltonian is derived by mapping from the multi-band constrained density functional theory Hamiltonian to a one band model. A Hartree-Fock mapping leads to $t = 0.66$eV, $t' = -0.14$eV, $U = 4.0$eV. Very similar parameters are obtained by exact diagonalization of finite clusters. The electron-phonon coupling to oxygen breathing modes gives $\lambda = 0.57$ for s-wave and $\lambda = 0.35$ for d $x^2 - y^2$ pairing. D-wave superconductivity is predicted to occur at 30K for doped La_2CuO_4, while the strong Coulomb repulsion suppresses the s-wave T_c to 10K.

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(submitted to Phys. Rev B., october 1994)
Revtex/Postscript version can be obtained from: James.Annett@bristol.ac.uk

Dielectric Function and local field effects of $TiSe_2$

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Abstract

The dielectric function (DF) for this prototype of the layered dichalcogenides has been determined on the basis of two different procedures. The first uses an *ab initio* method, the extended LAPW scheme, to calculate the microscopic DF, $\epsilon(0,0;\omega)$. The second relies on an empirical tight-binding fit to yield the full $\epsilon(\mathbf{q}+\mathbf{G},\mathbf{q}+\mathbf{G}';\omega)$, and the macroscopic DF via the inverse dielectric matrix. The former is especially suited to discuss the optical spectra whereas the latter accounts for the local field effects near the plasma frequency. The results are compared with experimental reflectivity and ellipsometric data.

(submitted to Phys. Rev. B)
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Electromagnetic Surface Response for a Solid with One-dimensional Crystallinity

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Abstract

To calculate the surface response the solid is modelled by a periodic modulated ionic density perpendicular and a translationally invariant density parallel to the surface. This model is designed for the purpose of physical systems like the layered crystals of the transition metal dichalcogenides. A Green's function procedure in position space is presented which allows to determine all the response quantities used in the standard jellium calculations. The algorithm is applied to a system with parameters adapted to TiS_2. Especially, the normalized response field and density near the surface are calculated in dependence of photon energy for the range below the plasma frequency. The results are compared with the jellium case.

(submitted to Phys. Rev. B)
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The extended-LAPW-based $\mathbf{k}\cdot\mathbf{p}$ method for complex band structure calculations

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Abstract

An *ab initio* $\mathbf{k}\cdot\mathbf{p}$ method has been developed, which employs the basis functions of the extended linear augmented plane wave method (ELAPW). To construct the solution of the Schrödinger equation inside the muffin-tin sphere the ELAPW method uses an extended set of radial basis functions, which is shown to be responsible for the high accuracy of the ELAPW-$\mathbf{k}\cdot\mathbf{p}$ method. The $\mathbf{k}\cdot\mathbf{p}$ method provides an efficient computational scheme for the complex band structure calculations. Results on the complex band structure of Cu are presented.

(submitted to Solid State Communications)
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Band theoretical investigation of circular magnetic x-ray dichroism in Fe and Co multilayers

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Abstract

A band theoretical study of circular magnetic x-ray dichroism (CMXD) in Fe and Co multilayers [$Fe(Co)_2Cu_6$ (001), $Fe_1Cu(Ag,Au)_5$ (001), Co_2Pd_4 (111) and Co_2Pt_m (111) (m = 1, 4,7)] has been carried out. The orbital magnetic moment given by the CMXD sum rule is found to be too small by up to 50%. Nevertheless, there is a linear relationship between the integrated CMXD signal and the orbital magnetic moment for each ion species. The calculated magnetic dipole moment is small in the Co systems, but is comparable to the orbital magnetic moment in the Fe systems. The CMXD sum rule for spin magnetization is found to give rather accurate spin magnetic moments (errors within 15%) for the Co systems, and also for the Fe systems if the magnetic dipole moment is included.

(J. Mag. Mag. Mat. (in press))
Postscript file can be obtained from: G.Y. Guo@dl.ac.uk

A relativistic description of spin- and angular-resolved core-level photoemission spectroscopy for magnetic solids

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Abstract

A fully relativistic description of the spin- and angular-resolved core level photoemission spectroscopy of magnetic solids based on multiple scattering theory is presented. This approach describing the corresponding final state as a time reversed LEED state allows a detailed investigation of the magnetic linear and circular dichroism in core level spectroscopy To simplify its application in practical calculations several approximations are suggested. Results for the 2p level spectra of pure Fe for linear polarization are presented which are in rather satisfying agreement with the linear dichroism observed by experiment.

(J. Mag. Mag. Mat. (in press))

Postscript file can be obtained from: H. Ebert (he@gaia.phys.chemie.uni-muenchen.de)

Pressure-induced polymorphism in CuCl: An ab initio study

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Abstract

We report the results of pseudopotential and full potential linear augmented plane wave (FP-LAPW) calculations on high pressure phases of copper chloride. It is found that non-local ionic pseudopotentials accurately describe the bonding in these strongly hybridised compounds over a wide range of densities. Successive transitions from CuCl-II (zincblende) to CuCl-IV (binary analogue of the BC8 structure) and then to CuCl-V (rocksalt) are predicted by both ab initio methods. Both these transitions have been observed in recent neutron powder diffraction experiments. The structural properties and electronic energy band structure of zincblende and NaCl structure CuCl as determined by the pseudopotential and FP-LAPW methods are compared and the band structure of CuCl-IV is, to our knowledge, reported for the first time.

(submitted to Phys. Rev. B)
Preprints can be obtained from: G.Y. Guo@dl.ac.uk

Cu-local density of states in CuAuI

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Abstract

We have determined the Cu-local density of states in CuAuI from photoemission measurements. To assist the analysis we carried out full relativistic x-ray photocurrent calculations using the potential functions and densities of states from electronic structure calculations of CuAuI based on the relativistic Korringa-Kohn-Rostoker method. The good agreement between the experiment and theory suggests that the latter scheme provides a realistic description of the Cu-local density of states in CuAuI.

(Phys. Rev. B (in press)
Preprints can be obtained from: R. G. Jordan (jordanrg@acc.fau.edu)

Density Functional Theory and Strong Interactions: Orbital Ordering in Mott-Hubbard Insulators

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Abstract

Evidence is presented that in strongly interacting electron systems orbital polarization has to be treated on an equal footing with spin polarization and charge density in density functional theory. Using a basis-set independent generalization of the LDA+U functional, we show that electronic orbital ordering is a necessary condition to obtain the correct crystal structure and parameters of the exchange interaction of the Mott-Hubbard insulator $KCuF_3$.

(submitted to Phys. Rev. Lett.)
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Momentum dependence of the linewidth of Raman-active phonons in the normal state of $YBa_2Cu_3O_7$

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Abstract

Previously we predicted a strong wave vector (q) dependence of the phonon linewidth for near-zone-center Raman phonons in $YBa_2Cu_3O_7$ (C.O. Rodriguez, A.I. Liechtenstein, I.I. Mazin, O. Jepsen, O.K. Andersen, and M. Methfessel, Phys. Rev. B **42**, 2692 (1990)). This prediction has now been qualitatively confirmed experimentally and in order to make a quantitative comparison with experiments we have calculated the linewidths with higher accuracy on an expanded q scale. We find that the thresholds for the Landau damping of the Raman phonons agree very well with the experiments which indicates that the renormalization of the electron velocities at the Fermi level is small. The size of the linewidths, which depend on the electron masses, are however too small in the calculations. This discrepancy is possibly due to renormalization of the electron masses.

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HIGHLIGHT OF THE MONTH

THE BOGOLIUBOV - DE GENNES (BDG) EQUATIONS FOR SUPERCONDUCTORS : WHY AND HOW WE SOLVE THEM.

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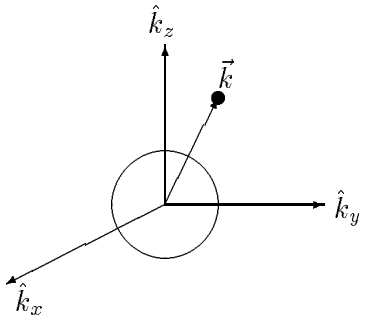
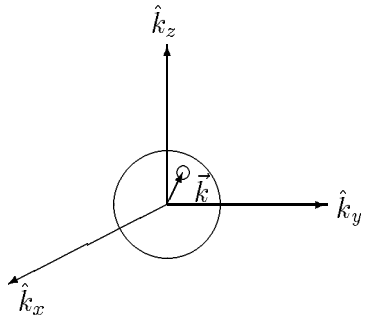
1 The Quasi-Particle Spectrum of Superconductors.

In the NORMAL STATE, the elementary excitations of a non interacting, degenerate Fermi system with a uniform background, are particles in the one particle plane wave states $|\vec{k}>$ for $|\vec{k}| > k_F$ and holes in the state $|\vec{k}>$ for $|\vec{k}| < k_F$ as shown below:





particle

$$\begin{aligned} \epsilon^p_{\vec{k}} &= E_0(N) + \varepsilon_{\vec{k}} - E_0(N+1) \\ &= \varepsilon_{\vec{k}} - \left(\frac{\partial E_0}{\partial N}\right)_N = \varepsilon_{\vec{k}} - \mu \end{aligned}$$

hole

$$\begin{aligned} \epsilon^h_{\vec{k}} &= E_0(N) - \varepsilon_{\vec{k}} - E_0(N-1) \\ &= -\varepsilon_{\vec{k}} + \left(\frac{\partial E_0}{\partial N}\right)_N = -\varepsilon_{\vec{k}} + \mu \end{aligned} \qquad (1)$$

where μ is the chemical potential.

Thus if we describe the particles by the wave function $u_{\vec{k}}(\vec{r})$ and the holes by $v_{\vec{k}}(\vec{r})$, we may say that the quasi-particle spectrum is given by the solutions of the following two component equations:

$$\begin{pmatrix} \epsilon + \mu - H_0 & 0 \\ 0 & \epsilon - \mu + H_0 \end{pmatrix} \begin{pmatrix} u_{\vec{k}}(\vec{r}) \\ v_{\vec{k}}(\vec{r}) \end{pmatrix} = 0 \qquad (2)$$

where $v_{\vec{k}}(\vec{r}) = 0$ for $|\vec{k}| > k_F$ and $u_{\vec{k}}(\vec{r}) = 0$ for $|\vec{k}| < k_F$, H_0 is the Hamiltonian for the non-interacting electrons and $\mu = \varepsilon_F$ is the Fermi energy.

In the SUPERCONDUCTING STATE an excitation will have both particle and hole amplitudes and the above equation generalizes to

$$\begin{pmatrix} \epsilon + \mu - H_0 & -\Delta(\vec{r}) \\ -\Delta^*(\vec{r}) & \epsilon - \mu + H_0 \end{pmatrix} \begin{pmatrix} u_{\vec{k}}(\vec{r}) \\ v_{\vec{k}}(\vec{r}) \end{pmatrix} = 0 \qquad (3)$$

where $\Delta(\vec{r})$ is the pairing potential. This is a fairly general form of the BdG equation [2] and as such it is the principle subject of this note.

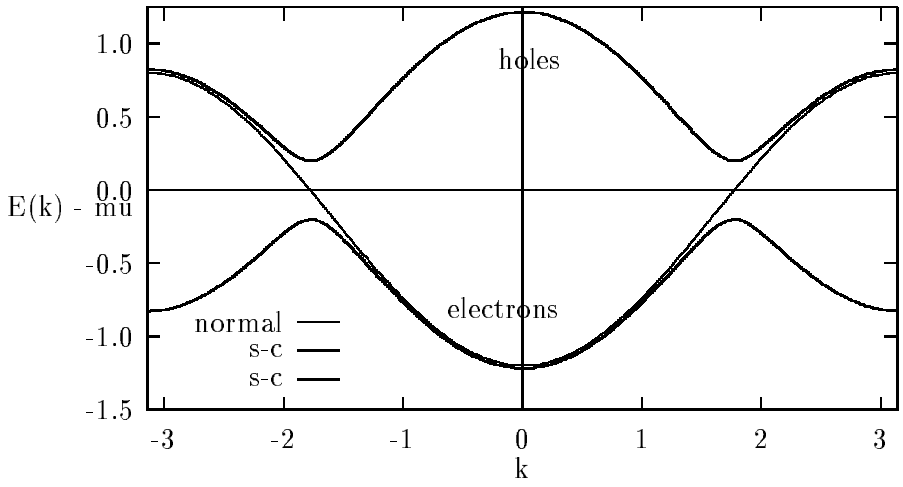


Figure 1: Normal, tight-binding band (continuous line) gapped by a pair potential, Δ (dashed lines).

In the Bardeen Cooper Schrieffer (BCS) theory the pairing potential is proportional to the pairing amplitude, $\langle \Psi_\uparrow(\vec{r}) \Psi_\downarrow(\vec{r}) \rangle$, an anomalous average which is zero in the normal state. It works out to be

$$\begin{aligned} \Delta(\vec{r}) &= -\lambda \langle \Psi_\uparrow(\vec{r}) \Psi_\downarrow(\vec{r}) \rangle \\ &= \sum_n u_n(\vec{r}) v_n(\vec{r}) \left[1 - 2 f(E_n) \right] \end{aligned} \tag{4}$$

where λ is the strength of the model electron-electron potential : $V^p(\vec{r} - \vec{r'})$, which is attractive for $\lambda > 0$, $\begin{pmatrix} u_n(\vec{r}) \\ v_n(\vec{r}) \end{pmatrix}$ is an eigensolution of the BdG equation in Eq. 3 corresponding to the quasi-particle energy eigenvalue E_n and $f(E)$ is the usual Fermi function. It should be stressed that Eq. 3 is to be solved self-consistently using Eq. 4 in each iteration.

If we assume that Δ is a constant, Eq. 3 leads to the well known BCS-formula

$$E_{\vec{k}} = \sqrt{\left(\varepsilon_{\vec{k}} - \mu \right)^2 + \Delta^2} \tag{5}$$

where $\varepsilon_{\vec{k}}$ is the dispersion relation, corresponding to H_0, in the normal state. This is displayed in Fig. 1.

What lends particular significance to the BdG equation in Eq. 3 is that it holds much more generally than the above simple BCS model implies. Indeed the recently formulated Density Functional Theory for superconductors [3] yields an Euler-Lagrange (Kohn-Sham) equation which is precisely of this form. Moreover, as is usual in density functional theories, it supplies exact recipes for calculating the effective one electron potential in H_0 and the pairing potential, $V^p(\vec{r}, \vec{r'})$. When these are approximated, in an LDA-like fashion for instance [4], the way is open to calculations of the ground state energy or ground potential as well as the quasi-particle spectrum in the superconducting states on a first principles basis.

Whilst from the point of view of our present concern the above generalization is decisive, it is relevant to note that the BdG equations are also studied in Nuclear Physics [1] and Astrophysics [5].

In summary, the BdG equations are of general significance in describing degenerate Fermi systems with anomalous pairing amplitudes like $\chi(\vec{r},\vec{r'})$. Since their structure is rather similar to those usually studied in calculation of the electronic structure of the normal state it is natural to deploy the powerful methods of 'band theory' for solving them. In what follows we shall describe some interesting examples of doing that. As it turns out these examples are the principle activities of Working Group Va in the Ψ_k-Network.

2 Density Functional Theory for Superconductors

For conventional superconductors the coherence length, $\xi_0 = \frac{\hbar v_F}{\pi\Delta}$, is large ($\approx 1000$Å) and therefore, $\Delta(\vec{r}) = \Delta$ a constant, is a good approximation. Consequently Eq. 5 describes well the quasi-particle spectra and it is sufficient to calculate $\varepsilon_{\vec{k},\nu}$, the normal state electronic structures. Indeed, when energies are rescaled by Δ and distances by ξ_0, the superconducting properties of most superconductors appear to be very similar. By contrast the new so-called 'high T_c' superconductors have short coherence length, $\xi_0 \approx 10 - 30\mathring{A}$, and their superconducting properties appear to be as varied among materials as the magnetic properties of itinerant magnets. Thus, in this case we may expect that first principles calculation may play an important role. In particular, since now $\Delta(\vec{r})$ will depend on $\vec{r}$, the quasi-particle spectra which has the general form

$$E_{\vec{k},\nu} = \sqrt{\left(\varepsilon_{\vec{k},\nu} - \mu\right)^2 + \left|\Delta_{\vec{k},\nu}\right|^2} \tag{6}$$

contains the 'gap' function, $\Delta_{\vec{k},\nu}$, as a new $\vec{k}$-dependent superconducting property. (Note that it is not the Fourier transform of $\Delta(\vec{r})$). The point is that, at least in principle, this most interesting quantity can be measured in angle-resolved photoemission [6], quantum oscillation [7] and neutron scattering experiments [8] and hence its study could provide the much needed differentiation between contending models.

Another novel feature of superconductors with small coherence length, like the superconducting cuprates, is that Δ may be different on inequivalent sites. This would show up in NMR experiments [9] and would be a natural consequence of a first-principles calculations.

The structure of the above density functional theory is very similar to that of Spin Density Functional Theory with the pairing amplitude $\chi(\vec{r})$ playing the role of the magnetization $m(\vec{r})$. Indeed, the Kohn-Sham equations of this theory for the two component wave-function $\begin{pmatrix} \Psi_\uparrow(\vec{r}) \\ \Psi_\downarrow(\vec{r}) \end{pmatrix}$ are very similar to the BdG equations given by Eq. 3 both in mathematical form and self-consistency logic. Thus the computational techniques necessary for solving the former can be expected to be a generalized version of 'spin-polarized band theory'.

Evidently, to get started we need a recipe, analogous to LSDA for an effective potential functional $V_{eff}\,(\vec{r},[n,\chi])$, to be used in H_0 of Eq. 3 and a pairing functional $V_p\left(\vec{r},\vec{r'};[n,\chi]\right)$. For the former we use the usual LDA and for the latter we take the following BCS-like form [4] :

$$V_p\left(\vec{r},\vec{r'};[n,\chi]\right) \equiv \frac{\delta E_{xc}[n,\chi]}{\delta\chi(\vec{r},\vec{r'})} = \lambda_i\delta(\vec{r}-\vec{r'}) \tag{7}$$

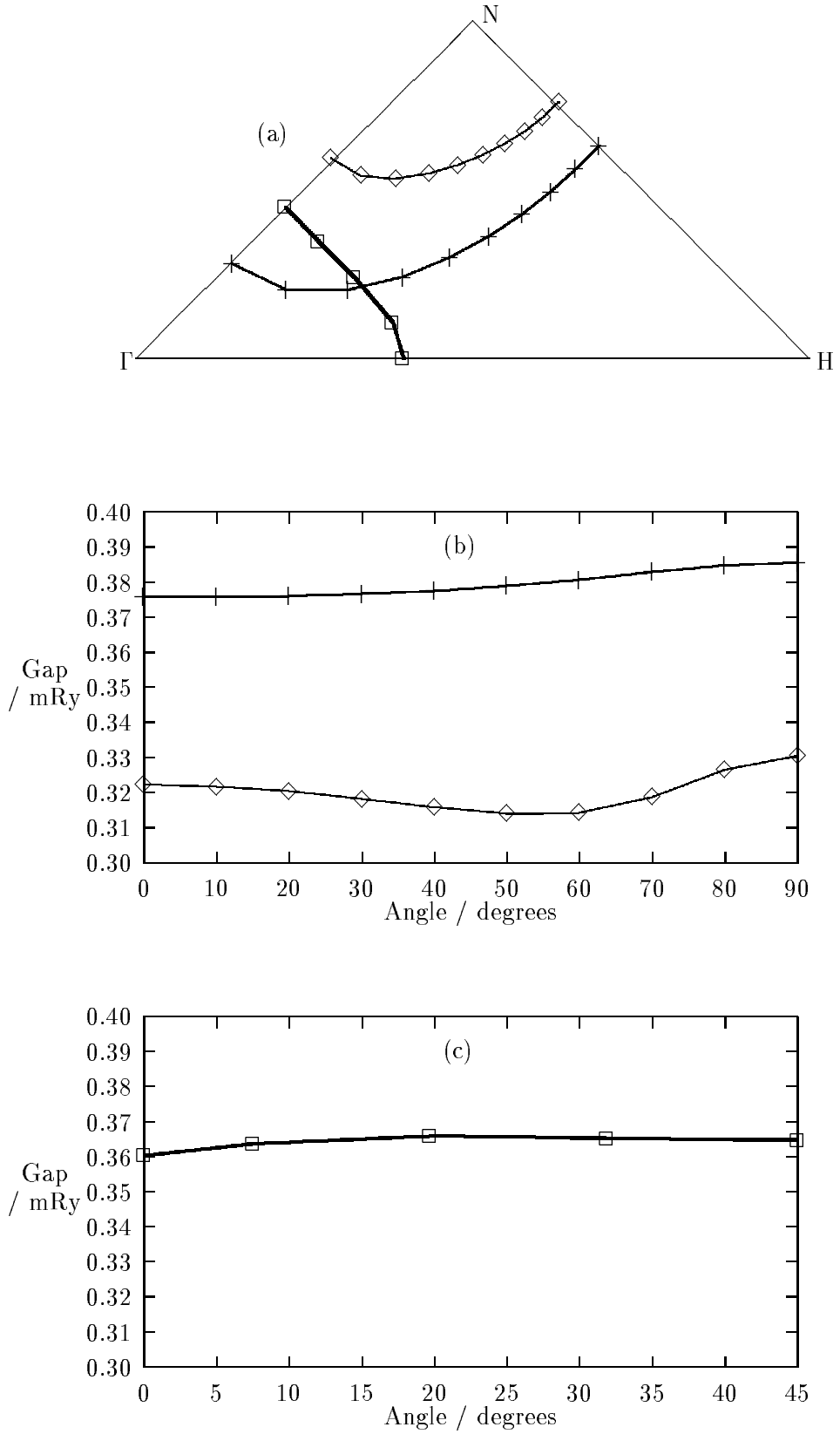


Figure 2: (a) Positions of sheets of Fermi surface in Nb, and (b), (c) the respective gaps for the directions indicated in (a). For (b) 0^o indicates the Γ-N line, while 90^o is on the N-H line. For (c) 0^o indicates the Γ-N line, while 45^o is on the Γ-H line.

where $\vec{r}$ and $\vec{r'}$ are within the muffin-tin well surrounding the i-th inequivalent site. Presently, we take the parameters λ_1, λ_2, *etc.*, one for each inequivalent site, as phenomenological parameters to be determined by requiring that some calculated properties like T_c, *etc.* agree with experiments. As was argued in the paper by Suvasini et al. [4] this semi-phenomenological, yet first principles, approach can be useful if there is a rich structure in $\Delta_{\vec{k},\nu}$ and only a few coupling constants, λ_1, λ_2, *etc.*, are needed.

The above strategy was fully implemented by Suvasini et al. [4] for Nb using the LMTO method. As an illustration of the results we show $\Delta_{\vec{k},\nu}$ on three sheets of the Fermi surface in Fig. 2. Since the coherence length of Nb is large ($\xi_0 \approx 1000\mathring{A}$) and hence Eq. 7 is not likely to be a good approximation, this example is only of computational interest. The code is now in the process of being scaled up to the HTC cuprates (YBCO *etc.*). The motivation behind such calculations is the hope that $\lambda_{Cu} \neq 0$, $\lambda_O = 0$ and $\lambda_{Cu} = 0$, $\lambda_O \neq 0$ in the CuO_2 planes will give sufficiently different quasi-particle spectra to enable us to identify which of the two configurations are favoured by experiments. Moreover, recently we began to experiment with finite range pairing potentials which are attracting for electrons on different sites. These have interestingly dramatic effects on the quasi-particle spectra [14]. Clearly, the novelty of this work is the fact that a very simple phenomenological pairing interaction, of unknown origin, is treated in the context of a realistic complex band structure. Viewed in this light this approach is very similar in spirit to the X_α method of Slater before the invention of proper density functional theory. Hopefully, some later time, we shall have a parameter-free local density approximation for the exchange-correlation energy functional $E_{xc}[n, \chi]$ in the superconducting phase. Thanks to our current work the numerical technique to exploit such circumstance will be available.

3 The Quasi-Particle Spectrum of the Abrikosov Flux Lattice

Type-II superconductors in magnetic fields $H > H_{c1}$ - the lower critical field - do not expel all external flux completely, but allow it to pass through in units of the flux quanta, $\Phi_0 = \frac{h}{2e}$. This is illustrated in Fig. 3. Where the flux is admitted the order parameter, $\Delta(\vec{r})$, drops to zero and the magnetic field reaches its external value. Such a configuration is called a vortex and, as was discovered theoretically by Abrikosov, these vortices form a two dimensional, usually triangular, lattice frequently referred to as the Abrikosov flux lattice [10]. His and almost all subsequent work on the subject was based on the phenomenological Ginzburg-Landau theory which describes the spatial variation of the order parameter $\Delta(\vec{r})$, or, to put it another way, the condensate of the Cooper pairs, but not the quasi-particle excitations of the superconducting ground state. The latter are described only by the fully microscopic BdG equations in a magnetic field. In this section we shall be concerned with the solutions of these.

Whilst such a fully microscopic theory of the flux state is clearly desirable in its own right, the recent discovery of de Haas-van Alphen oscillations [8] in the superconducting state makes this problem one of the burning issues of solid-state physics. Briefly, on the one hand even the precise mechanism of these oscillations is highly controversial, on the other, one would expect that seeing de Haas-van Alphen oscillations in the high $T_c$superconductors would prove that their normal state

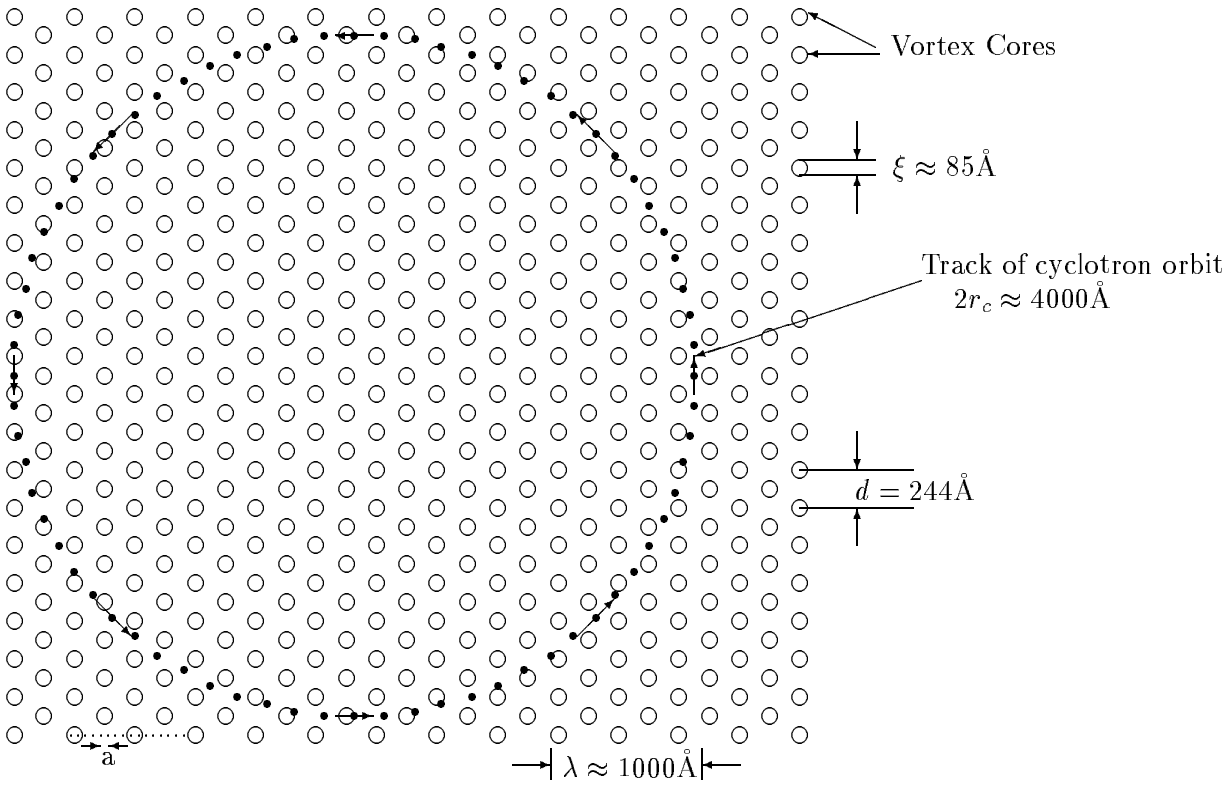


Figure 3: The various length scales for a field of 8 Tesla in $NbSe_2$

is a Fermi Liquid (since H_{c2} is several 100 Tesla and $T_c \approx 100K$, the only hope of seeing the de Haas-van Alphen effect in these materials is in the superconducting state) and their observation in the Heavy Fermion Superconductors like UPt_3 could be the 'smoking gun' experiment for exotic (p- or d-wave) pairing. To appreciate the difficulty of the problem at hand we illustrate the four different length scale on which we must do justice to the complexity of the electronic motion in Fig. 3.

They are the lattice parameter, a, the lattice parameter of the flux lattice, d, the size of the vortex cores, ξ_0 and the radius, r_c of the Landau orbits which, at least in the normal state, govern the dHvA oscillations. Note also that there are two separate flux quantizations in this problem: one is to do with the motion of the Cooper pairs and gives rise to the flux quanta, each Φ_0, piercing the superconductors at the vortices. The other is associated with the motion of individual electrons or quasi-particles, in Landau orbits which encircle integer multiples of the flux unit, $\frac{h}{e}(= 2\Phi_0)$.

Given the above complicated but interesting circumstances, an effective strategy is to take a simple model which contains all the principle ingredients of the physics and solve it exactly. In the present case such a model is a single band, tight-binding Bogoliubov-de Gennes equation with a magnetic field.

This may be written as follows :

$$\sum_j \begin{pmatrix} \left(\epsilon_0 + \frac{Un_i}{2} - \mu\right)\delta_{ij} + t_{ij} & \Delta_i\delta_{ij} \\ \Delta_i^*\delta_{ij} & -\left(\epsilon_0 + \frac{Un_i}{2} - \mu\right)\delta_{ij} - t_{ij}^* \end{pmatrix} \begin{pmatrix} u_j \\ v_j \end{pmatrix} = E \begin{pmatrix} u_i \\ v_i \end{pmatrix} \tag{8}$$

where the hopping amplitude, t_{ij}, is given in terms of the vector potential, $\vec{A}(\vec{r})$, by

$$t_{ij} = -t \exp\left\{-i\frac{e}{\hbar}\int_{\vec{R}_i}^{\vec{R}_j} \vec{A}(\vec{r})\cdot d\vec{r}\right\} \qquad \text{for } i \text{ and } j \text{ nearest neighbours,} \tag{9}$$

$$= 0 \qquad \text{otherwise} \tag{10}$$

ϵ_0 is the site energy, n_i is the charge density and Δ_i the pairing potential at the site i, and U is the electron-electron coupling constant in the negative-U Hubbard model, from which the above equation has been derived. As usual in electronic structure problems, Eq. 8 has to be solved self-consistently. Namely, for a set of $\{n_i, t_{ij}, \Delta_i\}$ one solves for $\{u_i, v_i\}$ and recalculates n_i , t_{ij} and Δ_i, using standard formulae (not given here) repeating this procedure until convergence. The most novel feature of such a calculation is the need to re-compute the hopping integral, t_{ij}, at each iteration. This involves finding the current, I_{ij}, on all the links $(i-j)$ and solving Ampères law for flux through each plaquette and the vector potential. In other words we are solving not only the usual electrostatic, but also the magnetostatic Maxwell equations self-consistently with the Many-Body Schrödinger's equation.

If the external magnetic field is such that the flux per plaquette is not a rational number times Φ_0, there is no lattice periodicity left in the above problem. This suggests that in solving it we throw out $\vec{k}$-space [11] altogether and solve the problem entirely in real space, by adopting the Recursion Method of Haydock and others [12] to deal with it. This turns out to be a very efficient procedure.

In the normal state $\Delta_i = 0$ and the energy eigenvalues of Eq. 8 are that of the celebrated Azbel'-Hofstadter spectra displayed in Fig. 4. Our real-space, Recursion-Method, solution for the local density of states $N_0(\varepsilon)$ at the centre of our coordinate system is shown in Fig. 5. Evidently the presence of the magnetic field has broken up the zero-field, square lattice band into sharp states. These are the tight-binding analogues of the Landau levels in the free electron (no periodic potential) limit. This is particularly clear near the band edges where the peak separations are quite uniform and are close to $\hbar\omega_c$ $\left(\omega_c = \frac{eB}{m^*}\right)$. Note that in the zero field case, our real space calculation reproduces satisfactorily the sharp features of the density of states due to van Hove singularities of the $\vec{k}$-space band structure. To achieve such accuracy we had to go to 10^3-10^4 approximate levels in the continued fraction representation of local density of states.

To solve the fully self-consistent superconducting version of the above problem is a very much greater computational task. However, it follows the logic of a real space, order N, self-consistent Density-Functional Calculation and it is particularly susceptible to treatment by parallel algorithms. In fact solutions were found for flux lattice unit cells containing up to 900 real lattice sites, by using up to 136 nodes of the Oak Ridge National Laboratory Paragon machine. For particular, unphysically large but computationally very convenient fields the solutions were for smaller flux lattice cells, and the density of states shown in figure 6 is for a vortex cell consisting of 16 unit cells of real lattice. The attractive interaction energy, $-U$, was also chosen to be unreasonably large,

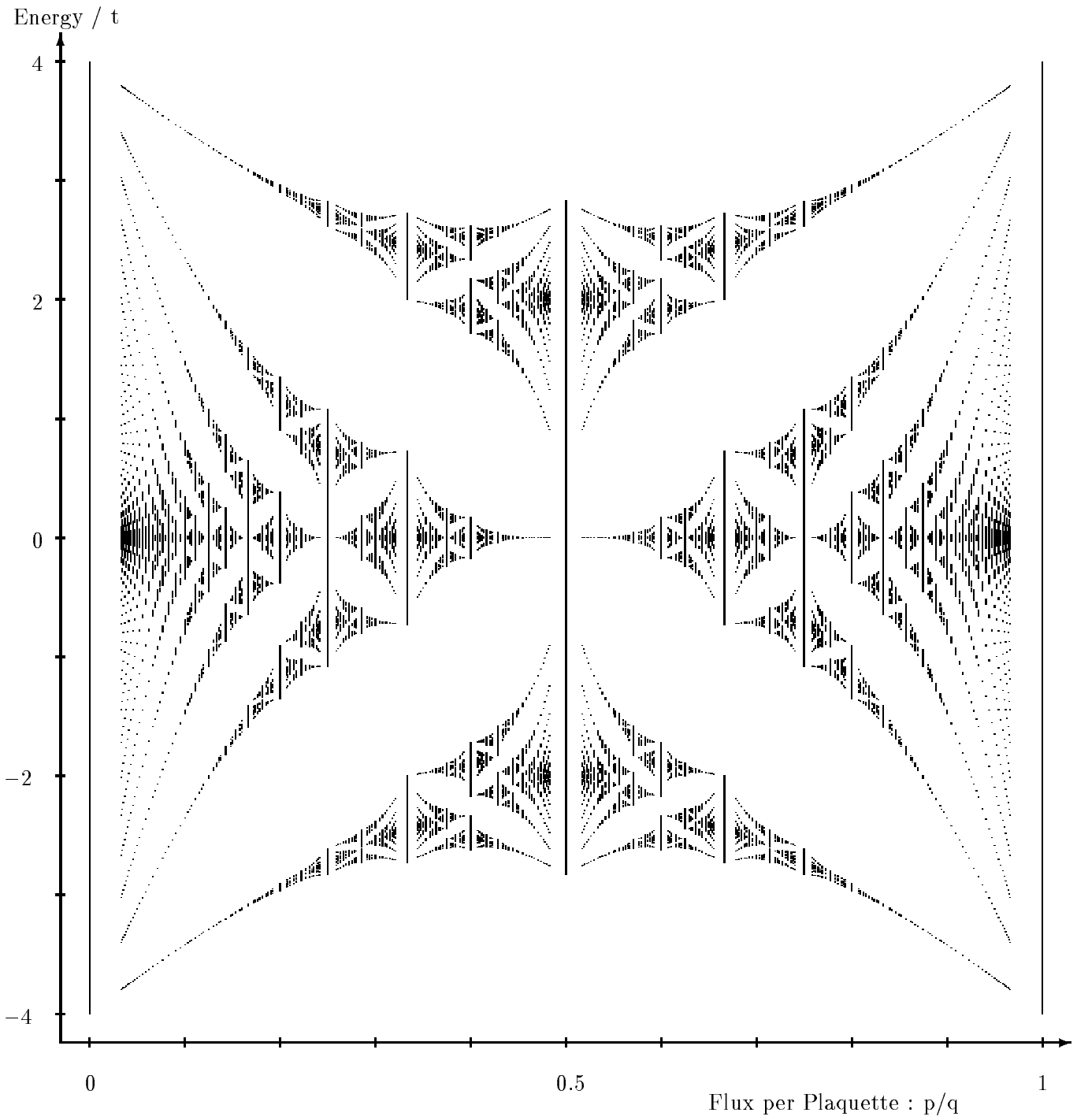


Figure 4: The Hofstatder Spectrum

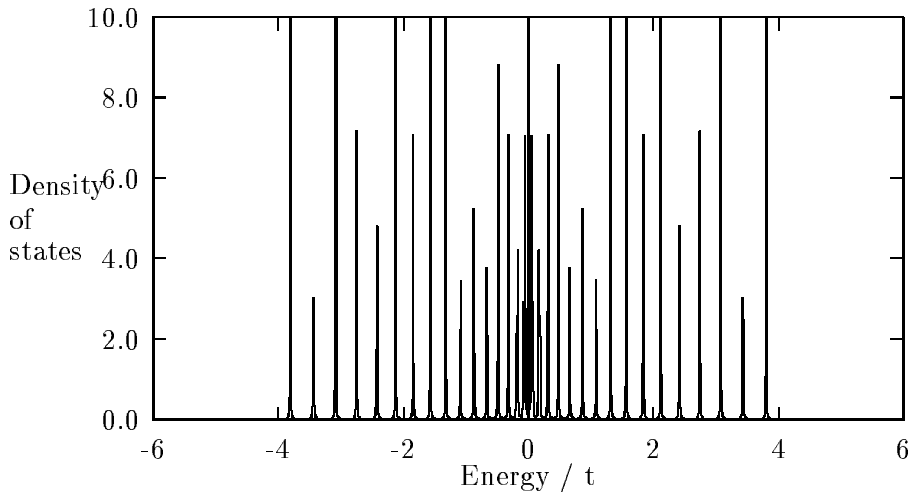


Figure 5: Normal state with a magnetic field, such that the flux per lattice plaquette, $Ba^2 = 1/32(h/e)$.

leading to a very large self-consistent order parameter, $\Delta(\vec{r})$, so that the coherence length, ξ_0, would be of the order a. The phase of the order parameter, $|\Delta_i|\, e^{i\theta_i}$ and the current vary cylindrically about the vortex core where the amplitude $|\Delta_i| = 0$. Away from the core, $|\Delta_i|$ recovers to more or less its value without the magnetic field in one step. In Fig.6 we show the quasi-particle density of states at such a healed lattice site (2,0) halfway between two vortex cores.

The quasi-particle local density of states, $N_{2,0}(\varepsilon)$ shown in Fig. 6 illustrates the central results of these calculations. Namely, as in the normal state the effect of a magnetic field in the superconducting state is that it breaks up the appropriate density of states into 'Landau level like' peaks. Of course these peaks are now pushed out from the gap region and squeezed together. The main point is that if a Landau level was below the Fermi energy, ε_F in the normal state it will be pushed down and will be found below the gap in the superconducting state. On the other hand if it was above ε_F, it will get pushed to energies above the gap as the system goes superconducting. Thus with increasing field there will be a steady migration of 'Landau levels' across the Fermi energy, ε_F, and the total energy will oscillate with changing $\frac{1}{B}$ as in the normal state. Naturally, the presence of the gap will change the phase and the amplitude of these oscillations, hopefully as observed in experiments, but the frequency remains the same.

Clearly, there is no hope of repeating the above calculation for such first principles Bogoliubov-de Gennes equation as we have discussed in Sec. 2. Yet if we are to interpret the very interested experimental data that is now beginning to be available we must make contact between them and quantitative calculations based on realistic models. To do this we retraced the history of the de Haas-van Alphen effect in the normal state during the late 50's and developed a semi-classical theory of the superconducting quasi-particle motion in a magnetic field.

In short, we took the solution of the Bogoliubov-de Gennes equation to be in the semi-classical

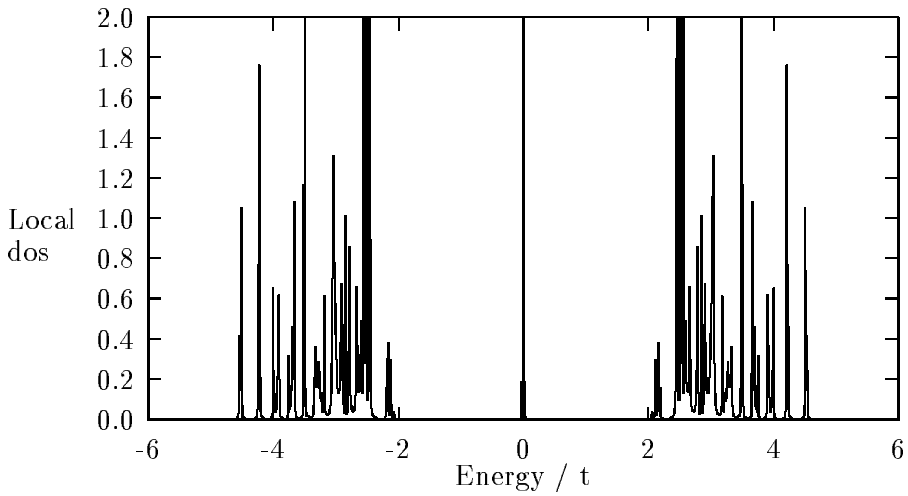


Figure 6: The local density of states on site (2,0) of a fully self-consistent solution with 16 lattice sites per vortex cell.

form

$$\begin{pmatrix} u(\vec{r}) \\ v(\vec{r}) \end{pmatrix} = \begin{pmatrix} u^0(\vec{r}) \\ v^0(\vec{r}) \end{pmatrix} \mathrm{e}^{\frac{i}{\hbar}\left[S(\vec{r})\underline{\underline{1}} + \Sigma(\vec{r})\underline{\underline{\tau}}_z\right]} \tag{11}$$

where u^0 and v^0 are slowly varying functions of $\vec{r}$, $\underline{\underline{1}}$ and $\underline{\underline{\tau}}_z$ are the unit matrix and z-component Pauli matrix respectively, and the phase functions, $S(\vec{r})$ and $\Sigma(\vec{r})$, are determined by the Bogoliubov-de Gennes equation to lowest order in $\hbar$. (To treat Eq. 8 we generalized the semi-classical theory of Wilkinson [5] for a tight binding model). An interesting novel feature of the theory is the presence of the two phase functions $S(\vec{r})$ and $\Sigma(\vec{r})$. They represent the sum and the difference phases of the two amplitudes, u and v, and give rise to the two, Landau and Abrikosov, flux quantizations.

As in the case of semi-classical theory for normal electrons, the Bohr-Sommerfeld quantization rules which follow from the requirement that $S(\vec{r})$ and $\Sigma(\vec{r})$ describe a single valued quasi-particle amplitude, $\underline{\Psi}(\vec{r}) = \begin{pmatrix} u(\vec{r}) \\ v(\vec{r} \end{pmatrix}$, determine the quasi-particle energies in terms of the band structure without the magnetic field. In the present, superconducting, case this is described by the normal state spectra $\varepsilon_{\vec{k},\nu}$ and the gap function $\Delta_{\vec{k},\nu}$, both of which we can aspire to calculate for a variety of pairing mechanisms.

The most remarkable upshot of this theory is that it relates the de Haas-van Alphen signal to extremal orbits on the Fermi Surface (in the normal state) and the average of the gap $\Delta_{\vec{k},\nu}$ over such orbits. This means that these experiments measure the gap average over selected portions of the Fermi Surface, namely the extremal orbits transverse to the external magnetic field. Given the track record of the de Haas-van Alphen measurements in providing detailed quantitative information about the shape and size of the normal state Fermi Surface, the above effect in the superconducting state can be expected to become a uniquely powerful probe of the superconducting gap's variation over the Fermi Surface. In particular, it is likely to be the 'smoking gun experiment' for detecting lines on the Fermi Surface along which $\Delta_{\vec{k},\nu} = 0$ and hence anisotropic superconductivity such

as expected in the high-T_c materials (d-wave pairing) and heavy fermion superconductors (UPt_3, UBe_{13} *etc.*).

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