Exact Results for Strongly Correlated Fermions in 2 + 1 Dimensions

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We derive exact results for a model of strongly interacting spinless fermions hopping on a two-dimensional lattice. By exploiting supersymmetry, we find the number and type of ground states exactly. Exploring various lattices and limits, we show how the ground states can be frustrated, quantum critical, or combine frustration with a Wigner crystal. We show that on generic lattices the model is in an exotic "superfrustrated" state characterized by an extensive ground-state entropy.

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Over the past few decades thousands of papers have been written exploring properties of itinerant-electron models in two spatial dimensions. Exact results, however, for such systems at strong coupling are few and far between. In this Letter we find the exact number and type of ground states in a model of spinless fermions with strongly repulsive nearest- and next-nearest-neighbor interactions. The strengths of these interactions are tuned to give an exact *supersymmetry.* The supersymmetry not only makes our exact computations possible, but also balances competing terms in the Hamiltonian. On most lattices, this results in an exotic "superfrustrated" state.

Our model is most transparently defined in terms of the supersymmetry generator Q and its Hermitian conjugate $Q^\dagger$, which are fermionic and obey $Q^2 = (Q^\dagger)^2 = 0$. These commute with the Hamiltonian defined by $H = \{Q, Q^\dagger\}$. This relation is at the heart of supersymmetric quantum mechanics; a number of important results follow [1]. All energy eigenvalues E satisfy $E \geq 0$, because $\langle s|H|s\rangle = \langle s|QQ^\dagger|s\rangle + \langle s|Q^\dagger Q|s\rangle$ cannot be negative. Any state with $E = 0$ is therefore a ground state; it is annihilated by both Q and $Q^\dagger$. Therefore, all we need to do to construct a many-body model with supersymmetry is to find a fermionic operator Q squaring to zero.

Our degrees of freedom are spinless fermions living on any lattice or graph of N sites in any dimension. A fermion at site i is created by the operator $c_i^\dagger$ with $\{c_i, c_j^\dagger\} = \delta_{ij}$. The sum $\Sigma_i c_i^\dagger$ squares to zero, but using this for Q results in a trivial Hamiltonian. The strongly interacting model we discuss was introduced in Ref. [2]. The fermions have a *hard core,* meaning that they are not only forbidden to be on the same site as required by Fermi statistics, but are also forbidden to be on adjacent sites. Their creation operator is $d_i^\dagger = c_i \mathcal{P}_{\langle i\rangle}$, where

$$\mathcal{P}_{\langle i\rangle} = \prod_{j \text{ next to } i} (1 - c_j^\dagger c_j) \tag{1}$$

is zero if any site next to i is occupied. A fermionic operator Q squaring to zero is then $Q = \Sigma_i d_i^\dagger$. This gives a nontrivial Hamiltonian

$$H = \{Q, Q^\dagger\} = \sum_{\langle ij\rangle} d_i^\dagger d_j + \sum_i \mathcal{P}_{\langle i\rangle}. \tag{2}$$

The latter term has a more conventional form on a lattice where every site has z nearest neighbors:

$$\sum_i \mathcal{P}_{\langle i\rangle} = N - zF + \sum_i V_{\langle i\rangle}, \tag{3}$$

where $V_{\langle i\rangle} + 1$ is the number of particles adjacent to i, unless there are none, in which case $V_{\langle i\rangle} = 0$. The operator $F = \Sigma_i d_i^\dagger d_i$ counts the number of fermions. So, in addition to the hard core, the Hamiltonian includes a hopping term, a constant (which we keep to ensure ground states have $E = 0$), a chemical potential z, and repulsive interactions between fermions two sites apart.

We use two mathematical tools to study the $E = 0$ ground states of (2). The first is the *Witten index* W [1]. It is similar to the partition function, but includes a minus sign for each fermion:

$$W = \mathrm{tr}[(-1)^F e^{-\beta H}]. \tag{4}$$

W is a lower bound on the number of ground states: it is the difference of the number of bosonic ground states and the number of fermionic ground states. This is because all energy eigenstates with $E > 0$ form boson-fermion doublets of the same energy E but opposite $(-1)^F$. The states in a doublet contribute to W with opposite signs and cancel, leaving only the sum of $(-1)^F$ over the ground states.

This argument shows that W is independent of β, so we can evaluate it in the $\beta \to 0$ limit, where every state contributes with weight $(-1)^F$. We compute this by dividing the lattice into two sublattices S_1 and S_2; we fix a configuration on S_1 and sum $(-1)^F$ for the configurations on S_2. Then we sum the results over the configurations on S_1. For a periodic chain with $N = 3j$ sites, we take S_2 to be every third site and the remaining sites S_1. Then the sum over configurations on any site on S_2 vanishes unless at least one of the adjacent sites on S_1 is occupied. There are only two such configurations:

$$|\alpha\rangle \equiv \cdots \bullet\square\circ\bullet\square\circ\bullet\square\circ\bullet\square\circ\bullet\square\circ\bullet\square\circ\ldots,$$
$$|\gamma\rangle \equiv \cdots \circ\square\bullet\circ\square\bullet\circ\square\bullet\circ\square\bullet\circ\square\bullet\circ\square\bullet\ldots, \tag{5}$$

where the square represents an empty site on S_2. Both $|\alpha\rangle$ and $|\gamma\rangle$ have $f = N/3$, so $W = 2(-1)^f$, requiring that there are at least two ground states.

The second tool we use is the computation of the *cohomology* H_Q of the operator Q. This tool is even more powerful, allowing us to obtain not just a lower bound, but rather the precise number of ground states, and the fermion number of each. The cohomology is the vector space of states which are annihilated by Q but which are not Q of something else (in mathematical parlance, these states are closed but not exact) [3]. Since $Q^2 = 0$, any state that is Q of something is annihilated by Q. Two states $|s_1\rangle$ and $|s_2\rangle$ are said to be in the same cohomology class if $|s_1\rangle = |s_2\rangle + Q|s_3\rangle$ for some state $|s_3\rangle$.

The nontrivial cohomology classes are in one-to-one correspondence with the $E = 0$ ground states [2]. To see this, consider an energy eigenstate $|E\rangle$ with eigenvalue $E > 0$. If $Q|E\rangle \neq 0$, then it is not in any cohomology class. If $Q|E\rangle = 0$ but $H|E\rangle \neq 0$, then $|E\rangle = Q(Q^\dagger|E\rangle/E)$. This is in the trivial cohomology class, so only the $E = 0$ ground states have nontrivial cohomology. Because they are annihilated by both Q and $Q^\dagger$, linearly independent $E = 0$ ground states must be in different cohomology classes. Precisely, the dimension of the vector space of ground states (the "number" of ground states) is the same as that of the cohomology. Since F commutes with the Hamiltonian, the cohomology class and the corresponding ground state have the same fermion number.

To illustrate these techniques, let us first generalize some of the one-dimensional results of Ref. [2] to a staggered (but still supersymmetric) chain. Let $Q(a) = Q_1 + aQ_2$ where a is a parameter and

$$Q_1 = \sum_{j=1}^{N/3}[d^\dagger_{3j-2} + d^\dagger_{3j}], \qquad Q_2 = \sum_{j=1}^{N/3} d^\dagger_{3j-1}. \tag{6}$$

Because $[Q(a)]^2 = 0$, the Hamiltonian $\{Q(a), Q^\dagger(a)\}$ is supersymmetric. It deforms (2) by multiplying the hopping term by a for hopping on or off S_2, and multiplying $\mathcal{P}_{\langle i\rangle}$ by a^2 when i is on S_2. For $a \to \infty$, the $E = 0$ ground states therefore are the states where $\mathcal{P}_{\langle 3j\rangle} = 0$ for all j. There are only two: $|\alpha\rangle$ and $|\gamma\rangle$ from (5). For large but finite a, there remain two ground states; for example, $|\alpha\rangle - 1/a|\alpha_2\rangle + \mathcal{O}(1/a^2)$, where $|\alpha_2\rangle$ is the sum of configurations differing from $|\alpha\rangle$ by shifting one particle one site to the right. When $a = 1$, we know from the Bethe ansatz solution that there are two ground states as well and that the model is gapless [4]. For $a \ll 1$, there are also two ground states, one localized on S_2 and the other with one particle for every two sites of S_1. The $a \ll 1$ ground states spontaneously break different parity symmetries than $|\alpha\rangle$ and $|\gamma\rangle$ do, and $a = 1$ is a quantum critical point separating the two phases.

We find the exact number of ground states by computing the cohomology H_Q by using a *spectral sequence.* A useful theorem is the "tic-tac-toe" lemma of Ref. [3]. This says that under certain conditions, the cohomology H_Q for $Q = Q_1 + Q_2$ is the same as the cohomology of Q_1 acting on the cohomology of Q_2. In an equation, $H_Q = H_{Q_1}(H_{Q_2}) \equiv H_{12}$. As with our computation of W, H_{12} is found by first fixing the configuration on all sites on the sublattice S_1, and computing the cohomology H_{Q_2}. Then one computes the cohomology of Q_1, acting not on the full space of states, but only on the classes in H_{Q_2}. A sufficient condition for the lemma to hold is that all nontrivial elements of H_{12} have the same f_2 (the fermion number on S_2).

We apply this theorem to the one-dimensional chain by using the decomposition of $Q = Q_1 + aQ_2$ given by (6). Consider a single site on S_2. If both of the adjacent S_1 sites are empty, H_{Q_2} is trivial: Q_2 acting on the empty site does not vanish, while the filled site is Q_2 acting on the empty site. Thus H_{Q_2} is nontrivial only when every site on S_2 is forced to be empty by being adjacent to an occupied site. The elements of H_{Q_2} are just the two states $|\alpha\rangle$ and $|\gamma\rangle$ pictured above in (5). Both states $|\alpha\rangle$ and $|\gamma\rangle$ belong to H_{12}: they are closed because $Q_1|\alpha\rangle = Q_1|\gamma\rangle = 0$ and are not exact because there are no elements of H_{Q_2} with $f_1 = f - 1$. By the tic-tac-toe lemma, there must be precisely two different cohomology classes in H_Q, and therefore exactly two ground states with $f = N/3$. Applying the same arguments to the periodic chain with $3f \pm 1$ sites and to the open chain yields in all cases exactly one $E = 0$ ground state, except in open chains with $3f + 1$ sites, where there are none [4].

We emphasize that for finite a, $|\alpha\rangle$ and $|\gamma\rangle$ are not the ground states themselves. A representative of a cohomology class is not necessarily unique, because adding Q of something to it does not change the class. A ground state is the one element in each class which is also annihilated by $Q^\dagger$. One can use this observation in principle (and in practice for small numbers of sites) to construct the exact ground states from $|\alpha\rangle$ and $|\gamma\rangle$ as a power series in $1/a$ [5]. The presence of states $|\alpha\rangle$ and $|\gamma\rangle$ in the ground states hints that the energy is lowest when particles are three sites apart. The chemical potential favors the creation of more particles, but putting them two sites apart causes an increase in potential energy and hopping energy. The two effects balance at an average separation of roughly three sites; we call this heuristic the "3-rule."

Having introduced the mathematical tools necessary, we now turn to the study of our spinless-fermion model on two-dimensional lattices. We find that generically, there is an *extensive ground-state entropy:* the number of ground states increases exponentially with the size of the system. This indicates that the system is frustrated; we explain how in the following.

The systematics of the one-dimensional case quickly extend to lattices of type Λ_3, which are obtained from any lattice (or even graph) Λ by putting two additional sites on every link. Letting S_1 be the original sites of Λ and S_2 the added sites, the only states in H_{Q_2} and H_{12} are the two where S_1 is completely full and completely empty. The first gives an $E = 0$ ground state with $f = N_\Lambda$ (the number of sites of Λ), while the latter gives an $E = 0$ state with $f = L_\Lambda$ (the number of links in Λ), with a possible exception when $L_\Lambda = N_\Lambda - 1$. When Λ is the square lattice, the two ground states on Λ_3 have filling $f = N/5$ and $f = 2N/5$. Lattices of type Λ_3 are the only two-dimensional ones we know of where the number of ground states does not grow with the size of the lattice.

Another exceptional case is the octagon-square lattice in the first part of Fig. 1. We take L rows and M columns of squares (hence $N = 4LM$ sites). Let S_1 consist of the leftmost site on every square. Then H_{Q_2} is trivial unless the M sites on S_1 in a given row are either all occupied or all empty. There are $2^L - 1$ such configurations that have at least one row in S_1 occupied. Because of the hard core, all the sites of S_2 adjacent to an occupied site on S_1 cannot be filled, and the remaining sites form independent open chains of length a multiple of 3. Such an open chain has just one element of H_{Q_2}, so each of these $2^L - 1$ configurations correspond to one element of H_{Q_2} and H_{12}. Now consider the configuration where all sites on S_1 are empty, so that the sites on S_2 form M periodic chains, each of length $3L$. We showed above that H_{Q_2} for *each* of these chains has *two* independent elements. Thus H_{Q_2} and H_{12} are of dimension $2^L + 2^M - 1$. Applying the tic-tac-toe lemma to this case is more involved, but the conclusion is that there are $2^L + 2^M - 1$ ground states, each with $N/4$ fermions.

We believe that on the octagon-square lattice, the model exhibits a combination of Wigner-crystal order with frustration. There are $2^L + 2^M$ configurations of $N/4$ particles that satisfy our heuristic 3-rule. 2^L of them are of the form displayed in Fig. 1: one can shift all the particles in a given row without violating the rule. This illustrates how frustration arises: in each row one can shift all the particles without violating the 3-rule. Likewise, 2^M of them have particles on the top or bottom of each square. For mysterious reasons, the state with $(k_x, k_y) = 0$ is not a ground state, but we believe the remaining $2^L + 2^M - 1$ ordered states dominate the actual ground states. In further support of this claim, we analyze the discrete symmetries commuting with Q. If a given element of the cohomology spontaneously breaks such a symmetry, the corresponding ground state will break it too. The ground states have spontaneously-broken parity symmetries like the Wigner-crystal states in Fig. 1. Again, like the crystal, all but one of the $2^L - 1$ ground states first considered spontaneously break translation symmetry in the vertical direction but not the horizontal; $2^M - 2$ of the remaining ground states spontaneously break translation symmetry in the horizontal direction. Moreover, the number of ground states here can be changed by requiring that just one site anywhere on the lattice be occupied. Consider the octagon-square lattice with one site on S_1 and its three neighbors on S_2 removed; this is equivalent to demanding that there be a particle on this S_1 site. On this lattice there are just 2^{L-1} ground states. Only in an ordered system should this type of change occur.

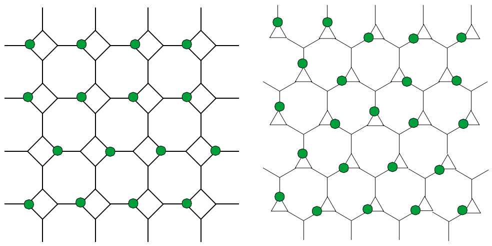

FIG. 1 (color online). Configurations obeying the 3-rule on the octagon-square and nonagon-triangle lattices.

The Λ_3 and octagon-square lattices are exceptional: on all other lattices we have studied the ground-state entropy is extensive. In many cases (including the triangular, hexagonal, and Kagomé lattices), this can be seen by computing the Witten index W as a function of the size of the lattice. Employing a row-to-row transfer matrix T_M, the index for $M \times L$ unit cells is expressed as $W_{L,M} = \mathrm{tr}[(T_M)^L]$. We found by exact diagonalization that the largest eigenvalues $\lambda_M^{\max}$ of the T_M here behave as $\lambda_M^{\max} \propto \lambda^M$, with $|\lambda| > 1$. Clearly, the absolute value $|\lambda|$ sets a lower bound on the ground-state entropy per lattice site. For n sites per unit cell, $S_{\mathrm{GS}}/N \geq \ln|W_{L,M}|/(nML) \sim \ln|\lambda|/n$. For the triangular lattice, $S_{\mathrm{GS}}/N \geq 0.13$ [6,7].

For the nonagon-triangle lattice shown in the right side of Fig. 1, the extensive ground-state entropy can be exactly computed. This lattice is formed by replacing every other site on a hexagonal lattice with a triangle. To find the ground states, take S_1 to be the sites on the triangles and S_2 to be the remaining sites. As with the chain, H_{Q_2} vanishes unless every site in S_2 is adjacent to an occupied site on some triangle. The nontrivial elements of H_{Q_2} therefore must have precisely one particle per triangle, each adjacent to a different site on S_2. This is because a triangle can have at most one particle on it, and (with appropriate boundary conditions) there are the same number of triangles as there are sites on S_2. A typical element of H_{Q_2} is shown in Fig. 1. One can think of these as "dimer" configurations on the original honeycomb lattice, where the dimer stretches from the site replaced by the triangle to the adjacent nontriangle site. Each close-packed hard-core dimer configuration is in H_{12}, and, by the tic-tac-toe lemma, it corresponds to a ground state. The number of such ground states $e^{S_{\mathrm{GS}}}$ is therefore equal to the number of such dimer coverings of the honeycomb lattice, which for large N is [8]

$$\frac{S_{\mathrm{GS}}}{N} = \frac{1}{\pi}\int_0^{\pi/3} d\theta \ln[2\cos(\theta)] = 0.161\,53\ldots. \qquad (7)$$

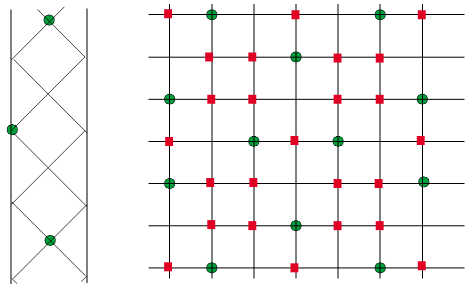

FIG. 2 (color online). "Ordered" states for the triangle-square ladder and the square lattice; the red squares are sublattice 2.

The frustration here clearly arises because there are many ways of satisfying the 3-rule.

For the staggered model, $Q = Q_1 + aQ_2$, on the nonagon-triangle lattice, the dimer states are the exact ground states when $a \to \infty$. In the singular limit $a = 0$ there are more ground states: $|\Psi_2\rangle$ with all particles on S_2, $2^{N/4}$ ground states $|\Psi_1^{(s)}\rangle$ with one particle on each of the triangles, and additional ground states at higher fermion numbers as well. For $0 < a \ll 1$, $|\Psi_2\rangle$ and $e^{S_{\rm GS}} - 1$ of the $|\Psi_1^{(s)}\rangle$ remain ground states, while the others develop energies of order a^2. The ground-state degeneracy can be lifted by including terms that break the supersymmetry. Consider changing the intratriangle hopping amplitude to $1 - \epsilon$ with $\epsilon > 0$. At $a = 0$, the $|\Psi_1^{(s)}\rangle$ have energy $E = N\epsilon/4$, so here the Wigner crystal $|\Psi_2\rangle$ is the unique $E = 0$ ground state. For a large and ϵ small, the leading piece in the effective Hamiltonian is a "flip" of 3 dimers around a plaquette, as in the quantum dimer model [9]. For generic potentials this model orders [10], leading to the possibility of a quantum critical point intermediate between this ordered phase and the $a = 0$ one. A quantum critical point, indeed, occurs for the chain at $a = 1$ [2,4], and so seems possible on general lattices for $a \sim 1$.

The situation on lattices with a higher coordination number is more complicated. There are ground states with more particles than the 3-rule allows: the increased chemical potential and possibilities for hopping compensate for an increase in potential energy. For the triangle-square ladder in Fig. 2 with $N = 3n + 1$ sites and open boundary conditions, we obtained a recursion relation for the ground-state generating function $P_n(z) = {\rm tr}_{\rm GS}(z^F)$:

$$P_{n+3}(z) = 2z^2 P_n(z) + z^3 P_{n-1}(z), \tag{8}$$

with $P_0 = 0$, $P_1 = z$, $P_2 = 2z^2$, $P_3 = z^3$. This shows the existence of $2^{n/3}$ ground states at fermion number $2N/9$, and also indicates additional ground states at higher fillings, up to $N/4$. An "ordered" state with $f = 2N/9$ violating the 3-rule is given in Fig. 2, but the frustration is evident in that there are many such states. Using the recursion relation, we find that the ground-state entropy is set by the largest solution $\lambda^{\max}$ of $\lambda^4 - 2\lambda - 1 = 0$, giving $S_{\rm GS}/N = (\ln\lambda^{\max})/3 = 0.1110\ldots$.

On a square lattice of $3L \times 3M$ sites with periodic boundary conditions, the situation is similar. When S_2 consists of the red squares in Fig. 2, there are two elements of H_{12} that have S_2 empty; one of them is displayed in Fig. 2. They have $2N/9 = 2LM$ particles, and also violate the 3-rule. Many more ground states with different fermion numbers can be found by introducing various types of defects in this pattern, but we have not found a way of counting them all [7].

Our exact results indicate that there is a new kind of exotic phase for itinerant fermions on a two-dimensional lattice with strong interactions. This superfrustrated state exhibits an extensive ground-state entropy, and occurs because supersymmetry ensures a perfect balance between competing terms in the Hamiltonian. Patterns with charge order can be distinguished in various limits and on special lattices, but the effect of (approximate) supersymmetry in general is that defects between different domains come at zero (very low) energy cost. For example, the charge order (stripes) found for hard-core fermions on the square lattice [11] becomes superfrustrated as the interactions and chemical potential are tuned to the supersymmetric point.

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