

# Lieb's Theorem and Maximum Entropy Condensates

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The maximum entropy steady states which form upon Floquet heating of the ground state of the Hubbard model on *unbalanced* bi-partite lattices are shown to possess uniform finite off-diagonal long-range order in the thermodynamic limit. For *repulsive* interactions the induced order corresponds to the formation of a spin-wave condensate, whilst for *attractive* interactions it instead corresponds to the formation of a superconducting,  $\eta$ -paired condensate. This creation of a 'hot' condensate can occur on *any* periodically driven unbalanced lattice where the relevant SU(2) symmetry is preserved. Our results provide an understanding of how strong driving can expose order which has been suppressed by the lattice geometry - independent of any microscopic parameters. We discuss the implications of this for recent experiments observing emergent superconductivity in solid-state photoexcited compounds.

*Introduction* - Geometry plays a decisive role in the properties of discrete lattice systems. In the fermionic Hubbard model - a successful, simple description of correlated fermions in solid-state materials - the lattice structure is known to significantly influence the system's equilibrium phases. The presence of triangles in the underlying lattice, for example, causes frustration, which prevents regular antiferromagnetic ordering [1–3] and induces the formation of exotic phases of matter such as a spin-liquid [4, 5].

Meanwhile, in the context of bi-partite Hubbard models, Lieb showed there is a strong distinction between the ground states on *balanced vs unbalanced* lattices [6] - with the former meaning the number of sites in each of the two sublattices are equal and the latter meaning they are not. For the balanced case, the ground state has a total spin of zero and is thus an antiferromagnet [7]. In the unbalanced case Lieb proved that the total spin is finite, resulting in a ferrimagnetic ground state [8–10].

Whilst the equilibrium properties of the Hubbard model on unbalanced lattices are well known, the system's response to external forces such as a periodic driving field is not. This is especially true in comparison to the extensive theoretical efforts on balanced, hypercubic lattices to engineer driven Hamiltonians which guide the system into ordered, prethermal phases whilst transiently mitigating the inevitable, deleterious Floquet heating [11–16]. These efforts are motivated by the opportunities arising from the realisation of coherently driven electronic systems in solid-state material experiments [17–19].

Solid-state materials, however, form a variety of complex, geometrical structures that are typically not balanced, hypercubic lattices [20–23]. Moreover, techniques such as scanning tunnelling microscopy and chemical synthesis mean that experimentalists now have an enormous

degree of control over the lattice structure of the correlated materials they can synthesise [24–31]. Moire superlattices - stacked sheets of Van der Waals heterostructures - are such a material [32–35]. The tunability of their geometry, physical dimension and frustration has made them a promising condensed matter alternative to ultracold atomic setups [36, 37], where the non-equilibrium physics of the Hubbard Hamiltonian can be directly simulated [38–40]. We thus consider it both pertinent and timely to determine the differences which arise in the response of correlated electronic systems to external driving fields when moving away from balanced, hypercubic setups and onto more complex lattices.

In this paper we show that, in the thermodynamic limit, the maximum entropy states which form upon continuous Floquet heating of the ground state of the Hubbard model on *unbalanced* bi-partite lattices can possess finite, uniform off-diagonal long-range order (ODLRO). These states are thus distinct from the featureless infinite temperature state which will always form under Floquet heating on *balanced* bi-partite lattices in the thermodynamic limit. This result is demonstrated by applying Lieb's theorems in conjunction with the constraints imposed by periodic driving which preserves the relevant SU(2) symmetry. These constraints, in tandem with the heating induced by the driving, force a dynamical renormalisation of the 'staggered', long-range correlations initially present in the ground state. The resulting maximum entropy state is completely translationally invariant and possesses ODLRO.

Using recently developed analytical methods we quantify this order for all possible bi-partite lattices in the thermodynamic limit. In the repulsive regime on any unbalanced lattice the steady state is provably a superconductor as the ODLRO is in the charge sector and the Meissner effect and flux quantisation are manifest. The same cannot be said for the ground state as it lacks translational invariance. We then detail how these or-

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dered, maximum entropy steady states can be realised and probed with current technology in ultracold atomic simulators. In this setting properties such as the optical conductivity spectrum can be determined, which is not possible with current computational methods.

Our results provide an understanding, independent of any microscopic parameters, of how strong driving can expose order which is suppressed by a system's geometry. We conclude by discussing the possible connection between this phenomenon and observations of emergent superconductivity in irradiated solid-state materials.

*Theory and Results* - Our starting point is the fermionic Hubbard model defined over some lattice  $\Lambda$ . The Hamiltonian reads

$$H = - \sum_{\substack{a,b \in \Lambda \\ a \neq b}} J_{a,b} \sum_{\sigma} c_{a,\sigma}^{\dagger} c_{b,\sigma} + U \sum_{a \in \Lambda} n_{a,\uparrow} n_{a,\downarrow}, \quad (1)$$

where  $n_{\sigma,a}$ ,  $c_{\sigma,a}^{\dagger}$  and  $c_{\sigma,a}$  are, respectively, number, creation and annihilation operators for fermions of spin  $\sigma \in \{\uparrow, \downarrow\}$  on site  $a$  within the lattice. The first summation in  $H$  runs over the sites of the lattice and kinetically couples them together with strength  $J_{a,b}$ ; for Hermiticity we have  $J_{a,b} = J_{b,a}$ . The second term in  $H$  represents an interaction of strength  $U$  between the two spin species on a given site  $a$ .

We assume that the lattice  $\Lambda$  is bi-partite, i.e the vertices can be split into two sublattices  $A$  and  $B$  with  $J_{a,b} = 0$  if both  $a$  and  $b$  are in the same sublattice. Without loss of generality we set  $N_A \geq N_B$ , where  $N_A$  and  $N_B$  are the number of sites in each sublattice. We can also assume, without loss of generality, that the system is connected, i.e. each site can be reached from any other by moving between pairs of sites where  $J_{a,b} \neq 0$ . Finally, for simplicity, we fix ourselves to half-filling, i.e.  $\sum_a \langle n_{a,\uparrow} + n_{a,\downarrow} \rangle = N = N_A + N_B$  and zero  $z$ -magnetisation, i.e.  $\sum_a \langle n_{a,\uparrow} - n_{a,\downarrow} \rangle = 0$ . Our results, however, should also apply at other intermediate fillings.

The Hamiltonian in Eq. (1) is  $SU(2) \times SU(2)$  symmetric. The first of these  $SU(2)$  symmetries, known as the 'spin' symmetry, can be introduced through the spin-raising operator  $S^+ = \sum_a S_a^+ = \sum_a c_{a,\uparrow}^{\dagger} c_{a,\downarrow}$ , its conjugate  $S^-$  and the total  $z$ -magnetisation  $S^z = \sum_a n_{\uparrow,a} - n_{\downarrow,a}$ . These each commute with  $H$ . The second, known as the ' $\eta$ ' symmetry, can be introduced via the  $\eta$ -raising operator  $\eta^+ = \sum_a \eta_a^+ = \sum_a f(a) c_{a,\uparrow}^{\dagger} c_{a,\downarrow}^{\dagger}$ , its conjugate  $\eta^-$  and the modified total number operator  $\eta^z = \sum_a (n_{\uparrow,a} + n_{\downarrow,a} - 1)$ . The latter of these commutes directly with  $H$  whilst the former commute with  $H$  once a trivial constant term is added to the Hamiltonian and the function  $f(a)$  is set to be  $\pm 1$  depending on whether the vertex  $a$  is in  $A$  or  $B$ . Importantly, the two symmetries are fundamentally related as the mapping  $U \leftrightarrow -U$  is effectively equivalent to swapping the spin and  $\eta$  degrees of freedom, i.e.  $\eta \leftrightarrow S$  [41].

This transformation, along with the theorems derived by E. Lieb [6], can be used to show that for  $U > 0$  the ground state of  $H$  satisfies  $\langle S^2 \rangle = X(X+1)$  and  $\langle \eta^2 \rangle = 0$  with  $X = (1/2)(N_A - N_B)$ . Meanwhile, for  $U < 0$ , we have  $\langle S^2 \rangle = 0$  and  $\langle \eta^2 \rangle = X(X+1)$ . The operators  $S^2 = (S^z)^2 + (1/2)(S^+ S^- + S^- S^+)$  and  $\eta^2 = (\eta^z)^2 + (1/2)(\eta^+ \eta^- + \eta^- \eta^+)$  are, respectively, the  $\eta$  and spin Casimir operators.

This result has significant implications for the ground state properties of  $H$ . For positive  $U$ , in *balanced* bipartite lattices where  $N_A = N_B$  (examples include any hypercubic lattice) the electron spins on sites in identical sublattices tend to align whilst those in separate sublattices misalign, creating an antiferromagnetic state. The distance dependence of these correlations varies with the lattice dimension; along any spin-axis the correlations in a 1D chain are known to decay algebraically with distance [41, 42] whilst in a 2D square lattice the correlations along the  $z$  spin-axis are oscillatory and long-range [43, 44].

Meanwhile, for *unbalanced* lattices, by definition, one of the sublattices is larger than the other and thus the same alignment tendencies force the system into a ferrimagnetic state instead. Moreover, regardless of the physical dimension, for *any* lattice where  $N_A - N_B \propto N$  the correlations along both the  $x$  and  $y$  spin-axes will not decay, creating a long-range, oscillatory profile with a non-zero average [45, 46]. For negative  $U$  the same is true, but for the correlations in the charge sector instead of the spin sector.

In Fig. 1 we illustrate some of these properties by using DMRG [47] to determine the ground state and its correlation profile for several quasi-1D Hubbard lattices. To aid our analysis we introduce the graph measure  $|a-b|$  which is the minimum number of edges (bonds between pairs of sites with non-zero  $J$ ) that must be traversed to move between sites  $a$  and  $b$ . Through this we can define the distance-dependent correlation function

$$C(d) = \frac{1}{\mathcal{N}} \sum_{\substack{a,b \in \Lambda \\ |a-b|=d}} \langle O_a^+ O_b^- \rangle, \quad (2)$$

where  $O$  is either  $S$  or  $\eta$  depending on whether  $U$  is positive or negative.  $\mathcal{N}$  is the number of pairs of sites which satisfy  $|a-b| = d$ .

For the ground states of the unbalanced lattices in Fig. 1 this correlation function is non-decaying and staggered in both sign and magnitude as a function of distance. On the balanced 1D chain this staggering is also present, but decays away with distance. For simplicity, we have taken the coupling strength  $J_{a,b}$  to be homogeneous, i.e.  $J_{a,b} = \text{const.}$  if it is non-zero. For inhomogeneous  $J_{a,b}$  on the unbalanced lattices the correlations in the ground state will become more disordered but they will still retain a similar, oscillatory, long-range structure as Lieb's theorems are independent of the specific  $J_{a,b}$ .

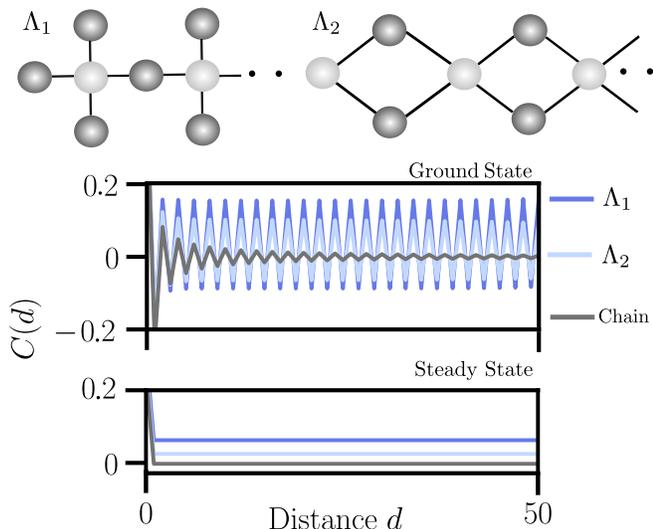


FIG. 1. Top) Two unbalanced bi-partite lattices  $\Lambda_1$  and  $\Lambda_2$ . The light vs dark sites indicate the two sublattices and the bonds correspond to coupled sites where the kinetic coupling  $J_{a,b} = J \neq 0$ . For all other pairs of sites  $J_{a,b} = 0$ . Bottom) Correlations versus distance (up to  $d = 50$ ) for the ground state and maximum entropy steady states of the half-filled Hubbard model on  $\Lambda_1$  and  $\Lambda_2$ , as well as a 1D chain. Each lattice is taken to have  $N = 100$  sites and we set  $U = \pm 5J$ . For  $U = 5J$ , the correlation function at a given distance  $d$  is defined in Eq. (2) with  $O = S$ . For  $U = -5J$ ,  $C(d)$  is of the same form but with  $O = \eta$ . The maximum entropy state is that which forms when the ground state is Floquet heated to infinite temperature whilst the relevant  $SU(2)$  symmetry (spin for  $U > 0$  and  $\eta$  for  $U < 0$ ) is preserved.

The central result of this work is that, in the thermodynamic limit, driving the ground states of unbalanced lattices to maximum entropy with some arbitrary field which preserves the relevant  $SU(2)$  symmetry forces the oscillatory correlations to become completely uniform with distance whilst remaining finite. Recent work has shown that, generally, the maximum entropy state which forms in the long-time limit of periodic driving will host completely uniform off-diagonal order in the preserved symmetry channel [48, 49]. Thus far, when driving an equilibrium state this induced order has only been shown to be finite for finite systems and on regular hypercubic lattices it will asymptotically decay to 0 as  $1/N$  [50]; preserving the intuition of Floquet heating as a deleterious effect in the thermodynamic limit. Here we show that on unbalanced lattices this will not be the case and periodic driving can be used to reach a maximum entropy condensate which hosts finite, uniform ODLRO.

This remarkable result can be proven independently of any specific parameters of the Hamiltonian and applied driving field. Consider  $U > 0$  and an arbitrary *unbalanced* Hubbard lattice in the thermodynamic limit. Provided both each  $N_A$  and  $N_B$  grow proportionally to  $N$  we have that, following Lieb's theorem, the ground state satisfies  $\langle S^2 \rangle \propto N^2$ . Under the application of continuous

periodic driving which preserves  $\langle S^2 \rangle$  then Floquet heating will occur but the system will be restricted to the subspace spanned by the eigenvectors of  $S^2$  which possess the same value of  $\langle S^2 \rangle$  as the ground state. The steady state  $\rho_{ss}$  is effectively the identity matrix in this subspace [50–52]. Such a probability distribution is translationally-invariant due to the permutational invariance of  $S^2$  and thus this state must have  $\langle S_a^+ S_b^- \rangle = C_{\text{off-diag}}$   $a \neq b$  as well as  $\langle S_a^+ S_a^- \rangle = C_{\text{diag}}$ , where both  $C_{\text{off-diag}}$  and  $C_{\text{diag}}$  are constant. By definition, it then follows that

$$\langle S^+ S^- \rangle = N C_{\text{diag}} + N(N-1) C_{\text{off-diag}}. \quad (3)$$

and as  $C_{\text{diag}}$  is a local on-site density we have  $0 \leq C_{\text{diag}} \leq 1$ . Moreover, as we are in the zero magnetisation sector we also have  $\langle (S^z)^2 \rangle = 0$  and  $\langle S^+ S^- \rangle = \langle S^- S^+ \rangle$ . Hence,  $C_{\text{off-diag}}$  must be non-zero in the thermodynamic limit in order for  $\langle S^2 \rangle = \langle S^+ S^- \rangle \propto N^2$  and the maximum entropy state hosts completely uniform ODLRO in the spin sector. If, instead, we have  $U < 0$  we can apply the same argument to show that the correlations  $\langle \eta_a^+ \eta_b^- \rangle$  will be completely uniform with distance and finite in the thermodynamic limit.

We now directly quantify the order of these maximum entropy states for different lattices. We utilise a recently constructed complete basis which simultaneously diagonalises both  $S^2$  and  $\eta^2$  [53]. This allows us to make analytical predictions for the size of the diagonal and off-diagonal  $\eta$  and spin correlations in the maximum entropy states on any lattice.

In Fig. 1 we plot the correlation function in Eq. (2) for the two pictured unbalanced lattices and the 1D Hubbard chain. Whilst the lattices used are of finite-size, any differences from the thermodynamic limit are minimal. We observe that in all cases the steady state possesses completely uniform correlations in the relevant symmetry channel. The chain is distinct from the two unbalanced lattices, however, as the steady state correlations are over an order of magnitude less and will become exactly zero as  $N \rightarrow \infty$ . Unlike the ground state, the steady state correlations are completely independent of the specific values of the  $J_{a,b}$  and  $U$ , only the sign of  $U$  is relevant.

The quasi-1D unbalanced lattices used in Fig. 1 were chosen because they are amenable to Matrix Product based routines, allowing us to compare the steady state correlations to the ground state. These results, however, apply to unbalanced lattices with any physical dimension  $D$ . In this vein, we can consider *any* bi-partite lattice in the thermodynamic limit and quantify the long-range order in the maximum entropy state as a function of the ‘imbalance’  $\lambda = (N_A - N_B)/(N_A + N_B)$ . The lattices  $\Lambda_1$  and  $\Lambda_2$  from Fig. 1 have  $\lambda = 1/3$  and  $\lambda = 1/2$  respectively whilst a 1D chain clearly has  $\lambda = 0$ . We directly access the thermodynamic limit  $N = N_A + N_B \rightarrow \infty$  by calculating the off-diagonal order for increasing  $N$  until convergence is achieved.

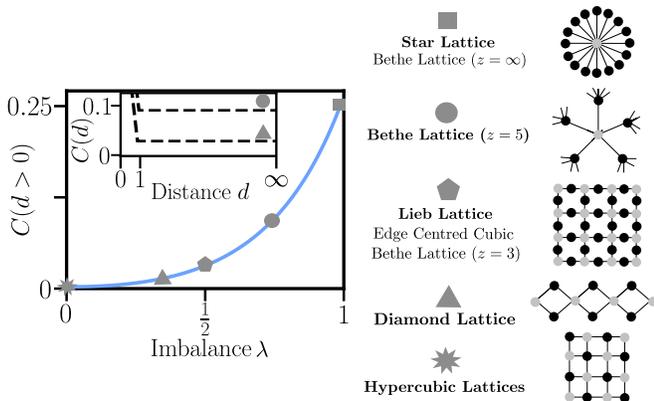


FIG. 2. Off-diagonal correlations versus lattice imbalance ratio  $\lambda = (N_A - N_B)/(N_A + N_B)$  for the maximum entropy steady states of the half-filled Hubbard model in the thermodynamic limit. These states are formed from Floquet heating the ground state whilst preserving the relevant  $SU(2)$  symmetry. If the ground state is for  $U > 0$ , the spin  $SU(2)$  symmetry must be conserved by the heating and the correlation function  $C(d)$  is defined in Eq. (2) with  $O = S$ . For  $U < 0$ , the  $\eta$   $SU(2)$  symmetry must be conserved by the heating and the correlation function is defined in the same way but with  $O = \eta$ . Inset) Correlation function  $C(d)$  versus distance  $d$  for the two indicated imbalances. Notable lattices and their corresponding imbalances are marked, those titled in bold are pictured.

In Fig. 2 we quantify this order, following Floquet heating of the ground state, for the full range of  $\lambda$ . We observe how the steady state order increases as the imbalance saturates to 1 and have marked some notable lattices on this diagram. These include the Lieb lattice and the edge-centred-cubic lattice - which are known to arise in materials such as the cuprates and perovskites [20, 21, 54]. Meanwhile, we see that the maximum entropy states on any *balanced* lattices ( $\lambda = 0$ ) are incapable of hosting off-diagonal order.

On any lattice in the thermodynamic limit with  $\lambda > 0$  the maximum entropy states satisfy Yang's definition for ODLRO [55] as we have that  $\lim_{|a-b| \rightarrow \infty} \rho(a, b) = \text{const} \neq 0$ . The matrix  $\rho(a, b)$  is the two-body reduced density matrix and corresponds to  $\text{Tr}(\rho_{ss} S_a^+ S_b^-)$  for  $U > 0$  and  $\text{Tr}(\rho_{ss} \eta_a^+ \eta_b^-)$  for  $U < 0$ . Whilst the ground state on an unbalanced lattice will also typically satisfy this ODLRO property there is a crucial difference. Specifically, unlike the steady state the two-body reduced density matrix for the ground state is not translationally invariant, i.e.  $\rho(a, b)$  is not constant for all  $|a - b| = d$ , an immediate consequence of the fact the lattice is not spatially symmetric.

The combination of particle-hole ODLRO and translational invariance has been proven to imply both the Meissner effect and flux quantisation [56, 57], meaning that our steady states are superconducting for  $U < 0$ . Without translational invariance these proofs no longer hold and thus we cannot say the same of the ground

state. The 'staggered', oscillatory nature of the correlations may be suppressing the state's underlying order.

Whilst the Meissner effect and flux quantisation will only be observable for  $U < 0$  and  $D \geq 2$  we anticipate that other crucial differences will arise when probing the steady state vs ground state on unbalanced lattices in both the attractive and repulsive case. Ultracold quantum simulators offer an experimental setting in which the steady states in this paper can be realised, and such differences identified.

The fermionic Hubbard model is realisable in this setting by loading an ultracold atomic gas into the potential landscape generated by standing wave laser beams [58]. The Hubbard interaction can be directly tuned to be both positive or negative via Feshbach resonances [38, 59]. The lattice geometry is dependent on the interference pattern the standing wave lasers create and an optical Lieb lattice has already been successfully realised and loaded with bosons [60, 61]. The setup necessary for creating the diamond lattice ( $\Lambda_2$  in Fig. 1) has also been theorised for both fermions and bosons [62].

In order to realise the desired steady states the ground state must be driven out of equilibrium and undergo Floquet heating whilst preserving the desired  $SU(2)$  symmetry. Inducing a periodic modulation of either the hopping strength or the interaction strength will do this and can be achieved by periodically 'shaking' the standing wave interference pattern [40].

The timescale on which the desired Floquet heating occurs and the uniform correlations are induced will depend on the specifics of the lattice geometry, driving field and the parameters of  $H$ . Nonetheless, using a moderate interaction strength and resonantly matching the driving frequency to it should dramatically reduce this timescale [63]. Studies of Floquet heating rates for infinite Bethe lattices suggest such a timescale is on the order of 10s of hopping times [64, 65].

Alongside direct measurement of two-point correlation functions via in-situ imaging [66–68], which would verify the results presented here, measurements can be taken in this setup which cannot be done computationally. The optical conductivity spectrum provides information about the transport properties of a state and can be used to distinguish superconductors, conductors and insulators. This cannot be calculated computationally for the steady states in this paper as it requires diagonalisation of the Hubbard Hamiltonian on an unbalanced lattice in the thermodynamic limit [69]. In optical lattices, however, this spectrum can be accessed via spectroscopic techniques [70–72].

Ultracold quantum simulators thus offer the opportunity to realise the states uncovered in this paper and identify distinctive features, outside of the two-point correlation function, which set them apart from the ground state.

*Conclusion and Outlook* - We have shown how, in

the thermodynamic limit, the maximum entropy steady states of the Hubbard model on unbalanced lattices possess finite, uniform ODLRO. These states can be formed by periodically driving the ground state of the system whilst preserving the  $SU(2)$  symmetries of the lattice; a process which renormalizes the staggered, inhomogeneous correlations initially present. For the attractive Hubbard model  $U < 0$  the steady state is provably a superconductor whilst the same arguments cannot be applied to the ground state. We quantified the induced steady state order as a function of the *imbalance* of the lattice, allowing us to make predictions for *any* bi-partite lattice. Finally, we discussed how such exotic, desirable steady states can be formed and probed with current technologies in optical lattice setups.

Our results here provide an understanding of how driving can expose and manifest order which is suppressed in equilibrium due to the lattice geometry - independent of any microscopic parameters. This phenomenon should be observable beyond the bi-partite, single-band Hamiltonian that we have studied here; equilibrium states with the desired, ‘suppressed’ long-range order have been observed in Hubbard models with more than two fermionic species [46], multiple-bands [73] and even frustration [74]. Moreover, regardless of how such states arise, we know that driving which preserves the requisite symmetry is guaranteed to transform the state into one which manifests uniform ODLRO in the thermodynamic limit.

Finally, and related to these points, the emergence of superconducting order has recently been observed in a number of solid-state materials upon exposure to strong driving [75–80]. These materials often contain layers of compounds such as  $CuO_2$  which can be described with single or multi-orbital Hubbard Hamiltonians on unbalanced Lieb lattices [81–83]. Whilst a microscopic description of these materials is beyond the scope of this paper, our results offer a possible phenomenological mechanism for these experimental observations. The optical conductivity spectrum is typically used as a fingerprint for the emergence of superconductivity in these solid-state experiments [84]. Measurement of this spectrum via an optical lattice realisation of our steady states could strengthen the connection between our work and these experiments.

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