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SUPERALGEBRAIC SOLUTION TO THE MEAN-FIELD HUBBARD MODEL

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ABSTRACT

We show that a mean-field Hubbard hamiltonian possesses a dynamical superalgebra $u(1|1) \oplus u(1|1)$, enabling diagonalization to be achieved and the obtention of a nonvanishing magnetic order parameter.

A classic lattice problem, recently revived as a possible paradigm for high T_c superconductors, is the Hubbard model [1]. We shall consider the following Hubbard hamiltonian (in any number of dimensions)

$$H^{Hub} = \Sigma \varepsilon n_{i\sigma} + \Sigma u \; n_{i\uparrow} n_{i\downarrow} + \Sigma \; t_{ij} \; a^+_{i\sigma} \; a_{j\sigma} \tag{1}$$

In the above, the number operator $n_{i\sigma}$ for electrons on the lattice site i with spin σ is defined by

$$n_{i\sigma} = a^+_{i\sigma} \; a_{i\sigma}$$

where the creation (annihilation) operators $a^+_{i\sigma}$ ($a_{i\sigma}$) obey the usual anti-commutation relations for fermions. The sums are taken over site indices i, j - it being assumed that only nearest neighbours contribute to the hopping-term t_{ij} = t - and spin $\sigma \equiv \uparrow$ or $\downarrow$.

The problem is trivially solvable either when $t_{ij} = 0$, so that H^{Hub} is already diagonal in the number operator, or when $u = 0$, for which the hamiltonian becomes $\Sigma\varepsilon_k n_{k\sigma}$ ($\varepsilon_k \equiv \varepsilon + t \cos k$) on taking the momentum representation. However, no exact solution exists for lattice dimension greater than one when both u and t are non-zero.

In this note we make a fermionic mean-field approximation (which we shall define) to H^{Hub} for which the dynamical algebra is a superalgebra, thus enabling a solution of the approximate model to be given involving non-zero parameters ε, u and t.

Consider first the identity for the hopping term:

$$a_i^+ a_j \equiv (a_i^+ - \langle a_i^+\rangle)(a_j - \langle a_j\rangle) + a_i^+ \langle a_j\rangle + \langle a_i^+\rangle a_j - \langle a_i^+\rangle\langle a_j\rangle \quad (2)$$

In (2), we may consider < > to be the expectation in some (thermodynamic) state. Now let us restrict ourselves to states such that the first term on the right-hand side of (2) is "negligible" in some sense. We may then approximate

$$a_i^+ a_j \sim a_i^+ \langle a_j\rangle + \langle a_i^+\rangle a_j - \langle a_i^+\rangle\langle a_j\rangle \quad (3)$$

[In (2) and (3) we have suppressed the spin index.] Note that this expression, in which necessarily $i \neq j$ so that a_i^+ and a_j anti-commute, is only consistent if the objects $\langle a_i\rangle$, $\langle a_i^+\rangle$ anti-commute with each other and with the operators a_i^+, a_j. This may be achieved by defining a basis $\{e_i, e_j^*\}$ $i,j = 1, \ldots N$ for a 2^{2N}-dimensional Clifford algebra

$$\{e_i, e_j\} = \{e_i^*, e_j^*\} = 2\delta_{ij},$$

$$\{e_i, e_j^*\} = 0.$$

Using the fermionic mean field approximation (3) we may approximate the hamiltonian (1) by

$$H^{MF} = \Sigma\varepsilon n_{i\varepsilon} + \Sigma u n_{i\uparrow} n_{i\downarrow} + \Sigma(\theta_{i\sigma} a_{i\sigma} + a_{i\sigma}^+ \theta_{i\sigma}^*) \quad (4)$$

where

$$\theta_{i\sigma} \equiv \Sigma t_{ji}\, e_j^*.$$

Thus we have written H^{Mf} as a direct sum, $H^{Mf} \equiv \Sigma_i H_i$, where H_i is (dropping the suffix i)

$$H = \varepsilon(n_+ + n_-) + u\, n_+ n_- + \theta_+ a_+ + \theta_- a_- + a_+^+ \theta_+^* + a_-^+ \theta_-^*. \qquad (5)$$

The dynamical algebra of this model is generated by the set

$$\{n_+ n_-,\ n_+,\ n_-,\ a_+,\ a_-,\ a_+^+,\ a_-^+\}$$

of elements of H. The algebra is generated under the natural (i.e. physical) commutation and anti-commutation relations; it is the superalgebra u(2|2) of the BCS-Umklapp model previously treated by the authors [2], together with the term $n_+ n_-$ characteristic of the Hubbard model. Assuming ↑↓ symmetry in our model ($\varepsilon_+ = \varepsilon_-$, $\theta_+ = \theta_- = \theta/\sqrt{2}$) we obtain the Hamiltonian $H = \varepsilon N + \mu W + \theta A + A^+ \theta^*$ with smaller dynamical algebra u(1|1) ⊕ u(1|1), closing under the 8 elements

$$\{I,\ A,\ A^+,\ B,\ B^+,\ N,\ W,\ U\}$$

where $A \equiv \frac{1}{\sqrt{2}}(a_+ + a_-)$, $B \equiv \frac{1}{\sqrt{2}}(n_+ a_- + n_- a_+)$, $N = n_+ + n_-$, $W = n_+ n_-$,

and $U = \frac{1}{2}(n_+ + n_- - a_+^+ a_- - a_-^+ a_+)$.

Defining $Z^{(1)} = \lambda A + \mu B + \text{h.c.}$, where λ, μ are anti-commuting elements of the Clifford Algebra, we find that

$$\exp(i\ \text{ad}\ Z^{(1)})(H) = \varepsilon N + \mu W + C\theta\theta^* U + D\theta\theta^*$$

where we have chosen $\lambda = i\theta/\varepsilon \quad \mu = -iu\theta/\varepsilon(u + \varepsilon)$

with $D(\varepsilon, u) = -\varepsilon^{-1}$

and $C(\varepsilon, u) = u/\varepsilon(u + \varepsilon)$.

Although H has thus been expressed in terms of mutually commuting elements (of a Cartan basis), these operators are not diagonal in Fock space. This is easily remedied by application of an outer autmorphison

$Z^{(2)} = \exp(\mathrm{ad}\ \frac{\pi}{4})\ (a_+^+ a_- - a_-^+ a_+)$. The resulting diagonal hamiltonian is

$$H = \varepsilon(n_+ + n_-) + u\, n_+ n_- + C\theta\theta^* n_\pm + D\theta\bar{\theta} I$$

(where the $n_\pm$ spontaneously generated term arises from ambiguity in the rotation $Z^{(2)}$). The coefficient $\theta\theta^*$ of this term plays the role of a magnetic order parameter; it has been evaluated self-consistently [3] and exhibits typical mean-field behaviour. This simple model does not exhibit pairing superconductivity, in that $\langle a_+ a_- \rangle = 0$.

References

[1] Hubbard, J., Proc. Roy. Soc. London Ser. A 227, 237 (1964).

[2] Montorsi, A., Rasetti, M., and Solomon, A. I., Phys Rev. Lett. 59, 2243 (1988).

[3] Montorsi, A., Rasetti, M., and Solomon, A. I., (to be published).