A Dynamical Supersymmetry in the Hubbard Model

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(Received 7 February 1997)

The Hubbard model, in the limit of infinite on-site repulsion and with hopping of unlimited range between all sites, is shown to be exactly and analytically soluble in terms of a dynamical spl(2, 1) supersymmetry. The complete spectrum is given. [S0031-9007(97)03223-7]

PACS numbers: 71.10.Fd, 02.20.Sv

The Hubbard model has proved to be a fertile framework for the study of the behavior of strongly interacting electrons [1,2]. The one-dimensional model has been solved exactly and completely by means of the Bethe ansatz together with an underlying SO(4) symmetry [3,4]. It has also been suggested that the superalgebra spl(2, 1) could be useful [5–7] in systematizing the study of the model in the limit of infinite on-site repulsion, which will be referred to as the Nagaoka limit. It is shown here that there is a special form of the model which admits an exact analytic solution by virtue of a dynamical supersymmetry of type spl(2, 1).

The usual form of the Hubbard Hamiltonian is

$$H = -t \sum_{\langle i,j\rangle,\sigma} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} \hat{n}_{i\uparrow}\hat{n}_{i\downarrow} ,$$

where the sum in the single-particle (hopping) term is over all nearest-neighbor pairs of sites and both spin projections, while the sum in the two-body term is over all sites. The hopping term involves electron creation and destruction operators at specific sites, while the interaction term involves electron number operators at each site. In most studies, the signs of the coefficients t and U are positive, representing an attractive hopping effect and a repulsive on-site interaction. The Hamiltonian is a spin scalar, so its eigenstates will have well-defined total spin. The form of the model to be investigated here has an infinitely repulsive on-site interaction, which effectively forbids double occupancy of any site. (Of course, the Pauli principle forbids two spin-up or two spin-down electrons at a single site, but it permits one spin-up and one spin-down electron at a given site, a spin-zero pair. This is ruled out by the infinite on-site repulsion.) In addition, the restriction on the summation in the hopping term is relaxed, so that all pairs of distinct sites are included. This infinite-range hopping is what admits the dynamical supersymmetry.

The special form of the Hubbard model which displays the dynamical supersymmetry is then defined by the Hamiltonian

$$H = -\sum_{i\neq j,\sigma} c^{\dagger}_{i\sigma} c_{j\sigma} = -\sum_{i,j,\sigma} c^{\dagger}_{i\sigma} c_{j\sigma} + \hat{n} ,$$

together with a prohibition on the double occupancy of any site. Here $\hat{n} = \sum_{i,\sigma} \hat{n}_{i\sigma}$ is the total number operator for electrons. The value of t has been chosen equal to unity, since it simply sets the energy scale. It should be noted that, in this form, the model is completely independent of the details of the "lattice," which could be in any number of dimensions and of any lattice type, including totally random or disordered. All that is required is a denumerable set of sites. The number of sites will be denoted by N. The Hamiltonian is still a spin scalar.

The constraint prohibiting double occupancy of a site can be implemented by introducing at each site the set of states $|i0\rangle, |i\uparrow\rangle, |i\downarrow\rangle$, where the first index labels the site and the second indicates a vacancy or a spin-up or spin-down electron at the site. There are nine Hubbard operators of the form $X^{(i)}_{ab} = |ia\rangle\langle ib|$ at each site, but the "no double occupancy" constraint can be expressed by the completeness condition

$$X^{(i)}_{00} + X^{(i)}_{\uparrow\uparrow} + X^{(i)}_{\downarrow\downarrow} = 1 ,$$

reducing the number of independent Hubbard operators at each site to eight. These operators satisfy the self-evident multiplication rule

$$X^{(i)}_{ab} X^{(j)}_{cd} = \delta_{ij}\delta_{bc} X^{(i)}_{ad} ,$$

from which can be deduced the commutators and anticommutators

$$[X^{(i)}_{ab}, X^{(i)}_{cd}]_{\pm} = \delta_{ij}(\delta_{bc} X^{(i)}_{ad} \pm \delta_{ad} X^{(i)}_{cb}) .$$

In terms of these operators, the infinite-range hopping Hubbard model with infinite on-site repulsion can be transcribed as

$$H = -\sum_{i,j,\sigma} X^{(i)}_{\sigma 0} X^{(j)}_{0\sigma} + \hat{n} .$$

By a suitable selection of the commutators and anticommutators, the eight independent Hubbard operators at each site can be chosen to be the infinitesimal generators of the algebra su(3) or of the graded algebra spl(2, 1) [7]. The former would be appropriate for the description of a boson model. For the present model, involving electrons, the appropriate choice is the graded algebra. The vacancy is a bosonic state; the spin-up and spin-down electron states are fermionic states. The even sector of the graded algebra is defined by the operators

$$S_+^{(i)} = X_{\uparrow\downarrow}^{(i)}, \qquad S_-^{(i)} = X_{\downarrow\uparrow}^{(i)} = S_+^{(i)\dagger},$$
$$S_0^{(i)} = (X_{\uparrow\uparrow}^{(i)} - X_{\downarrow\downarrow}^{(i)})/2,$$
$$\hat{n}_i = X_{\uparrow\uparrow}^{(i)} + X_{\downarrow\downarrow}^{(i)},$$

which generate su(2) $\times$ u(1). Their commutators are

$$[S_0^{(i)}, S_\pm^{(i)}] = \pm S_\pm^{(i)}, [S_+^{(i)}, S_-^{(i)}] = 2S_0^{(i)}, [\hat{n}_i, S_\alpha^{(i)}] = 0.$$

The su(2) algebra is just the electron spin. The odd sector includes the remaining independent Hubbard operators $X_{\uparrow 0}^{(i)}$, $X_{\downarrow 0}^{(i)}$, $X_{0\uparrow}^{(i)}$, and $X_{0\downarrow}^{(i)}$, whose anticommutators are

$$\{X_{\uparrow 0}^{(i)}, X_{0\uparrow}^{(i)}\} = 1 - \hat{n}_i/2 + S_0^{(i)}, \quad \{X_{\uparrow 0}^{(i)}, X_{0\downarrow}^{(i)}\} = S_+^{(i)},$$
$$\{X_{\downarrow 0}^{(i)}, X_{0\uparrow}^{(i)}\} = S_-^{(i)}, \quad \{X_{\downarrow 0}^{(i)}, X_{0,\downarrow}^{(i)}\} = 1 - \hat{n}_i/2 - S_0^{(i)}.$$

All other anticommutators between odd-sector operators vanish.

It is clearly more convenient to replace the operator $\hat{n}_i$ by the operator

$$\hat{Y}_i = 1 - \hat{n}_i/2,$$

which also commutes with all three spin operators. The commutators between operators in the even and odd sectors are then

$$[S_0^{(i)}, X_{\uparrow 0}^{(i)}] = X_{\uparrow 0}^{(i)}/2, \qquad [S_0^{(i)}, X_{\downarrow 0}^{(i)}] = -X_{\downarrow 0}^{(i)}/2,$$
$$[S_0^{(i)}, X_{0\uparrow}^{(i)}] = -X_{0\uparrow}^{(i)}/2, \qquad [S_0^{(i)}, X_{0\downarrow}^{(i)}] = X_{0\downarrow}^{(i)}/2,$$
$$[S_+^{(i)}, X_{\downarrow 0}^{(i)}] = X_{\uparrow 0}^{(i)}, \qquad [S_-^{(i)}, X_{\uparrow 0}^{(i)}] = X_{\downarrow 0}^{(i)},$$
$$[S_+^{(i)}, X_{0\uparrow}^{(i)}] = -X_{0\downarrow}^{(i)}, \qquad [S_-^{(i)}, X_{0\downarrow}^{(i)}] = -X_{0\uparrow}^{(i)},$$
$$[\hat{Y}_i, X_{\uparrow 0}^{(i)}] = -X_{\uparrow 0}^{(i)}/2, \qquad [\hat{Y}_i, X_{\downarrow 0}^{(i)}] = -X_{\downarrow 0}^{(i)}/2,$$
$$[\hat{Y}_i, X_{0\uparrow}^{(i)}] = X_{0\uparrow}^{(i)}/2, \qquad [\hat{Y}_i, X_{0\downarrow}^{(i)}] = X_{0\downarrow}^{(i)}/2,$$

with the remaining commutators between odd and even operators vanishing. From these it is evident that ($X_{\uparrow 0}^{(i)}$, $X_{\downarrow 0}^{(i)}$) constitutes a spin doublet with $Y = -1/2$ and ($X_{0\downarrow}^{(i)}$, $-X_{0\uparrow}^{(i)}$) constitutes a spin doublet with $Y = 1/2$.

The complete set of commutators and anticommutators at a particular site defines the graded Lie algebra spl(2, 1) [8]. This set can be generalized to pairs of sites by replacing the identical site indices in each commutator or anticommutator bracket by two different indices and including on the right-hand side of each relation a Kronecker delta between the two site indices. It is then possible to define a total or resultant spl(2, 1) in terms of the operators

$$S_\pm = \sum_i S_\pm^{(i)}, \qquad S_0 = \sum_i S_0^{(i)},$$
$$\hat{Y} = \sum_i \hat{Y}_i = N - \hat{n}_i/2, \qquad X_{\sigma 0} = \sum_i X_{\sigma 0}^{(i)},$$
$$X_{0\sigma} = \sum_i X_{0\sigma}^{(i)},$$

which satisfy the same set of (anti) commutation relations as the single-site operators.

The irreducible representations (irreps) of spl(2, 1) [8] are identified by a pair of indices, denoted $[Y, S]$, where Y, the eigenvalue of $\hat{Y}$, can in general be any complex number and S, the spin quantum number, can be a positive integer or half a positive odd integer, as usual. The irrep $[Y, S]$ contains at most four su(2) $\times$ u(1) multiplets of the form (S', Y'), namely, (S, Y), $(S - 1/2, Y + 1/2)$, $(S - 1/2, Y - 1/2)$, and $(S - 1, Y)$. The special cases in which an irrep contains less than four multiplets are $[S, S]$, which contains only the first two multiplets listed, and $[Y, 1/2]$, which contains only the first three multiplets listed. The dimension of the irrep $[Y, S]$ is thus $8S$ in general, and $4S + 1$ for the special cases. There are Casimir operators of orders two and three, of which only the former is of interest in the present application. This Casimir operator is

$$\hat{C}_2 = \vec{S}^2 - \hat{Y}^2 - (X_{\uparrow 0}X_{0\uparrow} + X_{\downarrow 0}X_{0\downarrow} - X_{0\uparrow}X_{\uparrow 0} - X_{0\downarrow}X_{\downarrow 0})/2$$

and has the eigenvalue $S^2 - Y^2$ in the irrep $[Y, S]$.

The Hamiltonian of interest here can be rewritten in terms of the operators of the total spl(2, 1) superalgebra,

$$H = -(X_{\uparrow 0}X_{0\uparrow} + X_{\downarrow 0}X_{0\downarrow}) + 2(N - \hat{Y}),$$

where N, it will be recalled, is the total number of sites. Using the anticommutators of the algebra and the definition of the Casimir operator, this can be brought to the form

$$H = \hat{C}_2 - \vec{S}^2 + \hat{Y}(\hat{Y} - 3) + 2N,$$

involving only the Casimir operators of the superalgebra and of the even-sector algebra. Its eigenvalues are thus immediately known once the relevant irreps are specified. When a Hamiltonian can be written as a linear combination of Casimir operators of a chain of algebras, there is said to be a dynamical symmetry. In this sense, the special limit of the Hubbard model here studied exhibits a dynamical supersymmetry.

To complete the explicit solution of the model, it is necessary to identify the relevant irreps of the spl(2, 1) superalgebra. In general, this algebra is not completely reducible; there exist reducible representations which cannot be broken down entirely into irreps [8]. However, the irreps of relevance to the Hubbard model turn out not to have this pathology. As a first step, it is helpful to identify the basic irrep which contains the fundamental single-site states. The three states $|i0\rangle$, $|i\uparrow\rangle$, and $|i\downarrow\rangle$, when acted upon by the generators of the superalgebra, are found to span the irrep $[1/2, 1/2]$, as follows:

$$S_0|i\uparrow\rangle = 1/2|i\uparrow\rangle, \quad S_+|i\uparrow\rangle = 0, \quad S_-|i\uparrow\rangle = |i\downarrow\rangle,$$
$$\hat{Y}|i\uparrow\rangle = 1/2|i\uparrow\rangle, \quad S_0|i\downarrow\rangle = -1/2|i\downarrow\rangle,$$
$$S_+|i\downarrow\rangle = |i\uparrow\rangle, \quad S_-|i\downarrow\rangle = 0, \quad \hat{Y}|i\downarrow\rangle = 1/2|i\downarrow\rangle,$$
$$S_0|i0\rangle = 0, \quad S_+|i0\rangle = 0, \quad S_-|i0\rangle = 0,$$
$$\hat{Y}|i0\rangle = 0, \quad X_{\sigma 0}|i\sigma'\rangle = 0, \quad X_{\sigma 0}|i0\rangle = |i\sigma\rangle,$$
$$X_{0\sigma}|i\sigma'\rangle = \delta_{\sigma\sigma'}|i0\rangle, \quad X_{0\sigma}|i0\rangle = 0.$$

The multiparticle states of the model thus all belong to $[1/2, 1/2]^N$. It is clear that n, the number of electrons, satisfies $0 \leq n \leq N$, since double occupancy of any site is excluded, so that $N/2 \leq Y \leq N$ and Y, like S, is either an integer or half an odd integer, in this specific application. Since S is the total spin of n spin-$1/2$ particles, it will be an integer for even n and half an odd integer for odd n. Since N is always an integer, Y will be an integer for even n and half an odd integer for odd n. So the sum of S and Y is an integer in any state.

Determination of the irreps included in $[1/2, 1/2]^N$ is facilitated by the branching rule

$$[Y, S] \otimes [1/2, 1/2] = [Y + 1/2, S + 1/2] \oplus [Y + 1, S] \oplus [Y + 1/2, S - 1/2],$$

where the third irrep on the right hand side is omitted if $Y = S$ or $S = 1/2$. This rule is easily established by combining the appropriate su(2) $\times$ u(1) multiplets in the two irreps being multiplied. It may be used to build up the irreps relevant to the N-site model, starting from $N = 1$ and increasing N by unity at each step by multiplying by the basic irrep. In this way it is found that, for given N, irreps occur for each value of Y from its minimum value $N/2$ to a maximum value $N - 1/2$, in steps of $1/2$. For each value of Y, irreps occur for each value of S from its maximum value $N - Y$ to a minimum value $1/2$ or 1 (depending on whether n is odd or even), in unit steps. A given irrep $[Y, S]$ may occur more than once in the decomposition. The multiplicity of each irrep needs to be determined.

For a given S and Y, the multiplet (S, Y) can occur in the irreps $[Y, S]$, $[Y - 1/2, S + 1/2]$, $[Y + 1/2, S + 1/2]$, and $[Y, S + 1]$. (Note that for certain extreme values of Y and S not all of these four irreps will in fact exist.) From the expression for the Hamiltonian in terms of the Casimir operators of spl(2, 1) and su(2) $\times$ u(1), the eigenvalue of the multiplet in each of these irreps can be written down immediately, and is $2N - 3Y - S$, $2(N - Y)$, $2(2Y - N)$, and $2N - 3Y + S + 1$, respectively. In terms of the number of electrons n, these are $-N + 3n/2 - S$, n, $-2(N - n)$, and $-N + 3n/2 + S + 1$, respectively.

A multiplet of the form (S, Y) has $n = 2(N - Y)$ electrons of total spin S. Since there are N sites available, with at most one electron at each site, an n-electron state of spin projection $M = (n_\uparrow - n_\downarrow)/2$, using a self-explanatory notation for the numbers of spin-up and spin-down electrons, can be made by distributing the electrons among the sites in $\nu(n, M) = \binom{N}{n_\uparrow}\binom{N-n_\uparrow}{n_\downarrow} = \binom{N}{n/2+M}\binom{N-n/2-M}{n/2-M}$ ways. So an n-electron state of spin S can be made in $\nu(n, S) - \nu(n, S + 1) = (2S + 1)N!/(N - n)!\,(n/2 + S + 1)!\,(n/2 - S)!$ ways. Restated in terms of Y and S, the model contains $(2S + 1)N!/(2Y - N)!\,(N - Y + S + 1)!\,(N - Y - S)!$ multiplets (S, Y), distributed among the various irreps of spl(2, 1).

The multiplet $(0, N)$, with $n = 0$ and $S = 0$, occurs exactly once, and belongs only to the irrep $[N - 1/2, 1/2]$. This irrep therefore has multiplicity one. It contains, in addition to the multiplet $(0, N)$, the multiplets $(1/2, N - 1/2)$ and $(0, N - 1)$. The former multiplet, with $n = 1$ and $S = 1/2$, occurs N times, so $N - 1$ of its occurrences must be in other irreps. It could belong to the irreps $[N - 1/2, 1/2]$ or $[N - 1, 1]$. So the irrep $[N - 1, 1]$ must have multiplicity $N - 1$. Similar arguments can be used to determine the multiplicities of other irreps, leading to a general formula for the multiplicity of the irrep $[Y, S]$ in the decomposition of $[1/2, 1/2]^N$, which can be established by mathematical induction. The multiplicity is $N!\,2S/(2Y - N - 1)!\,(N - Y + S)!\,(N - Y - S)!\,(Y^2 - S^2)$, except for the case $Y = S$, which occurs only in the exceptional irrep $[N/2, N/2]$ of multiplicity one.

Collecting together the above results, it is possible to write down the complete spectrum of the Hubbard model in the Nagaoka limit with infinite-range hopping. For n electrons on N sites, the ground state is highly degenerate. It occurs at energy $-2(N - n)$ (in units of the hopping strength t) and accommodates all spins from $n/2 - 1$ down to 0 or $1/2$ (for n even or odd, respectively), the multiplicity of the state of spin S being $N!\,(2S + 1)/(N - n)!\,(n/2 + S)!\,(n/2 - S - 1)!\,[(N - n/2)\,(N - n/2 + 1) - S(S + 1)]$. The ground state does not include the maximum spin $S = n/2$, so it cannot be ferromagnetic.

Next, in order of increasing energy, is a band of states at energies $-(N - 3n/2 + S)$, including states of spin from $n/2$ down to 1 or $1/2$ (for n even or odd, respectively), the multiplicity of the state of spin S being $N!\,2S/(N - n - 1)!\,(n/2 + S)!\,(n/2 - S)!\,[(N - n/2)^2 - S^2]$. The ferromagnetic state, $S = n/2$, occurs at precisely half the ground-state energy. This band does not include a state of spin $S = 0$, but all other spins occur. It is followed, at yet higher energy, by another band of states at energies $-(N - 3n/2 - S - 1)$, including states of spin from $n/2 - 1$ down to 0 or $1/2$ (for n even or odd, respectively), the multiplicity of the state of spin S being $N!\,2(S + 1)/(N - n - 1)!\,(n/2 + S + 1)!\,(n/2 - S - 1)!\,[(N - n/2)^2 - (S + 1)^2]$. This band does contain a state of spin $S = 0$, but not a ferromagnetic state of spin $S = n/2$.

Finally, the state of highest energy is again highly degenerate. It occurs at energy n and accommodates spins from $n/2$ down to 0 or $1/2$ (for n even or odd, respectively), the multiplicity of the state of spin S being $N!\,(2S + 1)/(N - n - 2)!\,(n/2 + S + 1)!\,(n/2 - S)! \times [(N - n/2)\,(N - n/2 - 1) - S(S + 1)]$.

All the above results hold for $n = 0$ to $n = N - 2$. For $n = N - 1$, the results are the same for the ground state and the two bands above it, but the state at energy n is a single state of spin $n/2$. Finally, for $n = N$, when all sites are occupied by electrons and there can be no hopping, all states occur at zero energy, there are states of all spins from $N/2$ down to 0 or $1/2$

(for N even or odd, respectively) and the state of spin S has multiplicity $N!\,(2S + 1)/(N/2 + S)!\,(N/2 - S - 1)!\,[N/2(N/2 + 1) - S(S + 1)]$, except for the state of spin $N/2$, which occurs only once.

For negative t, the spectrum described above would simply be inverted. The ground state would then also accommodate ferromagnetism.

In the thermodynamic limit, $N \to \infty$, the quantity of interest is the energy per site, expressed in terms of the fraction $f = n/N$ of occupied sites. Note that f takes values between zero and one. For $f = 1$, all states are degenerate at energy per site zero. For general f, the ground state has energy per site $-2(1 - f)$ and the spin structure previously described. It is followed by a band of states at energies per site from $-(1 - f)\,(S = n/2)$ to $-(1 - 3f/2)$ $(S = 1/2$ or $1)$, then by a band of states at energies per site of $-(1 - 3f/2)$ $(S = 0$ or $1/2)$ to $-(1 - 2f)\,(S = n/2 - 1)$. These two bands are separated by a gap in energy per site of $2/N$, twice the spacing between different spin states in each of the two bands. Finally, there is a state at energy per site f, with the spin structure previously given.

To summarize, it has been demonstrated that the Hubbard model, in the Nagaoka limit of infinite on-site repulsion and with infinite-range hopping between all sites, exhibits a dynamical supersymmetry of type spl$(2, 1)$ which admits an exact, analytic solution. The spectrum has been given, with its spin structure and multiplicity, and holds for any form of lattice at all (or even no lattice) and in any number of dimensions, provided the number of sites is denumerable. For attractive hopping, the ground state has no ferromagnetic component, though the highest state does. For repulsive hopping, the spectrum is inverted. This very unusual form of the model takes its place as one of the small class of exactly soluble strongly interacting many-fermion models.

The author is deeply indebted to Eytan Domany, who conceived of the special limit of the Hubbard model here discussed and brought it to the author's attention; to Ofer Megged, whose numerical results suggested an algebraic structure and served as empirical verification of the analytical results derived above; and to Baha Balantekin, whose description of the use of spl$(2, 1)$ in connection with the Hubbard model triggered the above approach and who supplied a key reference. Support from the Joseph and Bessie Feinberg Foundation is gratefully acknowledged.

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