The Hubbard model plays a key role in the study of magnetism, metal-insulator transitions, and high-temperature superconductivity. It is a simple model that captures the physics of phenomena of correlated systems. In view of the difficulty in establishing rigorous results of the model, the Nagaoka’s theorem is very significant, providing a good example, though of a restricted use, of metallic ferromagnetism in itinerant electron systems. The result of Nagaoka that the ground state of the Hubbard model with an infinite on-site repulsion with exactly one hole is a maximal-spin state is remarkable, given that for large on-site repulsion with no holes a maximal-spin state cannot be a ground state, due to the antiferromagnetic correlations that arise from kinetic exchange phenomenon. There have been several contributions extending or simplifying the original result of Nagaoka, and investigations on the instability of the Nagaoka state, when the number of holes is more than one. In the following we give a simple variational construction of a spin-wave state, and in conjunction with the fact that a degeneracy exists, and show that by lowering the spin one can lower the energy below that of the Nagaoka state. The simplest case where a degeneracy occurs is the one-hole case for a closed chain with an odd number of sites, and similarly the higher-dimensional lattices can be handled by lowering the spin one can lower the energy below that of the Nagaoka state. The result of Nagaoka that the ground state of the Hubbard model with an infinite on-site repulsion with exactly one hole is a ground state, due to the antiferromagnetic correlations that arise from kinetic exchange phenomenon. There have been several contributions extending or simplifying the original result of Nagaoka, and investigations on the instability of the Nagaoka state, when the number of holes is more than one. In the following we give a simple variational construction of a spin-wave state, and in conjunction with the fact that a degeneracy exists, and show that by lowering the spin one can lower the energy below that of the Nagaoka state. The simplest case where a degeneracy occurs is the one-hole case for a closed chain with an odd number of sites, and similarly the higher-dimensional lattices can be handled by lowering the spin one can lower the energy below that of the Nagaoka state. The result of Nagaoka that the ground state of the Hubbard model with an infinite on-site repulsion with exactly one hole is a ground state, due to the antiferromagnetic correlations that arise from kinetic exchange phenomenon. There have been several contributions extending or simplifying the original result of Nagaoka, and investigations on the instability of the Nagaoka state, when the number of holes is more than one.

Let us consider the Hubbard model on a hypercubic lattice with exactly one hole is studied. It is seen that a degeneracy can occur in the maximal-spin sector. It is proved variationally that the Nagaoka (maximal spin) state is not a ground state, if degeneracy exists. We give an explicit construction of a variational state, an incommensurate spin-wave state, with energy lower than that of the Nagaoka state. For the case of more than one hole, a few examples are discussed where a degeneracy exists.

The Hubbard model can be written as

\[ H = -t \eta \sum_{\langle i,j \rangle, \sigma} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} \]

where \( c_{i\sigma} (c_{i\sigma}^\dagger) \) annihilates (creates) an electron of spin \( \sigma \) at \( i \)’th lattice site, and \( n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma} \) is the number operator. The first sum in the above equation is for nearest neighbours only, with the hopping strength \( t \). The parameter \( \eta = 1 \) for the case of fermions (that we will discuss through out), and \( \eta = -1 \) for hard-core bosons. All the conclusions that we draw for the fermion problem carry through to hard-core bosons, by changing the sign of \( \eta \). We consider the case of the on-site repulsion \( U \) to be infinite large. This forces all the physical states with any number of electrons to consist of no doubly-occupied site orbitals, tantamounting to a super-Pauli exclusion. We choose a basis set of states, a 3\( N \)-dimensional Hilbert space, with this constraint built in and consequently the Hamiltonian consists of only the first term in the above equation. The total spin \( S \), and the \( z \)-component of the total spin \( S^z \) (at \( i \)’th site the spin operators are given as \( S_i^z = (n_{i\uparrow} - n_{i\downarrow})/2, S_i^z = c_{i\uparrow}^\dagger c_{i\uparrow} \)) are good quantum numbers of the model, and we use them to label the sectors of the Hilbert space. Let the number of electrons \( N_e = N - 1 \). The basis states consist of direct products of \( N - 1 \) site orbitals occupied each with either a spin-up or down electron. Also we note that all the matrix elements of the Hamiltonian have a definite sign, by choosing the set of basis states carefully. In the sector with \( S^z = S_{\text{max}} = N_e/2 \), the basis states can be labeled by the location of hole, and are obtained by operating with an annihilation operator on a reference ferromagnetic state (no holes and no down spins). The basis state \( i \) is given by

\[ |i > = c_{i\uparrow} |\uparrow\uparrow\uparrow\uparrow\uparrow\ldots > \equiv c_{i\uparrow} |\text{REF} > \]

where the hole is at the \( i \)’th site. The reference state \( |\text{REF} > = \prod_{i=1,N} c_{i\uparrow}^\dagger |0 > \) is created from the vacuum state by using the creation operators. With this choice of the basis set, the matrix elements have all one same sign, \( \langle \text{REF} | H |j > = t \zeta_{i,j} \) where \( \zeta_{i,j} = 1 \) if the site \( i \) and \( j \) are nearest neighbours on the lattice, and zero otherwise. For the sectors with \( S^z \neq S_{\text{max}} \) the construction is similar. For instance, for \( S^z = S_{\text{max}} - 1 \) sector, the basis states are \( \{|ik > \} \). A basis state is labeled by the locations of the hole (at \( i \)) and the down spin (at \( k \)), and is constructed from the reference state as \( |ik > = c_{i\uparrow} c_{k\downarrow}^\dagger |\text{REF} > \). The overlaps between the basis states are all of the same sign (using the fermion anticommutation relations),

\[ \langle i'k' | H |ik > = t \zeta_{i',k'} (\delta_{k,k'} + \delta_{i,k'} \delta_{i',k}) \]

\[ (3) \]

The sectors with
where the first term in the parenthesis comes from a movement of the up-spin electron, and the second term from that of the down-spin electron. It should be noted that the above equation does not change for hard-core bosons (by using the boson commutation relations), if we use $\eta = -1$ in Eq.(1).

As can be seen from the above equation, the Hamiltonian in a matrix form looks like $H = tA$, in any $S^2$ sector, where $A$ is matrix with positive-semidefinite elements, $A_{ij} \geq 0$, and the size of the matrix depends on $S^2$. The diagonal elements are zero, and there are exactly $z$ nonzero elements on any row (of magnitude unity). The largest eigenvalue is $\lambda_{\text{max}} \leq z$ independent of size, from Gershgorin theorem. And its easy to check that a uniform vector (which is a maximal-spin state) is eigenstate of the matrix, with eigenvalue $z$, implying $\lambda_{\text{max}} = z$. If the matrix is connected in the configuration space (i.e. the elements of $B = A^M$, for a finite $M$, are positive definite, $B_{ij} > 0$), $\lambda_{\text{max}}$ is a non-degenerate eigenvalue for any finite size from Perron-Frobenius theorem. For a bipartite lattice, where $N_1, N_2,$ are all even, the sign of $t$ is irrelevant. This can be seen by a canonical transform, changing the sign of the electron creation and annihilation operators on any size from size to size. It suffices to study one sign of $t$. So for $t < 0$, the lowest eigenvalue of the Hamiltonian corresponds to the highest eigenvalue of the matrix $A$. In this case, the Nagaoka state ($S = S_{\text{max}}$) is a ground state, with an energy $-zt$, and also it is nondegenerate (connectivity of $A$ is provable in more than one dimension). For nonbipartite lattices, where at least one of $N_1, N_2,$ is an odd number, we have to study both signs of $t$, and the nature of the ground state is quite different, as we shall see below. We proceed for $t < 0$ similarly as above, as the problem boils down to the investigation of $\lambda_{\text{max}}$, and the Nagaoka state is a ground state. The more interesting case, however, is for $t > 0$, where a degeneracy exists in the maximal-spin sector. Here we are confronted with the lowest eigenvalue $\lambda_{\text{min}}$ of $A$ and it very well could depend on the size of $A$; all the sectors of $S^2$ have to be examined. Table 1 shows a few examples of periodic two-dimensional lattices where a degeneracy occurs, along with the lowest eigenvalues from numerical diagonalizations for two spin sectors $S = S_{\text{max}}$ and $S_{\text{max}} - 1$, and the Nagaoka state fails to be a ground state. It can be shown from a variational construction that degeneracy disfavors high-spin states. We give a simple proof based on a spin-wave state that the Nagaoka state is not a ground state, as a direct consequence of a degeneracy. Our variational state has simple structure, and is similar to Roth-type wavefunctions investigated earlier. The strategy is to look at two sectors with $S^2 = S_{\text{max}}$ and $S^2 = S_{\text{max}} - 1$, and show that $\lambda_{\text{min}}(S_{\text{max}} - 1) < \lambda_{\text{min}}(S_{\text{max}})$, which implies that a state with total spin $S = S_{\text{max}} - 1$ has lower energy than the energy of Nagaoka state.

We focus on a one-dimensional closed chain with an odd-number of sites, and all the arguments used below can be trivially extended to higher-dimensional systems. In the sector with $S^2 = S_{\text{max}}$ we have only one species of electrons, which makes the system a spinless fermion problem. The term with the coulomb interaction $U = \infty$ in Eq. (1) does not come into play at all, and all the many-particle eigenfunctions are constructed as direct products of the single-fermion states. The translational invariance of the lattice helps us in diagonalizing the Hamiltonian in momentum $k$ space. The energy spectrum (the many-electron spectrum or the one-hole spectrum) is given by $\varepsilon_k = 2t \cos k$, where $k = 2\pi n/N$ and $n$ an integer. For $t > 0$ (and setting $t = 1$ from now onwards), the lowest energy of the spectrum is for $k = -\pi \pm \pi/N$ with a two-fold degeneracy (and the two degenerate states have a net momentum), and the highest energy is for $k = 0$ which is non-degenerate. Similarly for a square lattice with $N_1 \times N_2$ sites and $N_1$ odd and $N_2$ even, the lowest-energy state is two-fold degenerate. In this sector all the states carry a total spin of $S = S_{\text{max}}$, and hence this is an orbital degeneracy. Let us denote the two degenerate lowest-energy states in this sector as

$$\phi_1 = \sum a_i |i>; \phi_2 = \sum b_i |i>.$$  \hspace{1cm} (4)

We have $H|\phi_{1,2} > = E_M|\phi_{1,2} >$, where the energy is $E_M = -2 \cos \pi/N$, and the following conditions on the eigenfunctions from normalization and orthogonality

$$\sum a_i^* a_i = \sum b_i^* b_i = 1; \sum a_i^* b_i = 0;$$  \hspace{1cm} (5)

and further since the two states are eigenstates of the Hamiltonian, we have

$$\sum a_i^* a_j = \sum b_i^* b_j = E_M; \sum a_i^* b_j = 0.$$  \hspace{1cm} (6)

More importantly the two degenerate eigenfunctions are related by a phase

$$a_j = b_j e^{iq_o \phi_j}$$  \hspace{1cm} (7)

where $q_o = 2\pi/N$. As we shall see later this fact will be very crucial and useful.

We now turn to the sector with $S^2 = S_{\text{max}} - 1$, where an eigenstate of the Hamiltonian will either carry a total spin $S = S_{\text{max}}$ or $S = S_{\text{max}} - 1$, as no other spin is possible. To diagonalize the Hamiltonian in this sector is a
nontrivial problem as we have one down spin this time. However, we may not be impeded by that. The normalized eigenstates with \( S = S_{\text{max}} \) are easy to construct as the Hamiltonian commutes with the total spin, so a lowering of the \( z \)-component of the states we constructed above gives us the eigenstates we desire here. The two maximal-spin lowest-energy degenerate states are \( S^z \phi_{1,2} \), with an energy \( E_M \). The eigenstates with \( S = S_{\text{max}} - 1 \) are not easy to construct. We resort to a variational method. Let us construct a general variational spin-wave state

\[
\phi_a(q) = \frac{1}{\sqrt{N-1}} \sum_i \sum_{k \neq i} a_k e^{iqr_k} |ik >
\]

(8)

where the basis state \( |ik > \) has a hole at the site \( i \) and a down spin at \( k \), as discussed earlier. It is clear, from Eq.(5), that the above state is normalized. For \( q = 0 \) the state is an eigenstate of the Hamiltonian with maximal spin. For \( q \neq 0 \), the state does not have a definite spin, the expectation value of the spin is less than \( S_{\text{max}} \), as it has a component from both \( S_{\text{max}} \) and \( S_{\text{max}} - 1 \) spin sectors. If \( q \neq \frac{2\pi n}{N} \), with an integer \( n \), the above is an incommensurate spin-wave state. It is straightforward to evaluate the variational energy of this state using Eqs. (3) and (6), and we get

\[
E_a(q) = <\phi_a(q)|H|\phi_a(q)> = E_M + \frac{A(q) - E_M}{N-1}
\]

(9)

where the fourier-transform function

\[
A(q) = \sum_{<ij>} a_i^* a_j e^{iq(r_i-r_j)}.
\]

(10)

It is easy to show that \( A(q) \geq E_M \), by using a variational principle on a state \( \phi = \sum a_i \exp(iqr_i)|i> \) in the \( S^z = S_{\text{max}} \) sector, where \( \phi_1 \) (see Eq.(4)) is a ground state. This implies \( E_M \leq E_a(q) \). The equality holds at two points \( q = 0 \) and \( q = q_o \), as we will see below. From a similar construction of a spin-wave state \( \phi_b(q) \), using \( b_i \) instead of \( a_i \) in Eq.(8), we get the variational energy \( E_b(q) = E_M + [B(q) - E_M]/N-1 \), where

\[
B(q) = \sum_{<ij>} b_i^* b_j e^{iq(r_i-r_j)}.
\]

(11)

The two fourier-transform functions are related as the two degenerate states are related by a phase (see Eq.(7)); we have

\[
A(q) = B(q - q_o).
\]

(12)

The above equation, along with Eqs.(6), (10) and (11), implies \( A(q_o) = B(0) = E_M = A(0) = B(-q_o) \). We have now two different spin-wave states constructed from the two degenerate lowest-energy states with \( S = S_{\text{max}} \). Though both these states have energies higher than \( E_M \), we can now superpose these states to hope for a lowering in energy, as their overlap could be nonzero and useful. A precaution, that we have to take, is that the variational state should not become a spin eigenstate with \( S = S_{\text{max}} \). Let us try a variational state

\[
\psi = \frac{1}{2}(\phi_a(q) - \phi_b(q'))
\]

(13)

with a choice, from hindsight, \( q' = q - q_o \). Though we are restricting the variational parameter space, we shall see below that we still have enough freedom to minimize the variational energy below \( E_M \).

The above variational state has a norm \( <\psi|\psi> = N/N - 1 \), and the overlap between the two components of the state for the choice \( q' = q - q_o \) is \(<\phi_b(q')|H|\phi_a(q)>) = B(q) - B(q_o) - E_M/N - 1 \), where we have used Eqs. (3), (7) and (11). The variational energy \( E_\psi =<\psi|H|\psi>/<\psi|\psi> \) is, using the expressions for \( E_a(q) \), and \( E_b(q') \) from Eq. (9),

\[
E_\psi = E_M + \frac{1}{2N}(B(q + q_o) + B(q - q_o) - 2B(q))
\]

(14)

where we used Eq.(12) to write all the fourier-transform functions in terms of \( B(q) \). Now we seek values of \( q \) such that \( \gamma(q) \equiv B(q + q_o) + B(q - q_o) - 2B(q) \) is negative, which implies \( E_\psi < E_M \). We note that the function \( B(q) \) is periodic (with period \( 2\pi \)), and is non-constant, \( B(0) = B(-q_o) = E_M < 0 \), and \( B(\pi) = -E_M \). Then it is guaranteed that \( \gamma(q) < 0 \), for some value of \( q \), as the function \( B(q) \) necessarily has a local maximum. The expression for \( \gamma(q) \)
can be substantially simplified using Eq. (11) as \( \gamma(q) = -2(1 - \cos q_{\theta}) B(q) \). Now any value of \( q \) for \( B(q) > 0 \) would suffice to give us the desired result \( \gamma(q) < 0 \). For \( q = \pi \), we have \( \gamma(\pi) = -4(1 - \cos q_{\theta}) \cos (\pi/N) \), and

\[
E_\psi = E_M + \frac{2N}{N}(1 - \cos q_{\theta}) \cos \frac{\pi}{N} < E_M. \tag{15}
\]

This completes the proof that the variational state in Eq.(13), with \( q = \pi, q' = \pi - q_{\theta} \), has lower energy than that of the Nagaoka (\( S = S_{\text{max}} \)) state. The fact that we have two degenerate lowest-energy states with maximal spin is very crucial. The above arguments can be readily extended for more than one dimension. The structure of the proof does not change for higher-dimensional systems. For instance consider a two-dimensional lattice with periodic boundary conditions, with \( N = N_1 \times N_2 \) sites. And let \( N_1 \) be an even number and \( N_2 \) odd. The energy spectrum for the hole in \( S^z = S_{\text{max}} \) sector is \( \varepsilon(k_1, k_2) = 2(\cos k_1 + \cos k_2) \), with \( k_i = 2\pi n_i/N_i \). The lowest energy is for \( k_1 = \pi, k_2 = \pi \pm \pi/N \), with \( E_M = -2(1 + \cos(\pi/N)) \), with a two-fold degenerate. The various quantities \( q, q_{\theta}, \{r_i\} \) now become two-dimensional vectors. The phase between the two degenerate eigenstates is, in Eq.(7), is \( \mathbf{q}_0 = (0, 2\pi/N_2) \) and we choose \( \mathbf{q} = (0, \pi) \) in Eq. (14), to get the desired result \( E_\psi < E_M \). In a general case of a hypercubic lattice with \( N = N_1 \times N_2 \times N_3 \ldots \) sites, and with at least one of \( N_i \) is an odd number, we get a two-fold degenerate maximal-spin state for \( t > 0 \), where the Nagaoka state is not a ground state. We expect that a similar proof can be constructed for any lattice with exactly one hole, when a degeneracy exists. We would like to briefly comment on the nature of the actual ground state, if degeneracy exists. We expect similar arguments can be constructed to show that the lower the spin the better is the ground state energy, and most probably the ground state has the lowest possible spin. A heuristic argument can be given to understand the trend of minimal-spin ground state when degeneracy exists. In the non-degenerate case, the ground state eigenfunction is positive definite (i.e. a basis can be chosen such that the probability amplitudes of all the basis states in the ground state are positive), which is the key point of the Nagaoka state. If we have a degeneracy, the orthogonal states cannot be both positive definite, and at least one of them have negative probability amplitudes. A lowering of the spin introduces, by itself, negative signs. For instance, any state with \( S = S^z = S_{\text{max}} - 1 \) is of the form \( |S = S^z = S_{\text{max}} - 1 > = \sum \chi_{ik} |ik > \). It is necessarily accompanied by the constraints (as \( S^z|S = S^z = S_{\text{max}} - 1 = 0 \)) \( \sum \chi_{ik} = 0 \) for a fixed \( i \). This implies that the amplitudes come with both signs to satisfy the constraint equations. Now it may be expected that these negative signs, and the negative signs as a consequence of degeneracy may conspire to cancel out making the eigenfunction as much 'positive definite' as possible, and translate into a kinetic energy lowering. And by lowering the spin further, one lowers the energy further. Hence an expected minimal spin ground state.

We discuss the case when the number of holes \( N_H \) is more than one. It is easy to check if the maximal-spin sector has a degeneracy in the lowest many-hole energy state, as all we need to solve is a spinless fermion problem. We have the following interesting and simple examples where degeneracy occurs. (a) Consider the case of a bipartite lattice where for \( N_H = 1 \) we have no degeneracy and a Nagaoka ground state. For a closed chain with an even number of sites, the one-hole energy spectrum in \( S^z = S_{\text{max}} \) sector is \( \varepsilon(k) = -2|t| \cos k \). When we have two holes, the ground state in this sector is a direct product of single-hole \( k \)-space eigenstates (not true for hard-core bosons) with \( k_1 = 0, k_2 = \pm \pi/N \), which is two-fold degenerate. The same holds for \( N_H \) even and less than \( N - 1 \). And similarly for an \( N_1 \times N_2 \) lattice, for many values of \( N_H \) the lowest-energy state in the maximal-spin sector is degenerate. In the particular case of quarter filling \( N_e = N_H = N/4 \), for any \( N \), there is a degeneracy. (b) Consider the case of a non-bipartite lattice, with degeneracy for \( N_H = 1 \) (which implies Nagaoka is not a ground state from the proof outlined above). For example a closed chain with an odd number of sites has a degeneracy in the lowest-energy state of the maximal-spin sector when \( N_H \) is odd and less than \( N - 1 \). Similarly for higher-dimensional systems we encounter degeneracy for many values of \( N_H \). (c) Consider the case of a long-range hopping model, where the constraint of nearest-neighbour-only hopping that we have in Eq.(1) is relaxed, which exhibits macroscopic degeneracy. It is easy to diagonalize the maximal-spin sector, and the one-hole spectrum has only two energy levels, with energies \( -t(N - 1) \) (non-degenerate), and \( -t \) (degeneracy \( N - 1 \)). For \( t > 0 \), the lowest-energy many-hole state for \( N_H < N - 1 \) is degenerate. For \( t < 0 \), there is degeneracy for \( 1 < N_H < N - 1 \). The singular case of \( N_H = N - 1 \) also has a degenerate lowest-energy state, but there is only one spin sector \( S = 1/2 \).

In all the examples we considered above there is a degeneracy in the lowest-energy state of maximal-spin sector. We expect that the Nagaoka state is not a ground state in these cases. It would be interesting to see if one can generalize our simple proof for the above examples \( \mathbb{Q} \). Particularly, it should be investigated whether the ingredients that we used for \( N_H = 1, \) viz. the translational invariance, which is important to diagonalize the Hamiltonian in \( S^z = S_{\text{max}} \) sector and get a handle on the degenerate states (Eq.(7)), and the choice of a basis states such that all the overlaps have a single sign (Eq.(3)), are essential. Currently an investigation is under progress to extend our procedure in a more general context, viz. for non-cubic lattices with more than one hole.

In conclusion, we have seen that there is a general trend in the nature of the ground state. For \( N_H = 1 \), when the maximal-spin sector has a non-degenerate lowest-energy state, the ground state is a maximal-spin Nagaoka state.
and a degeneracy disfavors higher-spin states and a minimal-spin ground state is expected. An explicit proof, based on a variational construction of a spin-wave state, is given to exhibit that the Nagaoka state is not a ground state if degeneracy exists on hypercubic lattices, with an odd number of sites in at least one direction.

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Table 1 The lowest eigenvalue $E(S)$ for two spin sectors $S = S_{max}, S_{max} - 1$ for various sizes for $t = 1$.

| $N_1, N_2$ | Degeneracy in $S_{max}$ Sector | $E(S_{max})$ | $E(S_{max} - 1)$ |
|------------|-------------------------------|-------------|-----------------|
| 3,3        | 4                             | -2.0        | -2.732          |
| 3,4        | 2                             | -3.0        | -3.342          |
| 3,5        | 4                             | -2.618      | -3.115          |
| 4,4        | 1                             | -4.0        | -3.924          |
| 3,6        | 2                             | -3.0        | -3.278          |
| 4,5        | 2                             | -3.618      | -3.713          |