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Machine Learning Transport Properties in Quantum Many-Fermion Simulations

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In computational condensed matter physics, the influx of algorithms from machine learning and their combination with traditional numerical many-body approaches is one of the most enticing recent developments. At this confluence novel techniques have been developed that allow to characterise many-body wave functions and discriminate quantum phase of matter by adapting concepts from computer science and statistics, which have proved tremendously practical in completely different contexts. However, in order to actually turn into a productive and widely accepted tool for obtaining a deeper understanding of microscopic physics these novel approaches must allow for meaningful, comprehensible inference and go beyond the applicability of their traditional counterparts. In this contribution, we report on significant progress made in this direction by discussing a novel algorithmic scheme using machine learning techniques to numerically infer the transport properties of quantum many-fermion systems. This approach is based on a quantum loop topography (QLT), and capable of distinguishing conventional metallic and superconducting transport in quantum Monte Carlo simulations by learning current-current correlations from equal-time Green's functions. We showcase this approach by studying the emergence of s- and d-wave superconducting fluctuations in the negative-U Hubbard model and a spin-fermion model for a metallic quantum critical point. The presented results, combined with the numerical efficiency of the QLT approach, point a way to identify hitherto elusive transport phenomena such as non-Fermi liquids using machine learning algorithms.

1 Introduction

State-of-the art machine learning techniques have not only become ubiquitous in our daily life (sorting emails, suggesting movies to watch, or identifying users by the touch of a button or the scan of a face), they also promise to become a powerful tool in quantum statistical mechanics. Their core functions – dimensional reduction and feature extraction – are a perfect match to the goal of identifying essential characteristics of a quantum many-body system, which are often hidden in the exponential complexity of its many-body wavefunction or the abundance of potentially revealing correlation functions. The basic idea of interpreting collective states of matter, such as superfluids, superconductors, or insulating quantum liquids, as a source of complex data with unknown intrinsic structure immediately opens up all of condensed matter physics as a playground for established machine learning algorithms implementing supervised, unsupervised, or reinforcement learning schemes.

Groundbreaking initial steps in this direction[1] have demonstrated that convolutional neural networks can indeed be trained to learn sufficiently many features from the correlation functions of classical and quantum many-body systems[2] such that distinct phases of matter can be discriminated and the parametric location of the phase transition between them identified. In parallel, it has been demonstrated that machine learning of wave functions is possible,[3,4] which can lead to a variational representation of quantum states based on artificial neural networks like restricted Boltzmann machines that, for some cases, out-

performs entanglement-based variational representations.[3] In a parallel development, efforts to integrate machine learning perspectives into established numerical schemes have led to many methodological improvements such as new quantum Monte Carlo flavours with dramatically reduced autocorrelation times.[5,6]

This contribution reports on recent progress made in the use of machine learning to identify transport characteristics of itinerant electron systems. We will showcase that an innovative technique dubbed "quantum loop topography" (QLT), initially introduced by Eun-Ah Kim's group at Cornell to detect topological order in integer and fractional Chern insulators,[7] is capable of reliably distinguishing conventional metallic and superconducting transport by machine learning the essential features of longitudinal imaginary time current-current correlations. It should be noted that electronic transport properties are notoriously difficult to calculate – in the context of Monte Carlo approaches this typically asks for an analytic continuation, which is numerically ill posed, yielding no controlled framework to probe transport properties. As such, the QLT approach offers an intriguing alternative that is also vastly more efficient; the scaling of the computational cost differs by multiple orders of the considered system size. When compared to other machine learning protocols for quantum state recognition, the QLT stands out as a preprocessing step that, by using a correlation loop topography as a filter, selects and organises the input data with the physical response characteristic of the target phase in mind. It thereby distinguishes itself from, *e. g.* the application of convolutional neural networks (CNNs) whose motivation has been primarily rooted in image recognition techniques. Crucially, while making equally good transport predictions as CNNs, QLT requires a considerably smaller fraction of the input data, which is given by equal-time Green's functions produced in quantum Monte Carlo simulations. It has thereby become the method-of-choice for future applications in quantum statistical physics.

Although QLT is generally applicable, we will restrict our demonstration in this article to the particularly interesting case of transport in a quantum critical metal.[8] In the vicinity of an antiferromagnetic quantum critical point, which marks the onset of magnetic order at zero temperature, quantum critical fluctuations can interact with gapless excitations on a finite Fermi surface. In previous work, our group has established in numerically exact studies[9–12] of sign-free microscopic models that this interplay can give rise to novel non-Fermi liquid regimes and can lead to the emergence of unconventional d-wave superconductivity, making it a candidate mechanism responsible for some of the physics of many actively research materials such as the electron-cuprates, iron-pnictides, and heavy fermion materials - the high-temperature superconductors. We have reported on these activities in a previous contribution to this series.[13] As we will show in this article, QLT offers a new route for the exploration of transport properties across the phase diagram of such quantum critical metals[8] – an insight made possible through our large-scale simulations on the Jülich supercomputing facilities.

2 From Convolutional Neural Networks to Quantum Loop Topography

Arguably, one of the most striking applications of machine learning is pattern recognition in images, the prime examples being handwritten digit classification - for instance

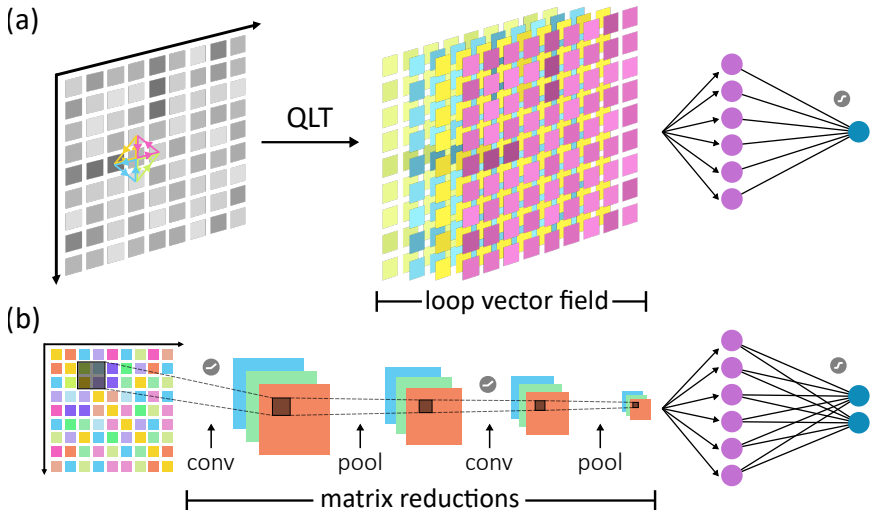

Figure 1. **Neural network architectures**. (a) QLT used as an input to a feed-forward fully-connected shallow neural network with one hidden layer of sigmoid neurons. Only triangular loops $L^{\triangle}_{jkl}$ are illustrated. (b) Deep convolutional neural network that convolves and pooles the unprocessed Green's functions $\widetilde{P}_{jk|\alpha}$ before threading them through a fully-connected layer of hidden neurons. Taken from Ref. 8.

of the famous MNIST data - and facial recognition. Conceptually, the employed strategy is straightforward: given a set of pre-classified images, a statistical model is trained until it has learned enough essential features to be able to distinguish between images of different categories. Hereby, the training amounts to minimising a cost function, which quantifies the deviation from the expected prediction across the training dataset, by a variant of gradient descent. However, despite its simplicity the performance of this approach will generally largely depend on the specific machine learning model and in particular its capability to extract and memorise correlation characteristics. As a consequence, many different architectures like multi-layer perceptrons, support vector machines, and feed-forward neural networks (FFNN) have been proposed over time. A key step in the success story of automated image recognition has been to combine such artificial neural networks with convolutional layers that systematically act as filters or preprocessors on the original data set. This way the identification of patterns is facilitated by exploiting the locality of correlations. In Fig. 1b we illustrate the typical architecture of such a so-called deep convolutional neural network, which consists of multiple successive convolutional layers eventually feeding into a regular FFNN.

Transferring this convolutional prefiltering approach to physics applications has allowed our group to take the first steps in identifying and discriminating different quantum states of many-fermion systems.[2] By interpreting the equal-time Green's functions of a spinful Hubbard-model, produced in quantum Monte Carlo simulations, as *image* snapshots of the physical system – real and imaginary parts are taken as separate colour channels, similar to the well-known RGB colour scheme – we were able to machine learn the distinction between an antiferromagnetic insulator and a semi-metal.[2] This original ap-

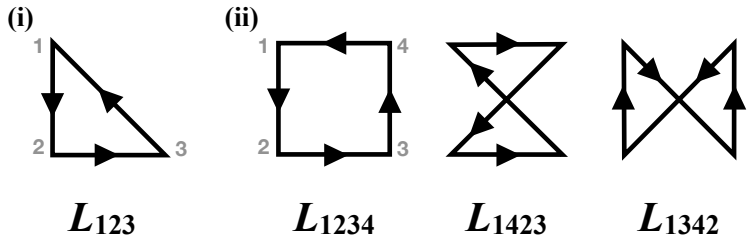

Figure 2. Illustration of the (i) triangular and (ii) quadralateral **loop operators** employed in the loop topography of the longitudinal current-current correlation function. Taken from Ref. 8.

proach, which employed a supervised learning strategy can be further generalised into an unsupervised setting, where the number of distinguishable quantum phases is not a priori known and learned in the process[14] – allowing for a semi-automatic determination of entire phase diagrams.

Some of the more intriguing many-fermion states like superconducting states and topologically ordered states, however, ask for more sophisticated, tailor-made "physics filters" in lieu of the simple convolutional layers in order to allow for a deeper understanding. In a recent work,[8] we have expanded one such approach dubbed "quantum loop topography" (QLT) by its developers,[7] which substitutes the generic convolutional layers by a loop topography scheme based on the specific physical response function of interest. More concretely, targeting longitudinal transport properties we consider the zero-frequency current-current correlation function

$$\Lambda_{xx}(\mathbf{r}_1,\mathbf{r}_2;\omega_n=0)\equiv\int d\tau\left\langle \hat{j}_x\left(\mathbf{r}_1,\tau\right)\hat{j}_x\left(\mathbf{r}_2,0\right)\right\rangle \tag{1}$$

where $\hat{j}_x(\mathbf{r}_1,\tau) = e^{H\tau}\hat{j}_x(\mathbf{r}_1)e^{-H\tau}$ with the current density operator $\hat{j}_x(\mathbf{r_1}) = -i[H(\mathbf{r}_1),\hat{x}]$. The Fourier transform of Λ_{xx} is famously related to the superfluid density ρ_s which, when surpassing a certain critical value, indicates superconducting transport.[15] For a gapped system it can readily be shown[8] that the current-current correlation at zero temperature breaks into a weighted combination of four-vertex loops and triangular loops of Green's functions $P_{\mathbf{r}'\mathbf{r}}=\langle c^\dagger_{\mathbf{r}'}c_{\mathbf{r}}\rangle$,

$$\begin{aligned}\Lambda_{xx}(\mathbf{r}_1,\mathbf{r}_2;\omega_n=0)=&\sum_{\mathbf{r}_3\mathbf{r}_4}P_{\mathbf{r}_2\mathbf{r}_4}P_{\mathbf{r}_4\mathbf{r}_1}P_{\mathbf{r}_1\mathbf{r}_3}P_{\mathbf{r}_3\mathbf{r}_2}\left(x_1-x_4\right)\left(x_2-x_3\right)\\&-\sum_{\mathbf{r}_4}P_{\mathbf{r}_2\mathbf{r}_4}P_{\mathbf{r}_4\mathbf{r}_1}P_{\mathbf{r}_1\mathbf{r}_2}\left(x_1-x_4\right)\left(x_2-x_1\right)\end{aligned} \tag{2}$$

The key idea of QLT is to approximate these current-current correlations by small loop operators (Fig. 2),

$$L^{\triangle}_{jkl}\equiv\widetilde{P}_{jk}|_\alpha\widetilde{P}_{kl}|_\beta\widetilde{P}_{lj}|_\gamma \tag{3}$$

and

$$L^{\square}_{jklm}\equiv\widetilde{P}_{jk}|_{\alpha'}\widetilde{P}_{kl}|_{\beta'}\widetilde{P}_{lm}|_{\gamma'}\widetilde{P}_{mj}|_{\delta'} \tag{4}$$

in which the Green's functions $\widetilde{P}_{jk}|_\alpha$ are typically obtained from individual samples α of quantum Monte Carlo simulations. Pictorially, as shown in Fig. 1a, the QLT amounts to constructing a loop vector field from the expectation values of $L^{\triangle}_{jkl}$ and $L^{\square}_{jklm}$ for different lattice sites in a preprocessing step before feeding the loop topography information into a regular feed-forward neural network. By processing the loop operators during the sampling process and avoiding an *a posteriori* Monte Carlo averaging, we quickly pass these fluctuation-laden data, which encodes partial information of the current-current correlation function, to the machine learning step.

Compared to regular convolutional layers, the QLT as a preprocessing unit has two important advantages. First, since being based on a particular physical correlation function, the information that is passed to the FFNN is transparent and physical. Hence one can draw inferences about the importance of certain physical correlations and can systematically improve the predictive powers of QLT by including higher order loop operators. Second, the QLT approach is vastly more efficient as it operates only a small fraction of the full Green's function data: in two spatial dimensions it scales as $L^2 \times D(d_c)$, where L is the linear system size and $D(d_c)$ denotes the loop vector dimension for a given maximal loop length d_c, compared to the full $L^2 \times L^2$ information. Remarkably, as we demonstrate below, this increased efficiency does not come with a loss in prediction accuracy and thus gives QLT a significant competitive edge over CNNs in transport characterisation applications.

3 Quantum Criticality in a Nearly Antiferromagnetic Metal

To showcase the power of the QLT approach for extracting transport characteristics of itinerant electron systems, we will apply it to the case of a two-dimensional metal near the onset of commensurate antiferromagnetic spin-density wave (SDW) order. Quantum phase transitions in metals pose a substantial theoretical and computational challenge since, in contrast to insulating systems, the order parameter modes can interact with gapless fermion excitations. The quantum critical physics of the system can be captured[11] by an effective Euclidean action $S = S_\psi + S_\phi + S_\lambda$ in terms of fermionic operators $\psi^\dagger, \psi$ (spin and other indices are left implicit) with dispersion $\epsilon_{\mathbf{k}}$ and chemical potential μ coupled to a bosonic order parameter ϕ,

$$\begin{aligned} S_\psi &= \int_{\tau,\mathbf{k}} \psi^\dagger_{\mathbf{k}} \left(\partial_\tau + \epsilon_{\mathbf{k}} - \mu\right) \psi_{\mathbf{k}} \\ S_\phi &= \int_{\tau,\mathbf{x}} \left[\frac{r}{2}\phi^2 + \frac{1}{2}\left(\nabla\phi\right)^2 + \frac{1}{2c^2}\left(\partial_\tau\phi\right)^2 + \frac{u}{4}(\phi^2)^2\right] \\ S_\lambda &= \lambda \int_{\tau,\mathbf{x}} e^{i\mathbf{Q}\cdot\mathbf{x}} \vec{\phi} \cdot \psi^\dagger(\mathbf{x}) \vec{\sigma} \psi(\mathbf{x}) + \text{h.c.} \end{aligned} \tag{5}$$

Here, $\vec{\sigma}$ are spin Pauli matrices, $\mathbf{Q} = (\pi, \pi)$ is the antiferromagnetic ordering wavevector and $\vec{\phi}$ is a 1-, 2-, or 3-component vector (depending on whether the SDW order parameter has easy-axis, easy-plane, or isotropic character, respectively). S_ϕ is a usual Landau-Ginzburg-Wilson ϕ^4-theory, written as an expansion in powers of the order parameter ϕ and its derivatives, where the tuning parameter r drives the system through a quantum critical point (QCP). The interaction term, S_λ, is of Yukawa type, linear in ϕ and quadratic in the fermion operators.

As usual, the central quantity of interest is the partition function $\mathcal{Z} = \int D\left(\psi, \psi^\dagger, \varphi\right) e^{-S}$ which after tracing out the fermion degrees of freedom can be written in determinant quantum Monte Carlo (DQMC) form as[16]

$$\mathcal{Z} = \int D\varphi \, e^{-S_\varphi} \det G_\phi^{-1} + \mathcal{O}\left(\Delta\tau^2\right) \tag{6}$$

Here, $G_\phi = \widetilde{P}_{jk}|_\phi = \langle \psi_j \psi_k^\dagger \rangle_\phi$ is the equal-time Green's function and $\Delta\tau^2$ is the usual controlled Trotter decomposition error.

Generally, quantum Monte Carlo simulations of the partition function for a model of interacting fermions will be hindered by a severe fermion-sign-problem - the integral kernel cannot be safely interpreted as a probability weight, as G_ϕ and its determinant are complex valued. However, as identified by Erez Berg and collaborators in a seminal work,[17] this issue is lifted for model (5) by an intrinsic anti-unitary symmetry (much like time reversal) which renders it amenable to a numerically exact analysis.

As our group was able to show in the first unbiased, numerically exact studies[9, 12] of model (5), which have been conducted on the JURECA and JUWELS supercomputers over multiple funding periods (see also our contribution[13] to this series in 2018), the phase diagram of the antiferromagnetic quantum critical metal clearly reveals a dome-shaped d-wave superconducting phase with a comparably high superconducting transition temperature $T_c \approx E_F/30$ compared to BCS theory (see the inset of Fig. 3). This transition from metallic to superconducting transport, which has been established by (costly) explicit calculations of the superfluid density, serves as a real-world benchmark for the QLT approach.

Applying a supervised learning scheme, we consider a finite-temperature scan cutting into the superconducting dome close to the maximal T_c and train a basic feed-forward neural network on QLT preprocessed equal-time loop correlations (Fig. 1a) at the extremal temperatures $T \approx 0.2$ and $T \approx 0.03$, where the system shows regular metallic and superconducting transport character, respectively. In Fig. 3 we show the neural output of the QLT architecture, which quantifies the confidence that the metal is in a superconducting phase, as a function of the inverse temperature. Clearly, the QLT model is able to reliably distinguish both transport regimes in the high and low temperature limits. Furthermore, it correctly identifies superconducting transport properties over an extended temperature range, as indicated by a high-confidence plateau. Remarkably, the entire trend of the neural output is in great agreement with quantum Monte Carlo results:[9] the notable increase of the confidence coincides with the onset of diamagnetic superconducting fluctuations (grey shaded region) before it indicates an extended superconducting phase at low temperatures, $\beta > \beta_c \approx 12.5$ (dashed line). In comparison to a conventional CNN (Fig. 3), which has been trained on the entire equal-time Green's function data, the QLT analysis provides similar accuracy while only relying on a subset of the data, namely physical small-loop correlations (Fig. 2). Overall, these findings suggest that the QLT model has efficiently identified and captured the superconducting transport characteristics across the phase diagram.

4 Concluding Remarks

In this article we have reported on a recent advance in the application of machine learning in condensed matter research: the probing of transport properties in itinerant quantum

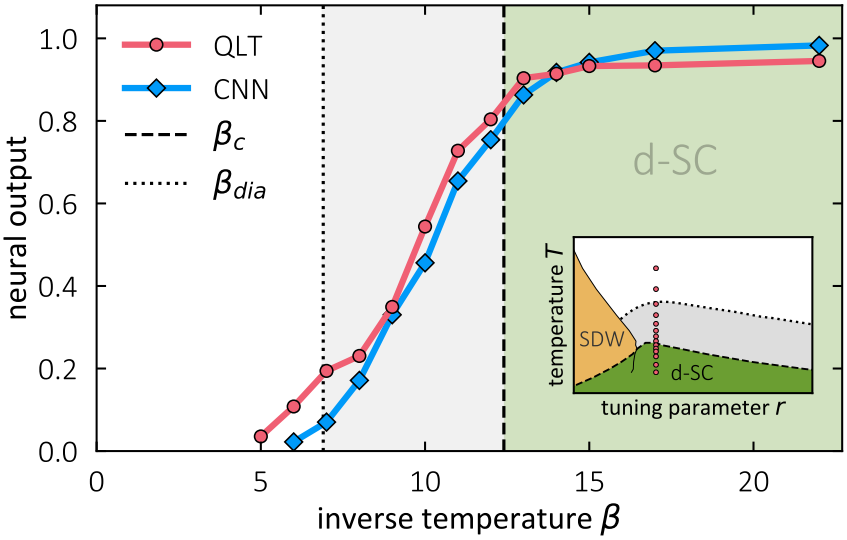

Figure 3. Neural network output for the superconducting transition near a **metallic easy-plane antiferromagnetic quantum critical point**. The training points were at $\beta = 30$ for superfluid transport and $\beta = 5$ for metallic transport. The vertical lines indicate the superconducting transition temperature $\beta_c \sim 12.5$ (dashed) derived from the superfluid density measurements and the onset of diamagnetic fluctuations $\beta_{\rm dia} \sim 6.9$ (dotted) where the orbital magnetic susceptibility changes sign.[9] The inset (modified from Ref. 9) illustrates the chosen finite-temperature scan cutting into the superconducting dome. Taken from Ref. 8.

many-fermion systems by quantum loop topography.[7,8] In contrast to directly applying feature extraction techniques (often originally developed for pattern recognition in images) to physics problems, the QLT approach stands out as a preprocessing scheme that filters the relevant correlations of a physical response function of interest. As we have showcased for a quantum critical metal the QLT approach is capable of reliably identifying a change in transport to reasonable accuracy while being vastly more efficient than traditional calculations, based on the superfluid density, and convolutional neural network architectures. Building upon these results, a natural question is whether, for a sufficiently suppressed superconducting dome, QLT can be used for the exploration of a potential fan-shaped quantum critical regime where transport is governed by the underlying QCP at $T = 0$. In this regard, we believe that the transparent physical basis of QLT is a valuable step in the implementation of machine learning methods that, when combined with analytical insight, will allow us to draw inferences about the physical mechanisms at play.

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