Coherent pairing states for the Hubbard model

1998 J. Phys. A: Math. Gen. 31 L355

(http://iopscience.iop.org/0305-4470/31/18/004)

J. Phys. A: Math. Gen. **31** (1998) L355–L360. Printed in the UK PII: S0305-4470(98)91905-9

LETTER TO THE EDITOR

Coherent pairing states for the Hubbard model

Allan I Solomon†§ and K A Penson‡∥

† Laboratoire de Gravitation et Cosmologie Relativistes, Université Pierre et Marie Curie-CNRS URA 769, Tour 22, 4ème étage, boite 142, 4, place Jussieu, 75252 Paris Cedex 05, France

‡ Laboratoire de Physique Théorique des Liquides, Université Pierre et Marie Curie-CNRS, URA 765, Tour 16, 5-ème étage, Boiî̂te 121, 4, place Jussieu, 75252 Paris Cedex, France

Received 19 February 1998

Abstract. We consider the Hubbard model and its extensions on bipartite lattices. We define a dynamical group based on the η-pairing operators introduced by Yang, and define coherent pairing states, which are combinations of eigenfunctions of η-operators. These states permit exact calculations of numerous physical properties of the system, including energy, various fluctuations and correlation functions, including pairing off-diagonal long-range order to all orders. This approach is complementary to BCS, in that these are superconducting coherent states associated with the exact model, although they are not eigenstates of the Hamiltonian.

1. Introduction

The Hubbard model plays a special role in condensed matter physics. It allows one, within appropriate limits, to model the electronic properties of systems ranging from insulators to superconductors. It is generally believed that high-T_c superconductivity may be described by some form of the Hubbard model. Although the model can only be solved in one dimension, some insight into its properties in general dimensions can be obtained through the so-called η-pairing mechanism introduced by Yang [1]. This mechanism allows one to construct a subset of the exact spectrum of the model. The eigenfunctions obtained through η-pairing possess the property of off-diagonal long-range order (ODLRO) and thus are superconducting. In this letter we introduce a new family of wavefunctions which are combinations of η-pairing eigenfunctions. The η-pairing procedure has been applied to a number of strongly correlated fermion systems [2–7]. Our wavefunctions are coherent pairing states (CPS) of the dynamical group of the Hubbard model. Although not eigenfunctions of the Hamiltonian, they permit exact calculations of numerous physical properties of the Hubbard model, including the energy, arbitrary moments of the Hamiltonian, fluctuations and correlation functions, including ODLRO which is shown to be non-vanishing. The CPS are mathematically related to the variational wavefunctions used in a mean-field treatment of Bardeen–Cooper–Schrieffer (BCS) type [8].

2. η-pairing and the dynamical group

For the Hubbard model we adopt the definition and notation of Yang [1]. Let $a_{\boldsymbol{r}}^{+}$ and $b_{\boldsymbol{r}}^{+}$ be real-space creation operators for spin-up and spin-down electrons respectively, i.e.

§ Permanent address: Faculty of Mathematics and Computing, The Open University, Milton Keynes MK7 6AA, UK. E-mail address: a.i.solomon@open.ac.uk

∥ E-mail address: penson@lptl.jussieu.fr

0305-4470/98/180355+06$19.50

$c^+_{r\uparrow} = a^+_r$, $c^+_{r\downarrow} = b^+_r$ with a^+_r and b^+_r satisfying the usual fermion anticommutation relations.

Consider a three-dimensional Hubbard model on a $L \times L \times L = M$ cube (L even) with periodic boundary conditions. The Hamiltonian is given by

$$H = T_0 + T_1 + V \tag{1}$$

$$T_0 = A\epsilon \sum_{\boldsymbol{k}} (a^+_{\boldsymbol{k}} a_{\boldsymbol{k}} + b^+_{\boldsymbol{k}} b_{\boldsymbol{k}}) \tag{2}$$

$$T_1 = -B \sum_{\boldsymbol{k}} (\cos k_x + \cos k_y + \cos k_z)(a^+_{\boldsymbol{k}} a_{\boldsymbol{k}} + b^+_{\boldsymbol{k}} b_{\boldsymbol{k}}) \tag{3}$$

$$V = 2W \sum_{\boldsymbol{r}} a^+_{\boldsymbol{r}} a_{\boldsymbol{r}} b^+_{\boldsymbol{r}} b_{\boldsymbol{r}} \tag{4}$$

where $\epsilon > 0$, $a^+_{\boldsymbol{k}}$ is the Fourier transform of $a^+_{\boldsymbol{r}}$, $2W$ is the on-site Hubbard interaction of arbitrary sign, and A and B are arbitrary constants. We introduce the η-operators which create (annihilate) a fermion pair with momentum $\boldsymbol{\pi}$:

$$\eta = \sum_{\boldsymbol{r}} \mathrm{e}^{\mathrm{i}\boldsymbol{\pi r}} a_{\boldsymbol{r}} b_{\boldsymbol{r}} = \sum_{\boldsymbol{k}} a_{\boldsymbol{k}} b_{\boldsymbol{\pi}-\boldsymbol{k}} \tag{5}$$

$$\eta^+ = \sum_{\boldsymbol{r}} \mathrm{e}^{\mathrm{i}\boldsymbol{\pi r}} a^+_{\boldsymbol{r}} b^+_{\boldsymbol{r}} = \sum_{\boldsymbol{k}} b^+_{\boldsymbol{\pi}-\boldsymbol{k}} a^+_{\boldsymbol{k}}. \tag{6}$$

It has been shown [1, 9] that the operator η^+ satisfies

$$[H, \eta^+] = E\eta^+ \tag{7}$$

with $E = 2A\epsilon + 2W$. Equation (7) is typical of a spectrum-generating algebra [10, 11] and implies that for any power-expandable $f(\eta^+)$

$$[H, f(\eta^+)] = E\eta^+ f'(\eta^+). \tag{8}$$

Note that E does not depend on B. The relation equation (7) for the Hubbard model was derived some time ago [9], but its consequences were only fully exploited by Yang [1]. The operators η satisfy the angular momentum commutation relations of $SU(2)$:

$$[\eta^+, \eta] = 2\eta_z \tag{9}$$

$$\eta_z = \tfrac{1}{2} \sum_{\boldsymbol{r}} (n^{(a)}_{\boldsymbol{r}} + n^{(b)}_{\boldsymbol{r}} - 1)$$

$$= \tfrac{1}{2} \sum_{\boldsymbol{r}} n_{\boldsymbol{r}} - \tfrac{1}{2} M \tag{10}$$

where the local occupation number $n_{\boldsymbol{r}}$ is equal to $n^{(a)}_{\boldsymbol{r}} + n^{(b)}_{\boldsymbol{r}} = a^+_{\boldsymbol{r}} a_{\boldsymbol{r}} + b^+_{\boldsymbol{r}} b_{\boldsymbol{r}}$. We also observe from equation (9) that the following relation holds

$$\left[\frac{\eta}{\sqrt{M}}, \frac{\eta^+}{\sqrt{M}}\right] = 1 - d \tag{11}$$

where d is the electronic density, $d = M^{-1}(\sum_{\boldsymbol{r}} n_{\boldsymbol{r}})$. Equation (11) indicates that for small electron density the operators $\eta/\sqrt{M}$ are approximately bosons [12]. The operators η also satisfy the relations $(\eta^+)^{M+1} = (\eta)^{M+1} = 0$, reflecting, according to the Pauli-principle, the impossibility of occupying a given site $\boldsymbol{r}$ by more than one pair (a^+b^+). For given M and using (7) one can produce M exact, normalized eigenstates of H by applying successive powers of η^+ on the vacuum state $|\mathrm{vac}\rangle$. So

$$|\Psi_N\rangle = \beta(N, M)(\eta^+)^N |\mathrm{vac}\rangle \qquad N = 1, \ldots, M \tag{12}$$

is a simultaneous eigenstate of H and of the operator N_2 counting the number of doubly occupied sites, $N_2 = \sum_{\boldsymbol{r}} n_{\boldsymbol{r}}^{(a)} \cdot n_{\boldsymbol{r}}^{(b)}$,

$$\begin{aligned} H|\Psi_N\rangle &= NE|\Psi_N\rangle \\ N_2|\Psi_N\rangle &= N|\Psi_N\rangle \end{aligned} \tag{13}$$

where $\beta(N, M)$ is a normalization factor equal to [1]

$$\beta(N, M) = \left[\frac{(M-N)!}{M!N!}\right]^{\frac{1}{2}}. \tag{14}$$

Evidently, $\langle\Psi_N|(\eta^+)^r|\Psi_N\rangle - \delta_{r,0}$. Note that $[H, N_2] \neq 0$. We observe that $|\Psi_N\rangle$ depend neither on the value nor on the sign of W. Generally $[\eta, H] \neq 0$ except for the half-filled band [13].

With this in mind, we embed the Hamiltonian H together with $\boldsymbol{\eta} = \{\eta, \eta^+, \eta_z\}$, in a larger, dynamical, group. Define a new operator J_0 by

$$J_0 = \frac{H}{E} - \eta_z. \tag{15}$$

Using equation (7) and its Hermitian conjugate we find that

$$[J_0, \boldsymbol{\eta}] = 0. \tag{16}$$

We conclude that the smallest group containing H is $\{J_0, \boldsymbol{\eta}\}$, where J_0 is the centre of the group but *not* the unit operator. The dynamical group of our Hubbard model is thus $U(2)$. This would appear to be the first instance of a dynamical group for an *exact* interacting many-body system. Relation (16) is essential for the calculation of any expectation values of H.

3. Coherent pairing states

We introduce a normalized spin coherent state by

$$\begin{aligned} |\mu\rangle &= \mathcal{N}^{-\frac{1}{2}} e^{\mu\eta}|0\rangle \\ &= (1+|\mu|^2)^{-\frac{M}{2}} e^{\mu\eta}|0\rangle \end{aligned} \tag{17}$$

where the state $|0\rangle$ is the filled pair state $|0\rangle = \frac{1}{M!}(\eta^\dagger)^M|\text{vac}\rangle$. We refer to $|\mu\rangle$ as a *coherent pairing state*. This step is reminiscent of the BCS wavefunction [8], which is however not related to any Hamiltonian with a local potential energy. In contrast, our states arise from the exact relations equations (7) and (16). In the limit $M \to \infty$, $|\mu\rangle$ becomes an eigenstate of $\eta/\sqrt{M}$ and apart from normalization is a harmonic oscillator coherent state [14]. The state $|\mu\rangle$ is not an eigenstate of H. In contrast to $|\Psi_N\rangle$ it involves components with different numbers of particles (pairs) and thus gives rise to non-zero values of $\langle\mu|\eta^r|\mu\rangle$. Further, using equations (7), (8) and (16) we may calculate $\langle\mu|H^p|\mu\rangle$ for any $p = 1, 2, 3, \ldots$ in terms of $\langle\mu|\eta^r|\mu\rangle$. We first calculate $\langle\mu|H|\mu\rangle$ by purely algebraic means:

$$\begin{aligned} H|\mu\rangle &= \mathcal{N}^{-\frac{1}{2}}\{[H, e^{\mu\eta}] + e^{\mu\eta}H\}\tfrac{1}{M!}(\eta^+)^M|\text{vac}\rangle \\ &= \mathcal{N}^{-\frac{1}{2}}\{-E\eta\mu e^{\mu\eta} + e^{\mu\eta}ME\}\tfrac{1}{M!}(\eta^+)^M|\text{vac}\rangle \\ &= (-\mu E\eta + ME)|\mu\rangle \end{aligned}$$

where $\mathcal{N}(\mu) = (1+|\mu|^2)^M$. The required expectation value $\langle\mu|H\mu\rangle$ becomes $ME - \mu E\langle\mu|\eta|\mu\rangle$, which, using the results of [14] (formula (4.2)), leads to

$$\langle\mu|H|\mu\rangle = \frac{ME}{(1+|\mu|^2)}. \tag{18}$$

Formula (18) indicates that the energy of the state $|\mu\rangle$ (which involves different numbers of pairs) is equal to the energy of the fully filled state $|0\rangle(ME)$ reduced by the factor $(1+|\mu|^2)^{-1} \leqslant 1$. The physical meaning of the parameter μ is obtained from the average number of pairs in a state $|\mu\rangle$, $\langle\mu|N_2|\mu\rangle$. Since $|\mu\rangle$ does not depend on the Hamiltonian's parameters,

$$\langle\mu|N_2|\mu\rangle = \frac{1}{2}\langle\mu|\frac{\partial H}{\partial W}|\mu\rangle = \frac{1}{2}\frac{M}{1+|\mu|^2}\frac{\partial E}{\partial W}. \tag{19}$$

We conclude that

$$|\mu|^2 = \frac{1}{\bar{n}_2} - 1 \tag{20}$$

where $\bar{n}_2 = \langle N_2\rangle/M$ is the average density of pairs in the state $|\mu\rangle$. We may extend the set of states for which exact analysis is available by introducing r-depleted states, defined by (normalized)

$$|\mu : r\rangle = \mathcal{N}_r^{-\frac{1}{2}}\eta^r|\mu\rangle. \tag{21}$$

These are analogues of the displaced number states of quantum optics [15]. These states give rise to a more interesting energy spectrum than the equidistant Yang case, with the gap between neighbouring depleted states $|\mu; r\rangle$ and $|\mu; r-1\rangle$ being given by

$$\Delta_r(|\mu|^2) = \frac{\langle\mu(\eta^+)^{r-1}H\eta^{r-1}|\mu\rangle}{\langle\mu|(\eta^+)^{r-1}\eta^{r-1}|\mu\rangle} - \frac{\langle\mu|(\eta^+)^r H\eta^r|\mu\rangle}{\langle\mu|(\eta^+)^r\eta^r|\mu\rangle}. \tag{22}$$

For $\mu = 0$ we evidently have Yang's functions for which all the gaps are strictly equal to E. For $\mu \neq 0$ we expect a structure in $\Delta_r(|\mu|^2)$. In fact all the quantities in equation (22) can be calculated using only $\mathcal{N}(|\mu|^2)$ and $\langle\mu|H|\mu\rangle$ equation (18). For a general operator Q we can calculate $\langle\mu|(\eta^+)^r Q\eta^r|\mu\rangle$ through the relation

$$\langle\mu|(\eta^+)^r Q\eta^r|\mu\rangle = (1+|\mu|^2)^{-M}\frac{\partial^r}{\partial(\mu^*)^r}\frac{\partial^r}{\partial\mu^r}[(1+|\mu|^2)^M\langle\mu|Q|\mu\rangle] \tag{23}$$

which indicates that for $\rho \equiv |\mu|^2$ the generating function for the matrix elements of Q between the depleted states is proportional to $(1+\rho)^M\langle\mu|Q|\mu\rangle$, which for $Q \equiv 1$ and $Q \equiv H$ furnishes all the input for equation (22).

The detailed analysis of equation (22) confirms a very interesting structure of Δ_r as a function of ρ, M and r. The precise description will be given elsewhere but we note here that the gaps as a function of ρ go through a maximum for $r \approx \frac{M}{2}$ which in turn disappears for $r > \frac{M}{2}$. This confirms that the half-filling point ($N = \frac{M}{2}$) plays a special role for the Hubbard model. Equation (23) may be used to obtain the following simple result for the energy dispersion in a coherent pairing state:

$$\frac{(\Delta H)^2}{\langle\mu|H|\mu\rangle^2} = \frac{\rho}{M} \tag{24}$$

where $\rho = |\mu|^2$. This indicates that the energy fluctuations are normal in the thermodynamic sense, as in the grand canonical ensemble. Similarly, in the first depleted state $|\mu; 1\rangle$

$$\frac{(\Delta H)_1^2}{\langle H\rangle_1^2} = \frac{\rho(2+2M\rho-M\rho^2+M^2\rho^2)}{(M-1)(1-\rho+M\rho)^2}. \tag{25}$$

Note that the dispersion in the first depleted state equation (25) is always greater than that in a spin coherent state (SCS), equation (24). Analogous, if more complex, results hold for higher depleted states.

Since the coherent pairing states are not eigenstates of the Hubbard Hamiltonian, they possess a non-trivial time dependence. This time evolution is easily calculable via the time-dependent Schrödinger equation due to the simple algebraic structure of the model. For the case of a conventional coherent state satisfying $a|z\rangle = z|z\rangle$ evolving under the action of a Hamiltonian $H = \omega(a^+a + \frac{1}{2})$, the evolution is simply expressed by the propagator ($\hbar = 1$)

$$|\langle z(0)|z(t)\rangle| = \exp(|z|^2[\cos\omega t - 1]). \tag{26}$$

In the case of the coherent pairing state equation (17), the analogous result, with equation (7) is

$$|\langle \mu(0)|\mu(t)\rangle| = \left|\frac{(1+|\mu|^2 e^{itE})^M}{(1+|\mu|^2)^M}\right|. \tag{27}$$

In the limit $M \to \infty$, $\mu \to z/\sqrt{M}$ (corresponding to the group contraction $\eta \to \sqrt{M}a^+$, compare equation (11)) we recover the conventional (bosonic) case equation (26).

4. Off-diagonal long-range order

The presence of ODLRO [16] is detected by the non-vanishing of correlators such as $\langle a_s^\dagger b_s^\dagger b_r a_r\rangle$ as $|r-s| \to \infty$. Yang has shown that his states display ODLRO which, in the thermodynamic limit, is proportional to $n_2(1-n_2)$, where $n_2 \equiv N/M$ is the pair density. We may similarly show that our SCS states $|\mu\rangle$, $\mu \neq 0$, exhibit ODLRO, also proportional to $\overline{n_2}(1-\overline{n_2})$ where the average pair density $\overline{n_2} = \langle N\rangle/M$. Additionally, the states $|\mu; r\rangle$ exhibit ODLRO and all the results reduce to those of Yang for $\mu = 0$ [17]. Thus the states $|\mu\rangle$, $|\mu; r\rangle$ are superconducting for all μ and r. It is worth noting that although $\langle\psi_N|\eta|\psi_N\rangle = 0$, which makes η unsuitable for defining an order parameter in the usual sense, $\langle\mu|\eta|\mu\rangle \neq 0$ as in the analogous BCS case.

5. Mean-field theory and related models

We may now write a mean-field version of the Hubbard Hamiltonian $H^{MF} = \sum_k H_k$

$$H_k = E_k(a_k^\dagger a_k + b_k^\dagger b_k) + 2W(\Delta_k^*\eta_k + \Delta_k\eta_k^\dagger) \tag{28}$$

with $\eta_q = \sum_k a_k b_{q-k} (q = \pi)$ and effective energies E_k which include the T_0 and T_1 terms of equations (2) and (3). The spectrum-generating algebra for the Hamiltonian equation (28) is u_k (2). The non-diagonal terms are the number-non-conserving analogues of a spin-density wave system (see, for example [18]) and were already observed in a multiphase $SU(8)$ model [19], where they were called 'anomalous' terms, their relation to the Hubbard model at that time not having been appreciated. Thus in the mean-field approximation the dynamical group is $\otimes_k U_k(2)$. The associated group parameters (Bogoliubov transformation angles) are μ_k, vector analogues of the μ parameter in the $U(2)$ which is what remains of the dynamical symmetry in the exact model.

It is possible to demonstrate that relation (7) (with modified E) can be fulfilled by Hamiltonians other than (1). Yang already mentioned the possibility [1] of non-local interactions satisfying equation (7) with appropriately modified η. It is interesting to observe that at least one case of a truly non-local interaction satisfies equation (7). It concerns an extension of the pair-hopping model [20] of the form [17]

$$H_{ph} = T_0 + T_1 + V\sum_{\langle rs\rangle}\boldsymbol{\eta}_r\cdot\boldsymbol{\eta}_s - \frac{V}{2}\sum_r n_r \tag{29}$$

which satisfies $[H_{ph} - (T_0 + T_1), \eta^+] = V\eta^+$. However, other extensions are possible for which the coherent pairing state $|\mu\rangle$ is a useful tool [17].

References

[1] Yang C N 1989 *Phys. Rev. Lett.* **63** 2144
[2] Essler F H L, Korepin V E and Schoutens K 1992 *Phys. Rev. Lett.* **68** 2960
Essler F H L, Korepin V E and Schoutens K 1993 *Phys. Rev. Lett.* **70** 73
[3] Arrachea L and Aligia A 1994 *Phys. Rev. Lett.* **73** 2240
[4] de Boer J, Korepin V E and Schadschneider A 1995 *Phys. Rev. Lett.* **74** 789
[5] Schadschneider A *Phys. Rev.* B **51** 10 386
[6] de Boer J and Schadschneider A 1995 *Phys. Rev. Lett.* **75** 4298
[7] Sato R 1996 *Phys. Rev.* A **221** 220
[8] Schrieffer J R 1964 *Theory of Superconductivity* (New York: Benjamin)
[9] Nowak E 1981 *Z. Phys.* B **45** 173
[10] Dothan Y, Gell-Mann M and Ne'eman Y 1965 *Phys. Lett.* **17A** 148
[11] Goshen S and Lipkin H J 1959 *Ann. Phys.* **6** 301
[12] Lipkin H J 1973 *Quantum Mechanics* (Amsterdam: North-Holland)
[13] Yang C N and Zhang S 1990 *Mod. Phys. Lett.* B **4** 759
[14] Radcliffe J *J. Phys. A: Math. Gen.* **4** 270
[15] de Oliveira F A M, Kim M S, Knight P L and Buzek V *Phys. Rev.* A **41** 2645
[16] Yang C N 1962 *Rev. Mod. Phys.* **34** 694
[17] Solomon A I, Penson K and Kunze K-K 1996 *Spin Coherent States in the Hubbard Model, 21st Int. Coll. on Group Theoretical Methods in Physics (Goslar, Germany)* ed H-D Doebner *et al* (Singapore: World Scientific)
[18] Solomon A I and Birman J L 1984 *Phys. Lett.* **104A** 235
[19] Solomon A I and Birman J L *J. Math. Phys.* **28** 1526
[20] Penson K A and Kolb M 1986 *Phys. Rev.* B **33** 1663