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Exact Results for the Many-Electron Problem: Competing Orders in a Nearly Antiferromagnetic Metal

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One of the most challenging problems in computational condensed matter physics is the simulation of many-electron systems by unbiased numerical techniques. Quantum Monte Carlo approaches – typically the method of choice for quantum many-body systems with bosonic or spin degrees of freedom – are oftentimes limited to handle many-electron systems due to the infamous fermion-sign problem that severely limits the computational efficiency of this otherwise very potent class of algorithms. Here we report on an elegant approach to overcome the fermion-sign problem in the study of competing quantum magnetism and superconductivity in metals. This approach allows us to study the onset of spin-density wave order in such itinerant electron systems via two-dimensional lattice models amenable to numerically exact, sign-problem-free determinantal quantum Monte Carlo simulations. The finite-temperature phase diagram of these models reveal a dome-shaped d-wave superconducting phase near the magnetic quantum phase transition. The striking similarity of these numerical results to the experimentally observed phenomenology of many unconventional superconductors points a way to a microscopic understanding of such strongly coupled systems in a controlled manner.

1 Introduction

Quantum many-body systems can give rise to remarkable collective states of matter that have no counterpart in their classical analogs. Archetypal examples include superfluids, superconductors, and insulating quantum liquids in the context of condensed matter physics, but collective quantum phenomena are also ubiquitous in nuclear physics, quantum chemistry, high-energy physics, traditional atomic physics as well as ultracold atoms. Quantum information technology not only takes quantum effects for granted, but goes a step further and aims at “taming the quantum” by controlling collective quantum states for applications like quantum computing.

In connecting such complex emergent behaviour to a microscopic picture in terms of short-ranged interactions between the elementary quantum mechanical degrees of freedom, analytical approaches on the level of mean-field theory or effective field theory descriptions can often provide qualitative guidance and occasionally understanding. However, the validity of such analytical approaches and their underlying abstractions are often a matter of debate, and unbiased numerical simulations play a crucial role in verifying these assumptions. Often quantitative guidance in mapping out phase diagrams (in terms of the microscopic interactions) and the respective phase transitions is obtained solely by numerical methods. In the interplay between theory and experiment, computational physics has thereby established itself as a vital discipline for quantum many-body physics.

The combination of analytical and numerical approaches has led to remarkable progress in understanding the general features of collective states of quantum systems constituted by bosonic degrees of freedom, such as a broad class of quantum magnets or ultracold atomic systems. However, there are a number of important outstanding problems that have for decades resisted solution, most prominently the many fermion problem.

The quantum statistics, which sets fermions apart from bosons, has profound implications not only on the intricate nodal structure of quantum mechanical wavefunctions of many-fermion systems and the resulting, enticingly complex variety of fermionic ground states but also on the ability to simulate many-fermion systems with the most powerful, unbiased numerical approach to quantum many-body systems – quantum Monte Carlo simulations. As realised early on, the fermionic exchange statistics leads to the infamous *sign problem*¹, i.e. the occurrence of negative statistical weights in the sampling of fermionic world-line configurations. Overcoming the sign problem by identifying a basis transformation to a sign-free basis (such as the basis of eigenstates) is known to be an *NP*-hard problem². Thus, in order to make progress on the many-fermion problem it will be paramount to employ entirely new perspectives on the many-fermion system and to develop novel numerical simulation schemes.

This short article reports on recent progress made in the understanding of competing magnetic and superconducting orders in itinerant electron systems, i.e. systems that in the absence of any electronic ordering instabilities typically form metals. Despite the itinerant character of the electrons, their spin degrees of freedom can nevertheless give rise to a spin-density wave order. Such antiferromagnetic metals exist in a variety of materials such as the electron-doped cuprates or the iron pnictides. Of course, these materials are much better known for another phenomenon that is intrinsically linked to the suppression of the spin-density wave order upon tuning some external parameter such as pressure or chemical composition for these materials – the emergence of high-temperature superconductivity.

While the conceptual link between the onset of magnetic order at a zero-temperature quantum critical point and the emergence of superconductivity overshadowing this quantum critical point at finite temperatures has been discussed over the last three decades from every conceivable analytical and phenomenological perspective, the discussion has been lacking unquestionable numerical data from exact many-body simulation techniques. However, following an ingenious insight³ into the modelling of such itinerant electron systems via effective, sign-free actions of microscopic spin-fermion models it has been the goal of this high-performance computing project to gather what has been the first numerically exact quantum Monte Carlo results for the finite-temperature phase diagram of such systems. This is precisely what we have been producing in JURECA runs over the last three years.

2 Sign-Problem Free Quantum Monte Carlo

The physics of a two-dimensional metal formed by itinerant, spinful electrons can be captured by a single-band Hamiltonian for electrons $c_{\mathbf{k}\sigma}$ with dispersion $\epsilon_{\mathbf{k}}$ coupled to an antiferromagnetic order parameter $\vec{\varphi}_{\mathbf{q}}$ has the form

$$H = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} + \lambda \sum_{\mathbf{k},\mathbf{q},\sigma,\tau} \left[c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}+\mathbf{Q}+\mathbf{q},\tau} \right] [\vec{\varphi}_{\mathbf{q}} \cdot \vec{\sigma}]_{\sigma\tau}, \quad (1)$$

where $\mathbf{Q} = (\pi, \pi)$ characterises the antiferromagnetic order and $\vec{\sigma}$ are the Pauli matrices. Generally, quantum Monte Carlo simulations of this Hamiltonian will have a severe sign-problem.

Over the last decade analytical work, in particular by Subir Sachdev and collaborators, has led to the identification of a quantum field theory⁴ describing the quantum fluctuations

which control the quantum critical point at the onset of magnetic ordering. One particularly intriguing feature of the so-derived quantum field theory is that it allows for an effective description of the non-trivial deviations from the Fermi liquid behaviour of conventional metals. This field theory further turns out to have many universal features, in particular it is independent of the detailed band structure of the model – only the Fermi velocities at a finite number of so-called *hot spots* on the Fermi surface are in fact relevant input parameters. Hot spots are those points on the Fermi surface that are connected by a momentum $\mathbf{Q}$, which correspond to states between which $\vec{\varphi}_{\mathbf{q}=0}$ scatters, see Fig. 1(a). However, without the help from numerics further progress in analysing this quantum field theory has not been straightforward as analytical approaches such as perturbation expansions or a renormalisation group analysis indicate a flow to the uncontrolled strong-coupling limit^{5,6}.

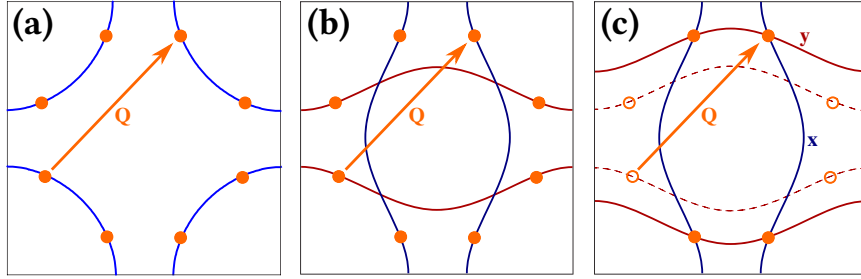


Figure 1. (a) 1st Brillouin zone with single band Fermi surface and hot spots. (b) Two-band model Fermi surfaces. (c) Additional shift yielding x - and y -bands. Figure adapted from Ref. 3.

A new inroad into understanding such quantum field theories was paved by a beautiful paper³ by E. Berg, M. A. Metlitski and S. Sachdev (published in Science in late 2012), which presents an ingenious approach that allows to analyse the onset of antiferromagnetism in determinantal quantum Monte Carlo studies completely free of the sign-problem. The key idea underlying this removal of the sign-problem of model (1) is to deform it into a two-band model with two *detached* Fermi surfaces, each containing hot spots that are separated by $\mathbf{Q}$ from those on the other surface, see Fig. 1(b). This procedure is performed in a *controlled* way such that the structure of the hot spots is sustained and close to them the Fermi surface does not change. In more technical terms, one introduces two flavours of fermions ψ_x and ψ_y (cf. Fig. 1c), which are coupled to a bosonic order parameter field $\vec{\varphi}$. A realisation of the new model at inverse temperature β is then given by the action $S = \int_0^\beta d\tau [L_F + L_\varphi]$ with

$$\begin{aligned}
L_F &= \sum_{\substack{\mathbf{i}, \mathbf{j} \\ \sigma=\uparrow, \downarrow}} \sum_{\alpha=x, y} \psi_{\alpha, \mathbf{i}, \sigma}^\dagger [(\partial_\tau - \mu)\delta_{ij} - t_{\alpha, ij}] \psi_{\alpha, \mathbf{j}, \sigma} \\
&\quad + \lambda \sum_{\substack{\mathbf{i} \\ \sigma, \tau=\uparrow, \downarrow}} [\vec{\sigma} \cdot \vec{\varphi}_i]_{\sigma, \tau} \psi_{x, \mathbf{i}, \sigma}^\dagger \psi_{y, \mathbf{i}, \tau} + \text{h.c.} \\
L_\varphi &= \frac{1}{2} \sum_{\mathbf{i}} \left(\frac{d\vec{\varphi}_i}{d\tau} \right)^2 + \frac{1}{2} \sum_{\langle \mathbf{i}, \mathbf{j} \rangle} (\vec{\varphi}_i - \vec{\varphi}_j)^2 + \sum_{\mathbf{i}} \left[\frac{r}{2} \vec{\varphi}_i^2 + \frac{u}{4} (\vec{\varphi}_i^2)^2 \right], \quad (2)
\end{aligned}$$

where τ runs through imaginary time and $i, j = 1, \dots, N$ are real space square lattice sites. The coefficients $t_{\alpha,ij}$ are appropriately chosen hopping constants and μ is the chemical potential. Antiferromagnetic order is favoured or impeded by tuning the control parameter r . To compute the partition function $Z = \int d(\psi_x, \psi_y, \vec{\varphi}) e^{-S}$ the fermionic degrees of freedom can be traced out, yielding an integral in $\vec{\varphi}$ -space over Slater determinants weighted by a bosonic action. This can be evaluated using the techniques of determinantal QMC (DQMC)⁷. One can easily prove that, in contrast to the original model (1), the action (2) then only leads to *strictly positive* weights in the Monte Carlo sampling.

3 Magnetism and Superconductivity in Itinerant Electron Systems

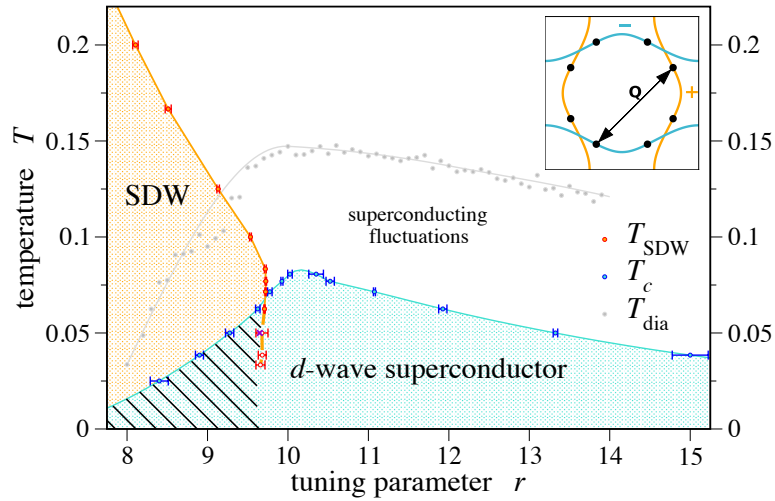


Figure 2. Phase diagram of model (2) showing the transition temperature T_{SDW} to magnetic spin density wave (SDW) order, the superconducting T_c , and the onset of diamagnetism at T_{dia} . Solid lines indicate a Berezinskii-Kosterlitz-Thouless transition. The SDW transition inside the SC dome, marked by a dashed line, possibly is a weakly first-order transition (see the main text). The shaded region indicates the coexistence region between SDW and SC quasi long-range orders. The inset shows the Fermi surface, with different colours indicating the sign of the superconducting order parameter. The hot-spots and the SDW ordering wave vector $\mathbf{Q}$ are marked. Figure taken from Ref. 8.

The main result of our simulation runs on JURECA is a careful determination of the finite-temperature phase diagram showing the competition between spin-density wave (SDW) order and superconductivity in the O(2) model variant of action (2) above. While the general features of this phase diagram have long been discussed in the context of various *uncontrolled* analytical approaches, our numerical results present the first *unbiased, controlled, and numerically exact* determination of this phase diagram – a key result which has been published in Physical Review Letters⁸. Our work has gathered broad attention from the strongly correlated electrons community after an early review of our work by Jörg Schmalian (KIT Karlsruhe) for the international condensed matter journal club^a.

^aSee <http://www.condmatjournalclub.org/?p=2727>

4 Numerical Simulations

All codes employed in our projects are high-end C++ codes developed in our group. Besides adhering to a number of advanced programming concepts including object-orientation, (expression) templates or code provenance we rely on a number of high-level C++ libraries, e.g. the boost, Intel MKL, or ALPS libraries. Scalability and parallelisation of our codes have extensively been tested and improved on the CHEOPS cluster at the regional computing centre (RRZK) located at the University of Cologne featuring a total of 9712 cores and a peak performance of 100 Teraflop/s – as such a machine whose fundamental characteristics (besides its size and processor generation) are thus very similar to the JURECA cluster.

The major bounds of the code performances are set by the complexity of the algorithm as well as the complexity of the problem studied. The computing time of an optimally implemented DQMC algorithm scales as $N^3\beta$, where N is the number of (fermionic) degrees of freedom in our system and β is the inverse temperature.

To illustrate some of the key performance features of our DQMC codes we put a particular emphasis on their parallelisation and scaling with number of cores in a production run setting. One of the simplest steps to ensure high efficiency of the algorithms is to parallelise the Markov chain sampling to simulate a given parameter of a model simultaneously on a multitude of cores – each of which initialised with a different random number seed. As expected this results in an optimal *linear* increase in measurements per minute versus the number of employed cores.

In many cases, the efficiency of the algorithms drops as we enter the domain of physics dominated by critical fluctuations or sometimes strong correlations, meaning that the exploration of the system’s configuration space becomes more difficult and autocorrelation times increase dramatically. To compensate for these intrinsically physical effects, we employ *parallel tempering* or *replica exchange* techniques. In the context of our DQMC codes we find that these parallelisation schemes are extremely valuable tools and we can significantly reduce the autocorrelation time of measurements as illustrated by the results in Fig. 3 and Tab. 1 obtained for an example problem.

		τ_{int} estimate
Canonical		11.9 ± 0.9
Replica exchange		
Cores:	5	12.0
	9	6.9
	15	3.6
	27	3.0
	45	1.6

Table 1. Numerical estimates of the integrated autocorrelation times τ_{int} for the canonical and replica exchange simulations of Fig. 3. The data reveals a significant improvement of the replica exchange mechanism as more cores are allocated.

The number of parameters that are run at the same time to enter the tempering process has to be adjusted according to the problem at hand, but will typically lie in the range of

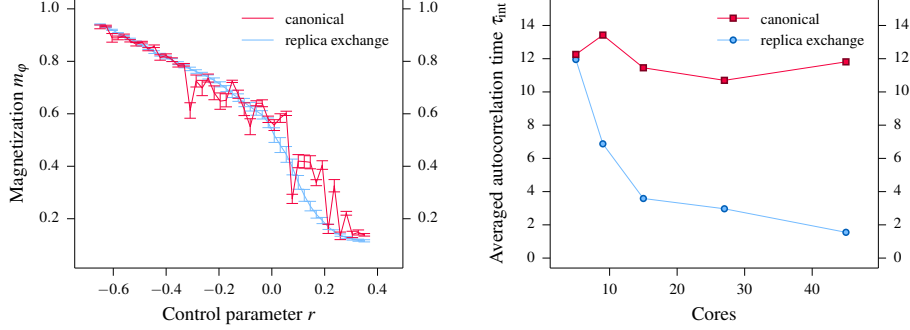


Figure 3. Example data obtained in short DQMC simulation runs of the $O(2)$ two-band itinerant electron model for the antiferromagnetic transition on an 8×8 square lattice at $\beta = 16$ highlights the benefits of the replica exchange (parallel tempering) algorithm, where the control parameter r is varied across the quantum phase transition. **Left:** The replica exchange mechanism greatly eases equilibration, especially near the continuous phase transition, yielding physical results instead of noise. **Right:** As more cores are allocated to a parallelised replica exchange simulation, autocorrelation times are further reduced.

20 – 100. In order to obtain sufficient statistical data for large systems at low temperatures, it has been necessary to combine the two optimisations and to run multiple simulations employing parallel tempering at the same time.

5 Concluding Remarks

Over the last two years, many leading analytical and numerical groups have followed up on our work^{9–20}. While our numerical competition^{14,15} has sometimes been using computational resources of an order of magnitude beyond those provided by the JURECA cluster (e.g. on the Milky Way II supercomputer, currently the world’s most potent HPC resource), probably the most interesting developments have been seen in the interplay with analytical approaches. Our own focus¹⁶ has been on a detailed comparison of our numerical results with the analytical predictions of the long-standing Hertz-Millis theory^{21,22} for the finite-temperature physics in the vicinity of the quantum critical point marking the onset of spin-density wave order. In parallel work, our collaborators have been running rigorous comparisons¹⁷ between numerical results for the superconducting transition temperature and analytical predictions of Eliashberg theory^{23,24}. To some initial surprise, both Hertz-Millis and Eliashberg theory have proved to be rather accurate, despite their sometimes crude and unjustified approximations. A more systematic understanding of this unexpected success of these decade-old theories has been provided over the last twelve months in a sequence of beautiful theory papers^{18–20} by Sung-Sik Lee and collaborators that convincingly argue that this agreement is mostly due to the fact that our numerical simulations have been carried out for an $O(2)$ magnetic order parameter – a deliberate choice we have made in order to observe a finite-temperature Berezinskii-Kosterlitz-Thouless (BKT) transition. Such a finite-temperature transition is absent for an $O(3)$ magnetic order parameter (as stated in the Mermin-Wagner theorem²⁵). However, the $O(2)$ order parameter also turns out to be special in other regards that reveal themselves only in a detailed analysis of the underlying

quantum field theory – it turns out¹⁹ that for the O(2) case certain diagrammatic corrections, the so-called vertex corrections, exactly cancel which explains the success of Eliashberg theory, neglecting precisely these vertex corrections, for the O(2) model. As such, it will be of paramount importance to repeat our simulations for the more general (and experimentally more relevant) O(3) model and check whether we can distill from future numerical data signatures of strongly correlated phenomena that have not been predicted by analytical theories and thereby allow for a deeper understanding of the many-electron problem.

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