Visualizing Correlations in the 2D Fermi-Hubbard Model with AI

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Phases of strongly correlated electronic systems are often described in terms of straightforward patterns, which are theoretically understood using Landau symmetry-breaking theory [1]. For instance, ferromagnetism on a square lattice involves a uniform pattern where the electrons’ spins align and create a magnetic state with a wavevector \( q = 0 \). Antiferromagnetism, slightly more complex, is revealed by a \( q = \pi \) alternation of the electrons’ spin state on two sublattices. These choices, and incommensurate (spiral) order which bridges them at general \( q \), can be characterized in a unified way through the magnetic structure factor, \( S(q) \), and further generalized to include time-domain patterns via the dynamic susceptibility. Similar statements apply to charge density wave and other phases involving diagonal long range order.

While many of our theoretical and experimental probes of interacting quantum systems have been constructed with coupling to these patterns in mind, there is an increasing realization that the most interesting strongly correlated phases might not be immediately accessible via such observables. Cuprate and iron-pnictide superconductors, which combine closely entwined conventional phases with well-established order parameters, and much less well-understood non-Fermi liquid (NFL) or pseudogap phases with so far ‘hidden orders’ are recent examples [2, 3], as is the zoo of orbital ferromagnetism, superconductivity, and Mott insulating behavior in twisted bilayer graphene [4, 5]. The community of strongly correlated quantum systems is thus faced with the challenge of developing new means of identifying complex phases.

Here, we introduce an unbiased approach in which AI is used to extract hidden features from raw images of quantum many-body systems. We test our approach using projective measurements on a two-dimensional (2D) Fermi-Hubbard model, obtained through quantum gas microscopy of ultracold fermionic atoms in an optical lattice. We find that filters of a convolutional neural network (CNN), trained to recognize snapshots of fermions, capture features at different densities that have clear interpretation in terms of short and long-range magnetic correlations of the model. We further show that a more complex CNN can produce an effective order parameter for the NFL phase, based on the interplay of multiple types of density fluctuations present in the system, reflecting the more enigmatic nature of the correlations in this phase.

In the experiment, the 2D Fermi-Hubbard model is realized using a spin-balanced mixture of the first and third lowest energy states of \(^6\)Li loaded into a square optical lattice. We work at a magnetic field of 615 G in the vicinity of the Feshbach resonance near 690 G, which gives us a scattering length of 1056(10) \( a_0 \). The lattice depth is 7.25(2)\( E_R \), where \( E_R \) is the lattice recoil energy and \( E_R/h = 14.66 \) kHz. For these parameters we obtain \( t/h = 850(20) \) Hz and \( U/t = 8.0(1) \). Here, \( t \) and \( U \) are the nearest-neighbor hopping matrix element and the strength of onsite repulsive interaction, respectively, in the Hubbard model.

Using quantum gas microscopy techniques [6], we image the atoms in the lattice with single site resolution with a fidelity of 98%. When a fluorescence image is taken, atoms on doubly occupied sites undergo light assisted collisions and appear empty. An image taken this way allows us to extract the local moment on each site. Alternatively, we can apply a short pulse of resonant light prior to taking an image to eject atoms of one of the two hyperfine states. This allows us to measure the single component density of the remaining hyperfine state.

Our lattice beams produce a harmonic trapping po-
FIG. 1. Phase diagram, sample snapshots, and CNN architecture. (A) Schematic phase diagram of cuprate high-temperature superconductors in the space of temperature and hole doping. AF, PG and SC stand for antiferromagnetic, pseudogap, and superconducting phases, respectively. (B) Sample experimental snapshots taken at the density \( n \sim 0.82 \). Left: Two 100 \( \times \) 100-pixel samples of occupancy snapshots of a single species of fermions taken at \( T \sim 0.35t \) (top panel) and \( T \sim 7.5t \) (bottom panel). Blue pixels indicate a particle on a site. Right: The 20 \( \times \) 20-pixel center part of four randomly chosen snapshots at each of the extreme temperatures, along with four snapshots at the same density whose pixels have been randomly shuffled, i.e., “fake” snapshots. (C) The main convolutional neural network architecture used in this study. The architecture contains a convolutional layer with one filter and one feature map followed by a global pooling layer. The output of the pooling layer is fed to 8 fully-connected neurons, followed by an output softmax layer with two neurons, each associated with a temperature limit. We use the rectified linear unit (ReLU) as the activation function in all but the output layer. In our experiments we observe that the presence of the fully-connected layer accelerates the training of the neural network. (D) Sample 10 \( \times \) 10-pixel single-species snapshots from DQMC at two different temperatures along with one obtained by shuffling pixels of the snapshot at the lower temperature.

tential, which if uncompensated leads to significant variations of the local density. To study regions of uniform density, we flatten the potential using light shaped using a spatial light modulator \([7]\). In the subsequent analysis, we work with a flattened region of 20 \( \times \) 20 lattice sites.

Figure 1 shows several randomly chosen samples of binarized occupancy snapshots at an average density of \( n = 0.82(2) \) at two extreme temperatures of \( T \sim U \) and \( T \sim 0.35t \) used in our study. These parameters place us within the NFL region of a typical cuprate phase diagram (Fig. 1A). Thermometry is performed using averages of various correlation functions taken over such snapshots \([7]\).

The increasingly large number of snapshots taken in quantum gas microscope experiments in various regions of the parameter space lends itself to data-driven approaches for science discovery, such as the enlisting of AI. In fact, early implementations of machine learning techniques for the study of quantum many-body systems demonstrated a great potential \([8-13]\). Recent applications to experimental data have either directly led to the discovery of new physics \([14-17]\), modeling of their distribution \([20]\), or the optimization of experimental processes \([18, 19]\), including those related to quantum gas microscopy.

CNNs offer an ideal platform for the detection of patterns in the experimental snapshots. Not only can they efficiently compress the information in images and use them for classification, but also their trained filters provide a window into the relevant features observed \([21]\). Figure 1C shows the main CNN architecture we have used. After labeling them according to their tempera-
We find that the CNN consistently makes the distinction with more than 91% accuracy, and it does so using filters showing a distinctive pattern indicative of short-range antiferromagnetic (AF) correlations. The nearest-neighbor checkerboard pattern emerging in the filters is consistent with the fact that the correlation length in the NFL region is about one lattice spacing. The appearance of this feature at different locations in the filter for different training runs points to a redundancy: on average the filter must reflect the translational symmetry of the underlying system.

Training the CNN using similar snapshots obtained at half filling results in filters that reflect a longer range anti-correlation between neighboring fermions of the same species (Fig. 2B). These findings suggest that the network effectively uses the strength of AF correlations as a measure for classifying snapshots of a single species of fermions. Figure 2D and E show that the density, distance, and temperature dependence of the magnetic correlations of the model, $C(r)$, which are calculated here on a $10 \times 10$ cluster using the determinantal quantum Monte Carlo (DQMC) [22], or in the thermodynamic limit using the numerical linked cluster expansion (NLCE) [24, 25], support this observation.

Quantum Monte Carlo simulations also provide a platform to corroborate these findings. However, except in one spatial dimension, these simulations cannot provide projective measurements in the density basis. Instead, theory “snapshots” can be constructed via expectation values of local charge or spin density using instances of auxiliary field variables during a simulation; for example, the $i$th pixel of a spin-up DQMC snapshot is $\langle \hat{n}_{i\uparrow} \rangle = 1 - G_{ii\uparrow}(h)$, where $G_{ii\uparrow}(h)$ is the $i$th diagonal element of the spin-up equal time Green’s function matrix for the auxiliary field instance $h$. We perform the simulations for a $10 \times 10$ site Hubbard system with $U = 8t$ at several average average densities and temperatures [22].

At high temperatures, of the order of $3t$, we find that density snapshots are fuzzy with no clear empty sites; mostly fluctuations about an average background density can be seen. This fuzziness is less of a concern for single-species snapshots (Fig. 1D), although they too lose their pixelated character at higher temperatures. For this reason, to eliminate fuzziness as an obvious feature for the CNN to learn, instead of high-temperature snapshots, we use low-temperature images whose pixels have been randomly shuffled, effectively destroying any physical correlations. In the following, we refer to the latter as fake (as opposed to real) snapshots.

Figure 2A shows a sample of four $5 \times 5$ filters after four different runs in which the CNN is trained to distinguish experimental snapshots of a single species of fermions at the highest temperature from those at the lowest temperature when $n \sim 0.82$. If we expect mostly random behavior at high temperature, of the order of the largest energy scale in the system, the features that spontaneously develop in the filters during training will most likely represent patterns found in the low-temperature snapshots.

Figure 2A shows a sample of four $5 \times 5$ filters for four independent runs are shown for (A) $n \sim 0.82$ and (B) $n \sim 1.00$. The CNN architecture is shown in Fig. 1C. The testing accuracies are between 91% and 95%. The visual pattern in each $5 \times 5$ filter in (A) is consistent with recognizing short range AF correlations. The four representative runs in (B) indicate patterns capturing long range order at half filling. (C) shows similar filters evolved from training runs using DQMC simulations. The testing accuracies are at least 68%. Panels (D) and (E) provide theory data for the nearest neighbor spin-spin correlation for $U = 8t$ vs. density at different temperatures (NLCE), and vs. distance for $n \sim 0.81$ and $n \sim 1.00$ at $T = 0.44t$ (DQMC). This figure illustrates that AI can capture the correct trends in magnetic behavior of the Hubbard model, and that the trained filters carry a clear physical interpretation.

FIG. 2. Analysis of single-species snapshots using CNNs with one filter. Sample $5 \times 5$ filters for four independent runs are shown for (A) $n \sim 0.82$ and (B) $n \sim 1.00$. The CNN architecture is shown in Fig. 1C. The testing accuracies are between 91% and 95%. The visual pattern in each $5 \times 5$ filter in (A) is consistent with recognizing short range AF correlations. The four representative runs in (B) indicate patterns capturing long range order at half filling. (C) shows similar filters evolved from training runs using DQMC simulations. The testing accuracies are at least 68%. Panels (D) and (E) provide theory data for the nearest neighbor spin-spin correlation for $U = 8t$ vs. density at different temperatures (NLCE), and vs. distance for $n \sim 0.81$ and $n \sim 1.00$ at $T = 0.44t$ (DQMC). This figure illustrates that AI can capture the correct trends in magnetic behavior of the Hubbard model, and that the trained filters carry a clear physical interpretation.
demonstrate that relevant spin correlations can be captured in an unbiased fashion through CNNs.

Studies of the origin of the NFL behavior, a central question in any theory of high-temperature superconductivity [26], have for decades been focused on its possible connections to the order parameter fluctuations of a magnetic quantum critical point [26,32]. Here, we are in a position to ask whether any such fluctuations manifest themselves in charge correlations too, and to what extent they can be inferred from the other type of snapshots available in the experiment, those of local moments.

A similar analysis using images at the two extreme temperatures, however, is largely affected by the abundance of doubly occupied sites at $T \sim 7.5t$, and their lack of representation in the snapshots of local moments. Upon lowering the temperature to $T \sim 0.35$, the fraction of doubly occupied sites at 18% doping reduces roughly by a factor of four from 12% to about 3%, providing the CNN again with an obvious feature with which to perform classification [22]. Removing this bias by randomly populating pixels to create “fake” replacements for high-temperature snapshots in the training, brings the accuracy down to only slightly above 50%. It becomes clear that snapshots of local moments in the NFL region of the Hubbard model do not contain a single dominant ordering pattern that can be captured by one filter in the CNN; a more advanced treatment is necessary.

In Fig. 3A we show results of a training with a CNN, modified to include six $7 \times 7$ filters in its convolutional layer [22]. The bigger dataset we have available for snapshots of local moments at this density allows us to experiment with different filter sizes and the number of filters. We find that including more than one filter in the CNN improves the best accuracies achieved, albeit not exceeding around 65%, while having too many, and/or much larger, filters can still result in overfitting.

Fig. 3A shows six filters of a sample CNN trained on the local moment snapshots. Unlike for the case of single-species snapshots, a single dominant feature does not emerge. The trained filters, however, do offer insight into possible spatial arrangements of local moments at low temperatures; filters $m = 1$ and 6, and to some extent 4 and 5, point to their clustering in small regions of a few sites. Filters 2 and 3, on the other hand, appear far more random with a slight tendency for local moments to be second neighbors. As we will see below, patterns in the first set of filters (filters 1, 4, 5, and 6) are more frequently associated by the network with real snapshots at this filling, whereas patterns in filter 2 are more frequently associated with fake snapshots.

The shape of the nearest-neighbor local moment correlation function and its zero crossing at $n \sim 0.8$, observed previously at a higher temperature [33], supports bunching of local moments, allowing holes to strongly avoid each other while positively correlating with doublons on neighboring sites. Theory results show that this behavior, which is consistent with the spatial arrangements favored mostly by filters 1 and 6 in Fig. 3A, persists to our low temperatures.

It is worth noting, however, that nonlinearities in the neural network model make the interpretation of features seen in the filters vis-à-vis correlations in the physical snapshots challenging since the knowledge of the network can be divided in nontrivial ways among its different components. An early example of this was the surprisingly successful classification of snapshots of the Ising lattice gauge theory at $T = 0$ and $T = \infty$, despite the lack of an order parameter, using CNNs with multiple filters [9].

By transferring the knowledge of the CNN to other densities, we find that the network is the most sensitive to correlations around the NFL region. Figure 3B shows the probability that a snapshot is categorized as belonging to the NFL region based on factors other than the density itself. We find this probability to be maximal in the vicinity of $n \sim 0.8$, suggesting that the CNN as a whole is in fact focusing on local moment correlations more unique to the NFL region and slightly lower densities. We have not been able to reproduce these results using CNNs with smaller, e.g., $5 \times 5$ filters, even if the number of filters is increased to eight.

While contribution of individual filters to the CNNs decision making cannot be completely isolated, we can study what the network output would be if each filter were to act alone [22]. Figure 3C shows this quantity averaged over samples at $n = 0.82$, after subtracting the value for the corresponding fake snapshot, for each of the six filters shown in Fig. 3A. The results suggest that filters 1 and 6, if acted alone, would have the largest effect on the decision making at this average density, followed by filters 4 and 5, while filter 3 plays almost no role at all and filter 2 has a negative effect. This implies that the clustering of local moments and their separation from holes/doublons over several sites may in fact be the dominant charge fluctuation in the NFL phase, although a definite conclusion is hindered by the less than ideal accuracy of the network. A similar analysis of snapshots with information about both species of particles in future experiments [34], may further reveal the interplay between spin and charge fluctuations in this region.

Using DQMC, we verify that similar trends can be observed in simulated snapshots of local moments. However, unlike with the experimental snapshots, here, we find that the accuracy increases steadily with increasing the number of filters in the CNN, while increasing the filter size does not necessarily improve the performance. We attribute these to the fundamental difference between the two types of snapshots (projective vs non-projective). Figure 3D highlights a representative sample of $5 \times 5$ filters of a CNN with sixteen such filters, trained on simulated snapshots reaching to an accuracy of 87%. They appear to measure, from left to right, nearest-neighbor correlations of local moments ($m = 1$ and 2), the likeli-
FIG. 3. Analysis of local moment snapshots using CNNs with multiple filters. (A) The six filters of a trained CNN. Training is performed with the 5023 experimental local moment snapshots taken at $n \sim 0.82$ and $T \sim 0.35$. The average testing accuracy in the last 20 epochs of the run is $62\% \pm 0.01\%$ [22]. (B) The difference in the average network output for $T \sim 0.35$ real and fake snapshots as a function of the density of local moments when all six filters are present: $\Delta \langle \text{Network Output}^{(1)} \rangle \equiv \langle \text{Network Output}^{(1)}(X^\text{real}) \rangle - \langle \text{Network Output}^{(1)}(X^\text{fake}) \rangle$. Superscript (1) indicates the value at the output neuron responsible for real low-temperature snapshots [22]. This quantity indicates roughly the percentage of the output attributable to factors other than the density. (C) Similar to (B) at $n \sim 0.82$ when it has access to one filter at a time. (D) Four representative filters of a CNN with sixteen $5 \times 5$ filters trained using DQMC snapshots of local moments [22]. (E) Same as (B) (C), but obtained using the CNN in (D).

hood of two empty sites being neighbors ($m = 3$), and the anti-correlation of neighboring local moments ($m = 4$). The first three have positive contributions that peak in the NFL region, while the fourth has a negative contribution in that region. These trends are consistent with those seen in Fig. 3C. Figure 3E shows the overall signal of the CNN for correlations unique to the NFL phase, plotted across densities. It has a broad peak around the NFL region. We find that including the information about doublons, i.e., using full density snapshots, generally improves the diversity of features seen in the trained filters while yielding the same basic trends [22].

The techniques developed in this work for the AI-assisted feature extraction in projective measurements can be adapted to peek into other mysterious phenomena for the Fermi-Hubbard model, such as the pseudogap phase, or the magnetic polaron which has been observed closer to half filling [35]. They can also be employed to study other microscopic models of correlated systems. Our work paves the way for AI related studies that go beyond mere categorization and the quest for gaining more predictive power and focus instead on the inner-workings of the machines to advance our understanding of complicated natural phenomena.

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Supplemental Information:
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THE MODEL

The Hamiltonian for the 2D Fermi-Hubbard model in particle-hole symmetric form is expressed as

$$\hat{H} = -t \sum_{\langle i,j \rangle} (\hat{c}_i^\dagger \hat{c}_j + H.c.) + U \sum_i (\hat{n}_{i\uparrow} - \frac{1}{2}) (\hat{n}_{i\downarrow} - \frac{1}{2}) - \mu \sum_i (\hat{n}_{i\uparrow} + \hat{n}_{i\downarrow}),$$  

where $\hat{c}^\dagger_{i\sigma}$ ($\hat{c}_{i\sigma}$) creates (annihilates) a fermion with spin $\sigma$ on site $i$, and $\hat{n}_{i\sigma} = \hat{c}^\dagger_{i\sigma} \hat{c}_{i\sigma}$ is the number operator. $\langle .. \rangle$ denotes nearest neighbors on a square lattice, $U = 8t$ is the strength of the onsite repulsive interaction in the numerical simulations, and $\mu$ is the chemical potential. $\mu = 0$ corresponds to half filling, although density fluctuations around half filling exist in our grand canonical ensemble. $t = 1$ (also $\hbar = 1$ and $k_B = 1$) sets the energy scale. The spin correlation function is calculated as $C(r) = \langle \hat{S}_{z,i} \hat{S}_{z,i+r} \rangle$, where $\hat{S}_{z,i} = \frac{1}{2} (\hat{n}_{i\uparrow} - \hat{n}_{i\downarrow})$.

NUMBER OF AVAILABLE EXPERIMENTAL SNAPSHOTs AT $T \sim 0.35$

|          | $n = 0.97$ | $n = 0.85$ | $n = 0.82$ | $n = 0.75$ | $n = 0.68$ | $n = 0.66$ | $n = 0.58$ |
|----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|
| Spin-up/Spin-down | 402       | -         | 302       | -         | -         | -         | -         |
| Singles     | 201       | 281       | 5023      | 290       | 345       | 281       | 330       |

DETERMINENTAL QUANTUM MONTE CARLO AND THEORY SNAPSHOTs

The implementation of determinantal Quantum Monte Carlo (DQMC) used in the work proceeds via the exact rewriting of the interacting electron-electron problem as independent electrons moving in a space-imaginary time auxiliary field $h(r, \tau)$. This reformulation involves first expressing the partition function $Z$ for the original Hubbard Hamiltonian as a path integral, and then the use of a Hubbard-Stratonovich transformation to decouple the electrons.
The original fermionic degrees of freedom are then traced out analytically, leaving an equivalent expression for $Z$ as an integral over $h(r, \tau)$. Detailed descriptions can be found in \[23, 36, 37\].

Here we focus on aspects of DQMC which have specific implications to the machine learning process. The most crucial is that, unlike world-line QMC methods or cold-atom experiments, which directly sample the 0 or 1 occupation of sites $r$ by the fermions, at any point (snapshot) in a DQMC simulation, the fermionic occupation is represented by a real number giving the probability of occupation of that site in the specific $h(r, \tau)$ currently being sampled. As the temperature is lowered below $t$, sharper images containing pixels more closely resembling binary pixels in the experimental snapshots emerge. In fact, one can show that in the atomic limit, local expectation values approach step functions as $T \rightarrow 0$. This ‘smearing’ of the occupation makes some aspects of machine learning via these snapshots more challenging. However, whether individual snapshots present (0,1) fermion occupations or not, the strong correlation physics (magnetism, superconductivity, strange metallicity) of the Hubbard model needs to be built up from many thousands of snapshots. It is the task of uncovering these many-body effects that is shared by the theoretical and experimental images investigated here with AI.

We have also generated projective measurements on small 8- and 10-site periodic clusters using exact diagonalization and sampling at finite temperatures. However, the significant boundary effects render comparison of training results at finite doping to experiments useless.

**FOURIER ANALYSIS OF THE SNAPSHOTS**

Figure 4 shows averages of the magnitude of Fourier coefficients of several different sets of snapshots at low temperatures. We find that, other than those corresponding to the expected $k = 0$ or $k$ in the vicinity of $(\pi, \pi)$ (for the single-species snapshots), there do not exist any other significant arrangements of fermions on the lattice captured through the linear Fourier transformation.

Figure 5 shows the percentage of weight associated with $k$ points other than $k = 0$ in the Fourier transform of the average snapshot. The suppression of this quantity as the number of snapshots increases makes clear that fluctuations inferred through Fourier transform are expected to decrease on average. They vanish for theory in the limit of infinite number of snapshots. However, inhomogeneities in the trapping potential can prevent that from happening for the experimental snapshots, even in the limit of infinite number of snapshots. As discussed below, we mitigate the issue when the CNN is sensitive to the inhomogeneities by creating fake snapshots that have the same average pixel values.
FIG. 4. Averages of the magnitude of Fourier coefficients of snapshots in different cases. (A), (B) and (C) show results for experimental snapshots of single-species fermions for $n \sim 1.00$ and $n \sim 0.82$ and snapshots of local moments (singles) for $n \sim 0.82$, respectively, all at $T \sim 0.35t$. (D), (E) and (F) show results for the theory snapshots at $T = 0.44t$.

as the corresponding real ones.

**UNSUPERVISED LEARNING**

We have employed two unsupervised learning algorithms, the linear principal component analysis (PCA) [38] and the nonlinear t-distributed stochastic neighbor embedding (tSNE) [39, 40], to perform dimensional reduction on the experimental snapshots at $n = 0.82$. In doing so, features may emerge in the low-dimensional space revealing certain repeated patterns in the snapshots.

In the PCA, one forms a matrix of data, $\mathbf{x}$ by flattening the matrix of pixel values for each snapshot and placing them as an array of 400 binary numbers in each row (of $\mathbf{x}$). In the next step, the covariance matrix of data is composed as $\mathbf{x}^T \cdot \mathbf{x}$. Diagonalizing the $400 \times 400$ matrix, we obtain its eigenvalues, whose magnitudes are a measure for the variance of the data along the principal axes, determined by the corresponding eigenvectors. As demonstrated for the two-dimensional Ising model in a pioneering application in physics [41], a dominant eigenvalue is indicative of a clear distinguishing pattern in the snapshots that can be represented as a linear combination of its pixels (their projection to the corresponding principal axis).

tSNE on the other hand, is a nonlinear method that minimizes the Kullback-Leibler divergences between pairwise
FIG. 5. **Percentage of \( k \neq 0 \) weight in the magnitude of the Fourier transform of the average snapshot.** Increasing the number of snapshots leads to the suppression of this quantity, showing that on average, there are no inhomogeneities in the data.

conditional probability distributions, representing similarity of points, from the high- and low-dimensional spaces (for a more detailed discussion see Ref. [39]). Here, we have used the implementation in Ref. [42].

Figure 6 shows our results in the two-dimensional space from both algorithms. Neither method seems to be able to draw any particular distinction between low and high temperature snapshots as there are no signs of any clustering of data points based on temperature. Figure 6A shows the eigenvalues of the covariance matrix of data and further proves that there is no linear combination of pixel values that could serve as a clear indicator for differences between snapshots at different temperatures. In Fig. 6B, we have projected the data into the space of the two linear combinations (principal axes) corresponding to the largest two eigenvalues. They represent the directions of the largest variance in data. As expected from Fig. 6A, all the points belong to one single symmetric cluster with no discernible features.

Likewise, Fig. 6C shows the same data projected into the space of tSNE’s two latent variables and does not display formation of any particular features. Changing the “perplexity” variable in the algorithm, the number of iterations, or the number of principal components kept from an initial PCA reduction before tSNE is applied does not significantly change this result.
FIG. 6. The application of the PCA and the tSNE algorithms to the quantum gas microscope snapshots at \( n \sim 0.82 \) across a range of temperatures. (A) The eigenvalues of the covariance matrix of data showing no outstanding principal components. (B) The projection of data to the two-dimensional space of the two largest principal components. The color bar denotes the temperature. Many of the high-temperature points overlap with their lower-temperature counterparts. No discernible patterns emerge in this projection. (C) Projection of data to the space of non-linear latent variables obtained in the tSNE analysis. A “perplexity” of 30 has been used here. No discernible patterns emerge.

**TRAINING THE CONVOLUTIONAL NEURAL NETWORK**

We implement our CNNs using Tensorflow [43]. The minimalistic design in Fig. 1C we have adopted reflects the need to reduce the number of free parameters to avoid overfitting given the sizes of our data sets. To train, we assign a label, \( Y \) to each snapshot based on the temperature at which it is taken, or whether it is real or fake. Each label is stored in the one-hot format, i.e., a binary array of two numbers, one of which is 1 and the other 0. The index for 1 indicates the category (high/low temperature, or real/fake) to which each snapshot belongs. Given an input image \( X \), the value arriving at the first of the two output neurons of the CNN shown in Fig. 1C, e.g., at the neuron we have associated in our labels to the low-temperature (or real) snapshots, is

\[
O_{1}^{\text{out}}(X) = \sum_{h} O_{h}^{\text{hid}}(X) \times W_{h}^{\text{out}}(1) + b_{h}^{\text{out}}(1),
\]

where the sum is over hidden neurons,

\[
O_{h}^{\text{hid}}(X) = \text{ReLU} \left( \frac{1}{N_s} \sum_{\text{strides}} \text{ReLU} (W_{\text{filter}} \cdot X(s) + b_{\text{filter}}) \right) \times W_{h}^{\text{hid}} + b_{h}^{\text{hid}}
\]

\( N_s \) is the number of strides the filter takes around the image convolving with different sections of it, \( W_{\text{filter}} \) is the matrix of pixel values for the filter, \( X(s) \) is the matrix of pixel values for the section of the image the filter is convolving with in stride \( s \), ReLU is the rectified linear unit activation function, and \( b_{\text{filter}} \), \( W_{h}^{\text{hid}} \), \( b_{h}^{\text{hid}} \), \( W_{h}^{\text{out}}(1) \) and \( b_{h}^{\text{out}}(1) \), are numbers representing other weights and biases in the network. \( O_{1}^{\text{out}} \), along with the value arriving at the second output layer \( O_{2}^{\text{out}}(X) \) are then passed through the softmax activation function in order to obtain two probabilities as
network outputs:

\[
[\text{Network Output}^{(1)}(\mathbf{X}), \text{Network Output}^{(2)}(\mathbf{X})] = \text{softmax}[O_{1\text{out}}(\mathbf{X}), O_{2\text{out}}(\mathbf{X})].
\]  

(4)

The input snapshot is classified as belonging to category \( i \) if \( O_{i\text{out}} \) is the higher probability. The accuracy is defined as the percentage of correct classifications given known labels \( Y \). The convolution of the trained filter with sections of the input image as it moves around in strides of one in every direction creates a “feature map” in which large overlaps between patterns in the filter and the image are highlighted.

For training, we use the Adam optimizer, which is an extension of stochastic gradient descent, to minimize the cross-entropy cost function, defined as

\[
ce = -\frac{1}{N_d} \sum_{\mathbf{X}} \sum_{i=1}^{2} \left( Y_i(\mathbf{X}) \ln [O_{i\text{net}}(\mathbf{X})] + [1 - Y_i(\mathbf{X})] \ln [1 - O_{i\text{net}}(\mathbf{X})] \right),
\]  

(5)

where \( O_{i\text{net}} = \text{Network Output}^{(i)} \) for brevity, \( N_d \) is the number of data. During the training, we keep between 10\% and 20\% of the snapshots from the CNN and use them to perform unbiased testing of the accuracy.

**CNN with More than One Filter**

In cases where we have more than one filter in the convolutional layer, we have modified the architecture to have no fully connected hidden layer in order to reduce the total number of network parameters; the output of each filter after pooling is instead fully connected to the output layer. The value arriving at the output neuron that is responsible for firing when a real snapshot \( \mathbf{X} \) is provided to the input, \( O_{1\text{out}}(\mathbf{X}) \), can then be expressed as a linear combination of contributions from individual filters:

\[
O_{1\text{out}}(\mathbf{X}) = \sum_{m=1}^{N_f} F_{m}^{(1)}(\mathbf{X})
\]

(6)

\[
F_{m}^{(1)}(\mathbf{X}) = \frac{1}{N_{s}} \sum_{s} \text{ReLU} \left( W_{m}^{\text{filter}} \cdot \mathbf{X}(s) + b_{m}^{\text{filter}} \right) \times W_{m}^{\text{out}(1)} + \frac{b_{m}^{\text{out}(1)}}{N_f},
\]

(7)

where \( N_f \) is the number of filters, and \( W_{m}^{\text{out}(1)} \) and \( b_{m}^{\text{filter}} \) are again numbers representing other weights and biases in the network. As in the case of the CNN with one filter, the network output is obtained using Eq. 4.
Effect of Individual Filters

To estimate the effect of filter \( m \) on the outcome, we replace \( O^{(1,2)}(X) \) with \( F^{(1,2)}_m(X) \) before the softmax function,

\[
[\text{Network Output}^{(1)}_{m}(X), \text{Network Output}^{(2)}_{m}(X)] = \text{softmax}[F^{(1)}_{m}(X), F^{(2)}_{m}(X)],
\]

so that we can interpret \( [\text{Network Output}^{(1)}_{m}(X^\text{real}) - \text{Network Output}^{(1)}_{m}(X^\text{fake})] \) as the percentage the network output for \( X \), based on the action of filter \( m \) alone, has to do with factors other than the density itself.

TRAINING PROGRESSION

To monitor the training progression and look for signs of overfitting, especially in the case of CNNs with more than one filter, we track the training and the unbiased testing accuracies over epochs. An epoch is when the network has gone over the entire dataset once. In Fig. 7A, we show these quantities for the case of training with experimental snapshots of local moment leading to the results in Fig. 3. Despite the deviation of the average of two accuracies from each other beyond \( \sim 1,000 \) epochs, signaling the beginning of overfitting due to the relatively large number of free parameters in the CNN, large fluctuations in the accuracies cause occasional overlapping of the two curves even after 5,000 epochs.

Figure 7B shows a similar training progression for CNNs used for DQMC snapshots of density with various numbers of filters. One can see signs of overfitting when the number of filters is increased to 64.

![FIG. 7. Progression of CNN’s accuracy during training for several different cases. (A) For the training with experimental snapshots of local moments using a CNN with six 7 × 7 filters (Fig. 3). (B) For trainings with DQMC density snapshots using CNNs with 2, 8 and 64 5 × 5 filters.](image-url)
ALTERNATIVE TRAININGS

Figure 8 displays results of a training with single-species experimental snapshots at \( n = 0.82 \), however, using a strategy similar to that adopted for the DQMC snapshots in Fig. 2C: using low-temperature snapshots with randomly shuffled pixels (fake snapshots) in place of those at the highest temperature in the training. We find that similar nearest-neighbor anti-correlation features observed in both Fig. 2A and C emerge in the trained filters in this case.

One may wonder what happens if we trained not on data with the most extreme temperature difference, but those from closer temperatures. Figure 9 shows the results for training using experimental snapshots at \( T \sim t \) and \( T \sim 0.35t \). Some of the same features as in Fig. 2 are visible in these panels. However, they appear messier and less refined. The accuracies also drop to around 70%, which are consistent with the limiting case expectation; that telling apart snapshots at the same temperature, only labeled differently, must be only 50% effective.

Changing the filter size does not significantly affect our findings. Figure 10 shows a sample of four \( 3 \times 3 \) filters trained on the same data as for Fig. 2A also yielding testing accuracies of at least 86%. The features obtained very much resemble those seen in Fig. 2A, albeit through a smaller lens; they too mostly point to nearest-neighbor anti-correlations between particles.

With DQMC, we also have access to \textit{spin} snapshots, as they can be obtained by subtracting snapshots of spin-up and spin-down density for the same instance of the auxiliary field. Figure 11 shows that training with those images yields the same features in filters as seen in training with spin-up or spin-down snapshots.

FIG. 8. \textbf{Training runs using real and fake experimental snapshots for} \( n \sim 0.82 \). Same as Fig. 2A, except that instead of experimental snapshots at \( T \sim 7.5t \) images generated by randomly shuffling pixels of low-temperature snapshots are used. The testing accuracy is at least 93%.
FIG. 9. Training runs using experimental snapshots for \( n \sim 0.82 \) at close temperatures. Similar to Fig. 2A, except that the training has been done to distinguish snapshots at \( T \sim t \) from those \( T \sim 0.35t \). The testing accuracies are around 70%.

FIG. 10. Training runs using smaller filters. Similar to Fig. 2A, except that the training has been done using \( 3 \times 3 \) filters. The testing accuracies are at least 86%.

No discernible features emerge in the filters trained on the snapshots of local moments (experimental singles) at the two extreme temperatures (see Fig. 12A) despite near perfect accuracies (> 95%) found for the CNN in predicting to which temperature each snapshot belongs. To reconcile the seemingly random patterns developing in the filters with the incredibly high predicting accuracies they provide for the CNN, we have examined the resulting feature maps and found that in every case, the network bases its decision essentially on the number of empty sites in every snapshot. This is a convenient feature for the network as there is a significantly larger number of them at the higher temperature due to the larger fraction of the doubly occupied sites (Fig. 12B), and the fact that they show up as fermion holes in the snapshots of local moments.

This is also supported by our observation that artificially increasing the value of pixels at occupied sites of high-temperature snapshots to match their average density of fermions with those in the low-temperature snapshots does
FIG. 11. Training runs using DQMC snapshots of spin. Same as Fig. 2C, except that DQMC snapshots of spin have been used in the training.

FIG. 12. Training runs using experimental snapshots of local moment at the extreme temperatures. (A) Same as in Fig. 2A, except that experimental snapshots of local moments are used in the training. The testing accuracies here are at least 95%. (B) Fraction of doubly occupied sites of the Fermi-Hubbard model in the thermodynamic limit as a function of temperature for $U = 8t$ at half filling and $n = 0.82$ from a numerical linked-cluster expansion. It decreases by about 70% when at $n = 0.82$, temperature decreases from $\sim 7.5t$ to $\sim 0.35t$.

not hinder the CNN’s predictive ability. On the other hand, using fake snapshots in place of high-temperature ones and keeping the average density at every pixel the same as for low-temperature snapshots to also account for the slight inhomogeneities in the trapping potential, leads to a sharp drop in the predicting accuracy to about 50%.
FIG. 13. **Output of a CNN with two convolutional layers trained on experimental snapshots of single species for** \( n \sim 1.0 \). (A) and (B) Trained filters in the first and second convolutional layers immediately after the input layer, respectively. (C) Nine sample inputs of single-species snapshots at the two extreme temperatures of \( T \sim 0.35t \) (marked by a red dot at the corner of the image) and \( T \sim 2.5t \). (D) Corresponding feature maps from the first convolutional layer. Stride of one in each direction has been used. The color bars are the same as in (A) with the maximum/minimum fixed at 0.0/1.5. (E) Corresponding feature maps from the second convolutional layer. Stride of one in each direction has been used. No pooling has been used between the two convolutional layers. The color bars are the same as in (A) with the maximum/minimum fixed at 0.0/1.4. After being trained, the network constructs feature maps in the second layer that have a lower density for low-temperature snapshots as a way to facilitate decision making.

**A DEEPER NETWORK FOR HALF FILLING**

Since we have access to more single-species snapshots at half filling than at \( n \sim 0.82 \), we have also tried training a CNN with two consecutive convolutional layers after the input layer, each with one \( 5 \times 5 \) filter. The trained filters and the output of each of the convolutional layers (feature maps) for nine sample input snapshots are shown in Fig. 13. Four of the sample snapshots, denoted by a red circle at their top right corner, belong to the low-temperature set with significant AF ordering present, and the other five are high-temperature snapshots. The first filter, directly in contact with the input, clearly picks up AF correlations as the feature to look for (Fig. 13(A), similar to those shown in Fig. 2B for a CNN with a single convolutional layer. Therefore, the resulting feature maps, shown in Fig. 13(D), reflect the same correlations, which appear stronger and more widespread for the low-temperature snapshots.

Here, the second convolutional layer operates directly on feature maps obtained by the filter in the first layer. The trained filter in the second layer is shown in Fig. 13(B). The pixels with relatively small negative values seen in this filter, along with the ReLU activation function, help the network identify the empty regions in the feature maps with which the filter convolves. This can be seen in the resulting feature maps of the second convolutional layer (Fig. 13(E)). Regions with significant checkerboard patterns in the first set of feature maps translate to mostly empty regions in the second set of feature maps. Pooling the pixel values in the latter results in a number that is smaller/larger than
FIG. 14. Analysis of experimental single-species snapshots using a convolutional autoencoder (CAE). (A) Input and output of a CAE for $n \sim 1.00$ quantum gas microscope snapshots. Left: Four sample inputs of single-species snapshots at the lowest temperature. Middle left: The filter used in the convolutional layer of the encoder immediately after the input layer. Middle right: Corresponding feature maps from the convolutional layer. Stride of one in each direction has been used. Right: Corresponding snapshots ‘dreamed’ by the CAE. The testing accuracy measured using mean square difference of the input and output is about 77%. (B) The CAE architecture used. The filter of the deconvolution layer of the decoder is chosen to be the same as for the convolution layer, deviating from a true CAE architecture, to further reduce the number of free parameters without compromising the physics. (C) Same as in (A), except that we have used experimental snapshots for $n \sim 0.82$. We have also used a filter already trained in a CNN (Fig. 2C) since there is a smaller number of snapshots available in this case.

a threshold value for the low/high-temperature snapshots and will be the basis for decision making.

ANALYSIS USING CONVOLUTIONAL AUTOENCODERS

The magnetic correlation for individual snapshots can be highlighted and studied with the use of another artificial neural network architecture known as a convolutional autoencoder (CAE) (Fig. 14B), specifically designed for feature extraction, dimension reduction and regeneration of data without the need to classify. During the training of the CAE, parameters of the network are optimized for the output to be, on average, as close as possible to the input. In general, one can think of the output images as quick impressions, or “dreams”, the neural network has of the input snapshots.
Figure 14A shows a random sample of four single-species experimental snapshots at half filling at the lowest temperature as inputs along with corresponding outputs of the CAE. The middle panels in the figure show the feature maps corresponding to each of the input snapshots in the left panels. They highlight the important feature promoted by the filter and its distribution by turning all the other seemingly unimportant fluctuations into an average background. Relatively large magnetically ordered domains can be clearly seen for each snapshot. We point out that due to the SU(2) symmetry of the model, AF ordering observed in the projected $S_z$ basis can on average only account for 1/3 of all spin ordering. The same analysis performed using single-species snapshots at $n = 0.82$ demonstrates the depleted nature of the magnetic correlation as a result of doping (Fig. 14C).

**TRAINING WITH DQMC SNAPSHOTS OF LOCAL MOMENTS**

Figure 15 shows the result of training a CNN with sixteen filters using 15000 $10 \times 10$ theory snapshots of local moments. This is the same CNN whose filters are featured in Fig. 3D of the main text. To obtain the snapshots in the DQMC, we note that for a particular auxiliary field, the expectation value of the local double occupancy reduces to its uncorrelated value; the product of the expectation values for spin-up and spin-down occupancies. Therefore, the local moment at site $i$ can be written as $\langle \hat{n}_{i\uparrow} \rangle + \langle \hat{n}_{i\downarrow} \rangle - 2 \langle \hat{n}_{i\uparrow} \rangle \langle \hat{n}_{i\downarrow} \rangle$, where $\hat{n}_{i\sigma}$ is the density operator for spin-$\sigma$ at site $i$.

Figure 15A shows the sixteen trained filters, which similar to what we find for spin, point to only short-range fluctuations. One can find many redundancies. However, a few representative patterns (those features in Fig. 3D of the main text) emerge. Figure 15B shows the average network output when the network trained at $n = 0.82$ is tested on configurations across a range of densities. We also test the network on fake snapshots. A non-monotonic behavior emerges in both cases. Subtracting the average network output for the real and fake snapshots at each density results in a curve that has a broad peak around $n = 0.85$ and showcases the extent of learned correlations between local moments in this CNN that have to do with factors other than the average density itself (Fig. 15C).

To attribute certain features seen in trained filters in Fig. 15A to correlations unique to the NFL region, we have to rule out their dominance at other densities. Figure 15D shows the performance of individual filters over the same range of densities we used to study the network output. Figure 15E further highlights the values in Fig. 15D at $n = 0.82$. Based on these results, filters that significantly contribute to CNNs’ decision making process and are unique to the NFL phase, and therefore, are the best candidates for offering insight into local moment fluctuations are $m = 1, 3,$
FIG. 15. Analysis of DQMC local moment snapshots using a CNN with sixteen filters. (A) Trained filters when \( n = 0.82 \) and \( T = 0.44t \). Note that pixel values or their range in one filter should not be compared with those in other filters since a filter-dependent bias is added to the result of the convolution before it is passed through the ReLU activation function (see Eq. 7). The testing accuracy is around 87%. (B) Average network output when a real or fake DQMC snapshot is provided as input, as a function of average density for this CNN. Here, 1 means all the snapshots are classified as likely to be real \( n = 0.82 \) snapshots, 0 means all the snapshots are classified as likely to be fake \( n = 0.82 \) snapshots, and 0.5 means neither of the two options is preferred. (C) The difference between the two curves in (B), representing the average percentage the decisions made by the CNN have to do with factors other than the density itself. (D) Similar to (C) when the CNN has access to one filter at a time (see Eq. 8). (E) Same as in (D), but at \( n = 0.82 \) for all the filters.

The most frequently seen correlation seems to be the one between two neighboring empty sites. This feature, which shows up in filters trained on density snapshots too (see below), is consistent with the picture emerging in Fig. 3 of the main text from training with experimental snapshots of local moments. Filters \( m = 6 \) and 13 signal that the network also partly uses the information about the density gradient near local moments to make a decision.
FIG. 16. Analysis of DQMC density snapshots using a CNN with sixteen filters. Similar to Figs. 15, but for the case in which the CNN is trained using DQMC full density snapshots. (A) The improvement in the prediction accuracy of the CNN by increasing the number of filters.

TRAINING WITH DQMC SNAPSHOTs OF DENSITY

Sample results for a CNN with sixteen filters trained on full density theory snapshots is shown in Fig. 16. In Fig. 16A, we show the improvement in accuracy as a function of the number of filters when 15,000 or 4,000 snapshots are used in the training. Remarkably, the unbiased testing accuracy can exceed 85%, however, we encounter signs of
overfitting when $N_f$ is increased to 32 for the former or 16 for the latter.

Figures 16B - F show the same quantities as in Fig. 15 but when training with density snapshots. We find that while the shape of the network output vs density in Fig. 16C can vary dramatically from one CNN trained at $n = 0.82$ to the next, the difference shown in Fig. 16D consistently takes a form that can be thought of as a NFL “order parameter”; a nonlinear function of the density profile represented by the CNN. Testing our CNN on snapshots for different temperatures, $U$’s, and system sizes all leads to results consistent with this possibility (see Fig. 18).

Performance of individual filters in Fig. 16E and F shows that most filters likely have an appreciable contribution to the overall network output, with filters $m = 3, 4, 10, 12$ and 13 providing the largest signals. Filter $m = 3$ has a feature resembling those seen in trained filters of the CNN in Fig. 15 measuring the correlation of two neighboring holes. Features seen in $m = 4$ and 5 indicate that the network is also partly using the knowledge of nearest-neighbor density correlations in its decision making process.

In Fig. 17, we show a sample of four density snapshots in the NFL region which are regarded as 100% real by the CNN presented in Fig. 16. It is very hard to discern any patterns with the naked eye using individual snapshots, although some particle-rich and particle-poor regions can be identified in each.

**PERFORMANCE OF CNNS ACROSS DENSITIES**

To further investigate the trends in the CNN’s signal in the NFL region and what that may teach us about the phase as model parameters change, in Fig. 18 we compare the signal we saw in Fig. 16D to one obtained by testing the same trained CNN with 16 filters on snapshots generated in DQMC under various circumstances. In Fig. 18A, we show that the signal is generally suppressed upon increasing the temperature, which is consistent with correlations being washed away at high temperatures.

We note that in the presence of the fermion “sign problem” [44, 45], we treat the network output during the testing
FIG. 18. **Performance of the 16-filter CNNs across densities under various circumstances.** (A) Same as Fig. 16C but testing performed also at other temperatures [the dark green curve in all panels is exactly what is shown in Fig. 16C]. We have used the same 16-filter CNN, trained with data at $n = 0.82$ and $T = 0.44t$, that is featured in Fig. 16. (B) Same as (A), but testing performed at different $U$’s. (C) Same as (A), but testing performed also on data from a larger $N = 20 \times 20$ cluster. The worst average sign is $\sim 0.4$ at densities around 0.85, leading to large errorbars. (D) Testing results for three different CNNs trained with data at the same $T = 0.44t$ and $U = 8t$, but at different densities.

process the same way the expectation value of a conventional observable, $\hat{O}$, is treated and use $\langle \hat{O} \times \text{sgn} \rangle / \langle \text{sgn} \rangle$ in place of $\langle \hat{O} \rangle$, where $\text{sgn}$ is the sign associated with the auxiliary field configuration resulting in a snapshot, as the average $[10]$. This is justified since like many other observables, the network output is simply a nonlinear function of the auxiliary field. Therefore, an exponentially small $\langle \text{sgn} \rangle$ at low temperatures, for large interaction strengths, or for larger cluster sizes $[45]$ increases the uncertainty in the average output dramatically and limits our calculations.

In Fig. 18B, we show that a stronger onsite repulsion of $U = 12t$ likely narrows the NFL region of the Hubbard model in the doping space while a weaker interaction of $U = 4t$ seems detrimental to the phase. Figure 18C further shows that charge correlations in fact grow by increasing the system size to $20 \times 20$ in the DQMC simulations. Again, the small average sign in this case ($\sim 0.4$) has led to much larger error bars as compared to the $10 \times 10$ case. The large number of $20 \times 20$ snapshots around $n = 0.82$ with a negative sign and the fact that training neural networks in sign-problematic regions to infer correlations of the Fermi-Hubbard model without a strategy to properly take the sign problem into account is not justified is the reason we have chosen to work mainly with the $10 \times 10$ cluster in this
Finally, Fig. 18D demonstrates what happens if we trained the same CNN with 16 filters not at $n = 0.82$, but at other average densities. We find that CNNs trained to distinguish real from fake density snapshots in the Fermi liquid region of the model ($n \sim 0.7$) and closer to half filling ($n = 0.9$) show peaks in the respective regions when tested on snapshots across the range of densities. This makes sense since each CNN is asked to focus on charge correlations specific to the respective regions and not necessarily on those relevant to the NFL phase.