Unsupervised phase discovery with deep anomaly detection

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We demonstrate how to discover unknown quantum phases in many-body systems using automated and unsupervised machine learning. In contrast to supervised learning, where data is classified using predetermined labels, we here perform anomaly detection, where the task is to differentiate a normal data set, composed of one or several classes, from anomalous data. As a paradigmatic example, we explore the phase diagram of the extended Bose Hubbard model in one dimension at exact integer filling and employ deep neural networks to determine the entire phase diagram in a completely unsupervised and automated fashion. As input data for learning, we first use the entanglement spectra and central tensors derived from tensor-networks algorithms for ground-state computation and later we extend our method and use experimentally accessible data such as low-order correlation functions as inputs. Our method allow us to reveal a supersolid state with unexpected properties, which appears in the system in addition to the standard superfluid, Mott insulator, Haldane-insulating, and density wave phases.

Introduction

Recent developments in machine learning (ML) have revolutionized the way how we can process and find correlations in complex data. These developments have impacted the physical sciences with a wide variety of applications [1]. Of particular interest is the classification and discovery of phase transitions [2–19]. Recent works concern studies of classical [2, 4], quantum [11, 14, 18] and topological phase transitions [12, 13]. The methods employed range from deep supervised [4, 18] and unsupervised [3, 6] to shallow unsupervised ML algorithms [2, 7, 8]. The input of the ML algorithms can vary from classical spin values [4], local observables [7, 8], correlation functions [14], entanglement spectra [3, 5, 15, 16] to the full state vector [11, 17]. At the same time, the development of the density matrix renormalization algorithm [20, 21] and its reformulation from a quantum information perspective in terms of tensor networks [22, 23] allows one to study large quantum many-body systems approaching the thermodynamic limit.

In this work, we demonstrate how to discover unknown quantum phases and to map out unknown phase diagrams in many-body systems using automated and unsupervised machine learning based on anomaly detection [24–26]. This approach is particularly useful when one is confronted with sufficient data from known classes of states and little or no data from unknown classes. Typical applications of anomaly detection are thus, for instance, credit card fraud detection [27], where one has to find fraudulent transactions in between orders of magnitude larger amounts of normal transactions or medical applications, where one attempts to detect a damaged tissue in an organism (as it is the case in [28] for retinal damage detection). Compared to previous unsupervised attempts in [2, 3, 6–8], this method needs only one or few training iterations and has better generalization properties from employing deep neural networks [29, 30]. This allows for efficient fully automatized phase discovery in the spirit of self-driving laboratories [31], where artificial intelligence augments experimentation platforms to enable fully autonomous experimentation. Intuitively, the method explores the phase diagram until an abrupt change, an anomaly, is detected, singling out the presence of a phase transition. The intuition is similar to the approach introduced in [32], where the authors proposed to detect quantum phase transitions by looking at the overlap between neighbouring ground states in the phase diagram. Here, the machine is used to detect these anomalies. Moreover, as we explain next, it does it from scalable data.

In principle, there are many possible choices as input data for training our method, including the full state vector. To improve scalability and reach large system sizes, we propose to use quantities that arise naturally in the state description and do not require complete state information. For instance, we obtain ground states with tensor networks, from which we use the tensors themselves or the entanglement spectrum (ES) as input data. These quantities arise naturally from the state description without further processing and contain crucial information about the phase, like ES for example [15, 16, 33]. We stress, however, that the choice of preferred quantities to be used for ML may in general vary and depend on the simulation method. In fact, we see that our method also works well with physical data accessible in experiments such as low-order correlation functions.

As a benchmark, we apply our method to the extended Bose Hubbard model in one dimension at exact integer filling. Its phase diagram is very rich and therefore provides a very good test to showcase our method. We are able to determine the entire phase diagram in a completely unsupervised and automated fashion. Importantly, our results point out the existence of a supersolid state that appears in the system in addition to the standard superfluid, Mott insulator, Haldane-insulating, and density-wave phases.

Anomaly Detection Method

In this work, we apply deep neural network autoencoders for anomaly detection,
which have been used in super computing systems to detect faulty states [26]. An autoencoder (AE) is a type of neural network that consists of two parts. The enco-
der part takes the $D$-dimensional input data point $x$ and maps it to a $k$ dimensional latent variable $z$ (typically $k < D$) via a parametrized function $z = f_{\phi}(x)$. The decoder part takes the latent variable $z$ and maps it back to $\bar{x} = g_{\theta}(z)$. The parameters $\phi$ and $\theta$ are trained via the minimization of a loss function $L(x, \bar{x})$ that measures the dissimilarity of the input $x$ and the output $\bar{x}$. The aim of the training is that the input is identical to the output for the whole training data set $\{x\}$. Heuristically, we find that the mean-square error $L(x, \bar{x}) = \sum_v |x_v - \bar{x}_v|^2/D$ suffices for this endeavour and provides good results.

The idea of this anomaly detection scheme is that for each state $|\psi\rangle$ we take corresponding data $x$, such as for instance its ES. That data has characteristic features that the AE learns to encode into the latent variable $z$ at the bottleneck [34], from which it is ideally able to reconstruct the original input. The loss $L$ directly indicates the success of this endeavour, which we improve by employing symmetric shortcut connections (SSC, see fig. 1), inspired from [35, 36] to typical losses $< 5\%$. Now, the intuition is that, when confronted with data from unknown phases, the AE is unable to encode and decode $x$. This leads to a higher loss, from which we deduce that the states do not belong to the same phase as the ones used to train the AE.

Deep learning architectures are known to generalize well [29, 30], such that it suffices to train in a small region of the parameter space. Compared to known supervised deep learning methods this anomaly detection scheme does not rely on labeled data. We train in one or several regions of the phase diagram (normal data), and ask whether a test data point is normal or anomalous. As we show later, this can be performed with no a priori knowledge and in a completely unsupervised manner. The computationally most expensive step, training, has to be performed only once to determine a boundary, as opposed to multiple times like in [3, 6]. Furthermore, it does not require a full description of the physical states in contrast to [32], where full contraction is necessary. Thus, for higher dimensional systems, [32] is infeasible as contraction is known to be generally inefficient for 2d tensor network states (commonly referred to as PEPS, see [23]).

The specific architecture in use consists of two 1d-convolutional encoding and decoding layers with SSCs, respectively, with 64 filters of size 3, activated by ReLU and followed by MaxPooling with size 2, such that the latent space is of size $D/2^2 \times 64$. We implement these layers using the open source library TensorFlow [37]. To ensure the reproducibility of our results, we made the source code available under an open source license [38].

**Simulation Method** We calculate the ground states by means of the Density Matrix Renormalization Group algorithm (DMRG) in terms of Tensor Networks, i.e. Matrix Product States (MPS) [22, 23]. A general multi-

![FIG. 1. Schematic one-dimensional convolutional autoencoder with symmetric shortcut connections (SSC).](image)

partite state of $L$ parties with local dimension $d$ $|\Psi\rangle = \sum_\sigma \psi_\sigma |\sigma\rangle$, where $|\sigma\rangle = \sigma_1 \ldots \sigma_L$ is the vector of local indices $\sigma_i = 1, \ldots, d$, can always be decomposed into products of tensors with the aid of the singular value decomposition. We use the convention of Vidal [39], and write our ground state in the MPS form

$$|\Psi\rangle = \sum_\sigma \Gamma_{\sigma_1} \Lambda^{[1]} \ldots \Lambda^{[L-1]} \Gamma_{\sigma_L} |\sigma_1 \ldots \sigma_L\rangle. \quad (1)$$

At site $i$, $\{\Gamma_{\sigma_i}\}$ is a set of $d$ matrices and $\Lambda^{[i]}$ the diagonal singular value matrix of a bipartition of the chain between site $i$ and $i + 1$, i.e. the Schmidt values (see [22]). One then approximates the exact ground state by keeping only the $\chi_{\text{max}}$ largest Schmidt values for each partition, where $\chi_{\text{max}}$ is known as the bond dimension. This is the best approximation of the full state in terms of Frobenius norm and enables us to handle big system sizes. Eq. (1) corresponds to finite length and open boundary conditions. The DMRG algorithm can also be formulated in the thermodynamic limit for infinite MPS (iMPS) [40–42]. In this case, instead of a finite chain we have a finite and repeating unit cell of length $L$. In either case, the entanglement entropy at bond $i$ is given by

$$S^{[i]} = - \sum_v \Lambda_v^{[i]} \log_2(\Lambda_v^{[i]}). \quad (2)$$

We use the Schmidt values $\Lambda^{[i]}$ as our input data $x$ to explore the phase diagram and ambiguously refer to it as ES. Our numerical results support the functionality of using this anomaly detection scheme with ES as we get near-constant losses for states of the training region and significantly higher losses for unknown phases. The method generalizes well with similar losses for states inside and outside the training region. As we will see below, the method works even well for transitions of Berezinskii-Kosterlitz-Thouless (BKT) type, where the exact transition point is hard to determine in terms of observable correlation functions, and symmetry protected topological (i.e. global) order.
Hamiltonian We test our method on the extended Bose-Hubbard Model

\[ H = -t \sum_i \left( b_i^\dagger b_{i+1} + b_{i+1}^\dagger b_i \right) + \frac{U}{2} \sum_i n_i(n_i - 1) + V \sum_i n_in_{i+1}, \]

with nearest neighbour interaction on a one dimensional chain. It serves as a highly non-trivial test ground with its rich phase diagram that, beside a critical superfluid and two insulating phases, admits a symmetry protected topologically ordered phase at commensurate fillings \([33, 43–51]\). Here, \(n_i = b_i^\dagger b_i\) is the number operator for Bosons defined by \([b_i, b_j^\dagger] = \delta_{ij}\). Typically, we are interested in varying the on-site interaction \(U\) and nearest-neighbour interaction \(V\) and fix the hopping term \(t = 1\). We explicitly enforce filling \(\bar{n} := \sum_i \langle n_i \rangle / L = 1\) by employing \(U(1)\) symmetric tensors \([52]\), which we implement using the open source library TeNPy \([53]\) (easily readable code accessible in \([38]\)).

One way to physically classify these phases is to look at the correlators

\[ C_{\text{SF}}(i, j) = \langle b_i^\dagger b_j \rangle \]  
\[ C_{\text{DW}}(i, j) = \langle \delta n_i (-1)^{|i-j|} \delta n_j \rangle \]  
\[ C_{\text{HI}}(i, j) = \langle \delta n_i \exp \left( -i\pi \sum \delta n_{0 \leq j < 1} \right) \delta n_j \rangle \]

with \(\delta n_i = n_i - \bar{n}\), which are decaying exponentially in the Mott-insulating (MI) phase and with a power-law in the superfluid (SF), density-wave (DW) and Haldane-insulating (HI) phases, respectively. The non-local string term in eq. (6) is characteristic of topological order, where the translational symmetry remains protected with a transition in the Luttinger liquid universality class from MI and gets broken with a transition in the Ising universality class to DW \([51]\). We visualize the phase diagram by computing \(O_i = \sum_{i,j} C_{\text{SF}}(i, j) / L^2\) in fig. 2 in the thermodynamic limit for a repeating unit cell of \(L = 64\) sites with a maximum bond dimension \(\chi_{\text{max}} = 100\) and assuming a maximum occupation number \(n_{\text{max}} = 3\), which results in a local dimension \(d = n_{\text{max}} + 1 = 4\).

Numerical Results Assuming no a priori knowledge, we start by training with data points at the origin of the parameter space \((U, V) \in [0, 1.3]^2\), which in our case accounts to training in SF. By testing with data points from the whole phase diagram we can clearly see the boundaries to all other phases from SF in fig. 3. The BKT transition between SF and MI is matched by an abrupt rise in loss (fig. 3, inset a)). In this particular case, we can already determine the different phases inside the anomalous region due to their different loss levels and the appearance of two valleys at the phase boundaries between MI, HI and SF (fig. 3, inset b)). Physically, we can explain these valleys by the criticality of these Luttinger and Ising type transitions, which lead to a slowly decaying ES at the boundary, just like in the critical SF phase.

It is not necessarily always the case that one can differentiate the different phases inside the anomalous region. Thus, as a systematic approach, we propose picking homogeneous and high contrast anomalous regions after the initial training, as we did in fig. 4 for \((U, V) \in [4, 4.8] \times [2, 4]\), which accounts to DW. We can confirm the previously determined boundaries to the anomalous region, which is very sharp due to the Ising type transition. Further, we can again separate MI and HI due to different loss levels but without a valley in between (fig. 4, inset a)).

We also test our method on other input data. Instead of ES, we can also use a tensor \(\Theta_{\sigma_i}^{\nu_{i-1}, \nu_i} = \sum_{a,b} \Lambda_{\nu_{i-1},a}^{\nu_i} \sigma_i^{a,b} A_{b,v_i}^{\nu_i}\) from the chain, from which one can compute all single-site expectation values \([22]\). This quantity has three indices, which is why we interpret it as a colored image, because two indices \(\nu_{i-1}\) and \(\nu_i\) can be interpreted as the two dimensions of the image and the third index \(\sigma_i\) can be interpreted as the color channel. Instead of 1d convolution, we now use 2d convolution with otherwise identical architecture. Even though translational invariance is broken in DW, we find it suffices to use only one tensor \(\Theta\) from the center of the unit cell.
FIG. 3. Anomaly detection after training near the parameter space origin. Phase boundaries are determined by a rise in loss (inset a) and c)). Anomalous regions are already well-separated by valleys due to the criticality at the phase boundaries (inset b)), which share similarities with the critical SF phase.

FIG. 4. Training in the region of high loss from after the first iteration confirms the boundaries. MI and HI are well separated inside the anomalous set as depicted in inset a). This isn’t necessarily the case as indicated in inset b) for SF and SS.

This is because, despite the broken translational symmetry, entanglement is still distributed uniformly in the unit cell, which is implicitly encoded in $\Theta$. Furthermore, we find that the network is capable of encoding more than one phase in the normal dataset, seen in fig. 5. We still find the boundaries between MI, HI and DW due to the criticality of the transitions (see fig. 5, inset a)), similar to the valleys in fig. 3.

This is not necessarily the case, as we can see in fig. 6, for the BKT transition. Here, instead of unprocessed data from simulation, we use physically motivated quantities, i.e. we calculate $\{C_{SF(i,j)}\}_{i,j=1}^{64}$ and train in MI and SF. We interpret rows as color channels for 1d convolution again. Because $C_{SF}$ does not contain any information about the topological order in HI, the method does not recognize this region as we would expect (fig. 6, inset a)). Overall, the boundaries match perfectly with a sharp increase onto a plateau at the transition points. This opens the possibility to use physical observables from experiment with the caveat of requiring physical knowledge a priori.

FIG. 5. Instead of ES, we use $\Theta$ as input data and use 2D convolutional layers. The same AE can encode both MI, HI and SF data. The marks in DW are consistently in every training.

By close inspection of figs. 3 and 6, we see a region with noticeable contrast for small $U$ and large $V$, indicating the presence of a separate phase. This is interesting because, initially, we did not expect to find a fifth phase in the diagram. Upon further physical inspection, we suspect it to be supersolid (SS). While SS has been discussed in previous literature for incommensurate fillings [19, 43–46], to the best of our knowledge, considering $\bar{n} = 1$ and obtaining SS was merely mentioned in [33], and has not been discussed before. In order to show its character in this specific setting, we compute the Fourier transform of the local density $\tilde{n}(k) = \sum_j \langle n_j \rangle e^{-ikj/L}$ and detect long-range solid order by looking at

$$S := \max_{k \neq 0} |\tilde{n}(k)|^2$$

in fig. 7 [54]. Additionally, we find non-zero $O_{DW}$ and $O_{SF}$, showing both superfluid and crystalline behavior, from which we conclude supersolidity. However, what we find is very different from previously observed supersolids. If the number of atoms fluctuates, or the filling is smaller than one, the system incorporates vacancies, and
FIG. 6. Instead of ES, we use $C_{SF}$ as input data. The same AE can encode both MI and SF data. HI is not recognized as the data does not contain information about the topological order of this phase.

may develop the SS via the so called Andreev-Lifshitz-Chester scenario [55–57]. Here, this cannot happen because we explicitly fix the number of particles to the number of sites. We find periodically repeating regions of crystalline order in $\langle n_i \rangle$. $C_{SF}$ matches these checkerboard regions, additionally to the non-trivial decay, as indicated exemplarily for $V = 4$ in the inset of fig. 7. Note, that the demonstration of the SS phase at the fixed integer filling equal to one is novel and challenging itself and the mechanism describing this phase at integer filling has yet to be determined. The detection of this new phase demonstrates the power of our approach.

Conclusion We have shown an unsupervised method to map out the phase diagram of a complex quantum many-body system with no physical a priori knowledge. By using tensor networks we can reliably compute ground states of many-body systems in the thermodynamic limit and at the same time extract the desired data without further processing. Entanglement spectra and central tensors serve as natural quantities in this context, but the method also proved successful for physical observables. Hence, this method can be applied in both purely computational platforms like self-driving laboratories as well as experimental setups.

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Appendix A: Tensors as input data

We briefly summarize Matrix Product States (MPS), a special form of one-dimensional tensor-network states. This is important to understand how we use the central tensor $\Theta$ as input data for our training.

There is a natural graphical language for tensor networks, where eq. (1) corresponds to fig. 8 [22]. In this graphical representation, connected lines correspond to index contractions, which in the case of eq. (1) corresponds to matrix multiplication. This representation has the advantage that one can readily obtain the mixed canonical form,

$$\Psi = \sum_\sigma A^{\sigma_1} \ldots A^{\sigma_{i-1}} \Theta^{\sigma_i} B^{\sigma_{i+1}} \ldots B^{\sigma_L},$$  \hspace{1cm} (A1)

from combining $\Gamma$s and $\Theta$s accordingly, where $\{A^{\sigma_i}\}_{j=1}^{i-1}$ and $\{B^{\sigma_j}\}_{j=i+1}^{L}$ are left- and right-normalized, i.e.

$$\sum_{\sigma_j} (A^{\sigma_j})^\dagger (A^{\sigma_j}) = \sum_{\sigma_j} (B^{\sigma_j})^\dagger B^{\sigma_j} = \mathbb{I}$$ (see [22] for details).

Hence, in order to calculate local observables at site $i$, one only needs the single site pseudo-wavefunction

$$\Theta^{\sigma_i}_{v_{i-1},v_{ii}} = \sum_{a,b} \Lambda^{[i-1]}_{a,v_{i-1},\sigma_i} \Gamma^{\sigma_i}_{a,b} \Lambda^{[i]}_{b,v_{ii}}.$$  \hspace{1cm} (A2)

For example, single-site operator expectation values are simply calculated in terms of $\langle O_i \rangle = \sum_{\sigma_i,\sigma'_i,v_{ii},v_{i-1}} \Theta^{\sigma_i}_{v_{i-1},v_{ii}} O_{\sigma_i,\sigma'_i} (\Theta^{\sigma'_i}_{v_{i-1},v_{ii}})^\dagger$ and similarly two-point correlation functions, as graphically depicted in fig. 9.

![Graphical representation of a finite MPS](image)

FIG. 8. Graphical representation of a finite MPS with open boundary conditions, physical indices $\sigma_i$ and virtual indices $v_{ii}$. $\Gamma^{\sigma_i}_{\sigma'_i,v_{i-1},v_{ii}}$ is the local description of site $i$ with singular values $\Lambda$ connecting to the left and right part of the chain (entanglement spectrum).

To input $\Theta$ into a neural network, we simply treat the tensor as an image, that, instead of the typical red green blue (RGB) channels, has ‘spin channels’. Each excitation value $\sigma_i = 0, \ldots, n_{\text{max}}$ now corresponds to a “colour channel”, yielding a $\chi_{\text{max}} \times \chi_{\text{max}}$ image for that channel. This way, we can use classical machine learning methods that are optimized for image processing for our physical problem.

Heuristically, we found that already a tensor or the ES from a site is sufficient for our method to discriminate the phases. A possible explanation is the translational invariance of the model, which, in our case also results in uniformly distributed entanglement. By this, we mean that the entanglement spectrum is the same at all bonds, resulting in a uniform entanglement entropy distribution along the chain. This is true even for the DW phase, where translational invariance is broken. Only for the SS phase this is not the case anymore, where the ES admits a periodic pattern. To improve the results one could take several spectra or tensors from the chain by concatenating them, keeping the input data scalable. Yet, we find that one tensor or ES suffices for discrimination.

Appendix B: Extended Bose Hubbard model phases

We briefly summarize the phases of the extended Bose Hubbard model at integer filling, that have not been discussed in the main text.

1. MI-HI-DW transition

Another way to locate the phase transitions, as has been discussed in the main text, is by looking at the entanglement entropy eq. (2)

$$S[i] = -\sum_v \Lambda_v^{[i]} \log_2(\Lambda_v^{[i]}),$$  \hspace{1cm} (B1)

and the correlation length $\xi$, defined in terms of

$$\mu_2 = \exp(-L/\xi),$$  \hspace{1cm} (B2)

where $\mu_2$ is the second largest eigenvalue of the transfer matrix of the $L$-site unit cell. Note that here all entanglement entropies are equal along the chain, such that we will simply speak of $S$. We fix $U = 5$ and compare these two quantities with the order parameters in fig. 10. We note that due to the infinite nature of the states, $\xi$ and $S$ were not susceptible to $L$, only to $\chi_{\text{max}}$. Since the order parameters do not notably change with $\chi_{\text{max}}$, we fix $\chi_{\text{max}} = 100$, for which $S$ and $\xi$ indicate well the transitions.

As mentioned in the main text, another way to indicate quantum phase transitions without any a priori knowledge is by calculating overlaps (fidelity) between ground states in the phase diagram [32],

$$F(V_i, V_j) = \langle \Psi(V_i) | \Psi(V_j) \rangle.$$  \hspace{1cm} (B3)
Order parameters; $L = 64, \chi_{\text{max}} = 100, U = 5$

Entanglement entropy; $L = 64, U = 5$

Correlation length; $L = 64, U = 5$

For example, we depict the MI-HI-DW transition for $U = 5$ in fig. 11. We can see how the states in the different phases separate into quasi non-overlapping regions. The off-diagonal $\mathcal{F}(V_i, V_{i+1})$ accurately yields the transition points, indicated by drops in fidelity [32].

2. Critical Superfluid phase

The best results are obtained from looking at the overlaps, eq. (B3), in fig. 13. Though, the contrast in the off-diagonal as indicated in the inset is very low. Note that the criticality of SF leads to the valleys between MI, HI and DW, depicted in fig. 3 in the main text.

3. Critical Supersolid phase

We perform consistency checks of our findings in the main text regarding the supersolid phase. There is an implicit bias to our ground states from fixing a repeating unit cell size. We look at the ground state at $(U, V) = (0.5, 4.0)$ and vary $L$ in fig. 14(a). Between $L = 2$ and $L = 32$ we find DW-like patterns of damped amplitude (e.g. $(0.8, 1.2, 0.8, 1.2\ldots)$) in inset of fig. 14(a) for $L = 16$). Formations that roughly make up half of the unit cell emerge from there and grow accordingly. An energetically optimal configuration is reached around $L = 150$. From there on, the formation does not grow.
but splits into smaller parts, such that for \( L = 300 \) we obtain the same structure and energy as for \( L = 150 \). In between we find energetically worse configurations. We exemplarily show stable configurations for \( L = 128, 256 \) and 512 in fig. 14(b). To compare different runs with different unit cell sizes, we shift the strings of expectation values \( \langle n_i \rangle \) accordingly. We find matching positions and widths of these formations for different unit cell sizes. We note that DMRG often gets stuck in local minima with higher ground state energy, even when we employ a mixer [58, 59].

We note that inside the solid formations, there is a non-trivial power law decay in \( C_{SF} \) as indicated in fig. 14(c). The same is true when we start with a site outside the solid formation. Further, we want to check what happens when we deviate from integer filling. We fix again \((U,V) = (0.5, 4.0)\) and a unit cell size of \( L = 64 \) and gradually subtract particles. In this case, the existence of solid formations survives up to 2 of 64 holes, with an intermediate configuration for 3 and uniform distribution beyond, as indicated in fig. 14(d).

FIG. 12. 1) Correlators for the superfluid phase for fixed nearest neighbour interaction \( V = 0.1 \). 1a) deep in SF phase, 1b) near the transition point and 1c) deep in MI phase. 2) Superfluid to Mott-Insulator transition characterized 2a) by vanishing charge energy gap, 2b) diverging entanglement entropy and 2c) diverging correlation length.
FIG. 13. \( \mathcal{F}(U_i, U_j) \) for all possible combinations on 100 equally spaced \( U_i \in [0, 5] \) for fixed \( V = 0 \). Inset: Off diagonal indicating transition point with drops in overlap. Note the low contrast.

FIG. 14. a) Energy scaling for unit cell sizes \( L \). Insets are corresponding density profiles. The solid formations reach an optimum around \( L = 150 \) and start to break into smaller parts that are energetically less optimal. For multiples of \( L = 100, 128 \) and 150, respective configurations and energies are repeated (see inset and fig. 14(b)). b) Matching solid formations for different unit cell sizes in the supersolid region at \((U, V) = (0.5, 4.0)\). Because positions of these formations seem to appear arbitrarily, we manually shifted the start and end point in order to better see the matching size and positions. c) \( C_{SF}(21, j) \) inside the solid formation for \( L = 150 \) at \((U, V) = (0.5, 4)\). We use every second value to visualize the power-law decay by plotting in double logarithmic (inset 1) and single logarithmic (inset 2) scale. Inset 3) shows the global context of the correlator. d) Gradually removing particles leads to the breakdown of solid formations after 3 of 64 holes, exemplarily for \((U, V) = (0.5, 4)\).