Exact spectrum analysis of a one-dimensional Hubbard model

1990 J. Phys. A: Math. Gen. 23 L389

(http://iopscience.iop.org/0305-4470/23/8/007)

J. Phys. A: Math. Gen. 23 (1990) L389-L392. Printed in the UK

LETTER TO THE EDITOR

Exact spectrum analysis of a one-dimensional Hubbard model

Philippe Audit

Laboratoire PMTM, Université Paris-Nord, 93430 Villetaneuse, France

Received 8 January 1990

Abstract. For a one-dimensional Hubbard model with a half-filled band and one extra hole the single-hole Green function is calculated analytically; the spectrum analysis shows that the N electrons tend to move so as to form identical and consecutive packets to satisfy rules fixed by arithmetical properties of the integer N.

Investigations of the Hubbard model have been numerous, but exact results are rare though often enlightening [1-3] and unattainable by approximate methods, as in the present exact spectrum analysis of a one-dimensional Hubbard model with a half-filled band and one extra hole in the strong correlation limit ($U=\infty$). This model was considered long ago by Nagaoka [1], who proved some exact results for the ground state of 3D lattices, whereas the hole propagation has been studied [4, 5] by approximate Green function calculations. Moreover, the one-dimensional Hubbard model is exactly solvable [2] and even exactly integrable [6], and some exact asymptotic results have been obtained recently [7] for the infinite chain. But the size-dependent properties are of interest from a theoretical point of view [8], and also for extrapolation to the bulk limit Monte Carlo results on finite systems; moreover fragmented chains play a role in some high-temperature superconductors [9]. However, in the present work, although the number of electrons indeed plays a usual role through its size, the surprising main result appears to be that the behaviour of the N electrons is entirely determined by the arithmetical properties of the integer N and so is in fact ruled by the elementary theory of numbers.

Considering a Hubbard chain of $N+1$ atoms and N electrons with strong intra-atomic Coulomb repulsion ($U=\infty$) and assuming periodic boundary conditions and N odd, in the basis of states

$$|i\boldsymbol{\sigma}\rangle = (-1)^i c^{\dagger}_{0\sigma_0} \ldots c^{\dagger}_{i-1,\sigma_{i-1}} c^{\dagger}_{i+1,\sigma_{i+1}} \ldots c^{\dagger}_{N\sigma_N}|\rangle$$

where i and $\boldsymbol{\sigma}$ denote respectively the site where the hole is located and the spin's configuration $\boldsymbol{\sigma}=(\sigma_1, \sigma_2, \ldots, \sigma_N)$, σ_α being the spin at site $i+\alpha$, the Hamiltonian

$$H = t \sum_{i=0,\sigma=\uparrow,\downarrow}^{N} c^{\dagger}_{i\sigma} c_{i+1,\sigma} + c^{\dagger}_{i+1,\sigma} c_{i\sigma}$$

has the matrix representation

$$H = -t(m_{N+1} \otimes G_N + m^{-1}_{N+1} \otimes G^{-1}_N) \tag{1}$$

where the double periodicity of the model is properly taken into account by a $(N+1)\times(N+1)$ cyclic matrix

$$(m_{N+1})_{ii'} = \delta(i-i') \mod(N+1) \qquad i, i' = 0, 1, \ldots, N$$

0305-4470/90/080389+04$03.50

and a $2^N \times 2^N$ spin's cyclic permutation matrix

$$(G_N)_{\sigma\sigma'} = \delta(\sigma m_N - \sigma') \qquad \text{where } \delta(k) = 1 \text{ (or 0) if } k = 0 \text{ (or } \neq 0).$$

The pth power of these matrices have diagonal elements in the form

$$(m_{N+1}^p)_{ii} = (N+1)^{-1} \sum_{\alpha=0}^{N} \omega_{N+1}^{\alpha p} \qquad \omega_n = \exp(2i\pi/n) \tag{2}$$

$$(G_N^p)_{\sigma_d\sigma_d} = N^{-1} \sum_{\beta=0}^{N-1} \sum_{l=1}^{d} \omega_d^{\beta l} \omega_N^{\beta p} \tag{3}$$

where, for $d|N$ (means d divides N), σ_d denotes a N-tuple which is partitioned in exactly d identical and consecutive N/d-tuples; if that is not the case, the notation still holds since σ_1 can be used to denote such vectors; and likewise the two ferromagnetic configurations will be denoted by σ_N.

With these notations and by using (1), (2) and (3) we readily obtain

$$\langle i\sigma_d | H^p | i\sigma_d \rangle = N^{-1}(N+1)^{-1}(-t)^p \sum_{\alpha=0}^{N} \sum_{\beta=1}^{N-1} \sum_{l=1}^{d} \omega_d^{\beta l} (\omega_{N+1}^{\alpha} \omega_N^{\beta} + \omega_{N+1}^{-\alpha} \omega_N^{-\beta})^p \tag{4}$$

from which we deduce for the one-particle Green function $R(z) = (z - H)^{-1}$, through its power series, the diagonal elements in the form

$$\langle i\sigma_d | R(z) | i\sigma_d \rangle = N^{-1}(N+1)^{-1} \sum_{\alpha=0}^{N} \sum_{\beta=0}^{N-1} \sum_{l=1}^{d} \omega_d^{\beta l} \left[z + 2t \cos 2\pi \left(\frac{\alpha}{N+1} + \frac{\beta}{N} \right) \right]^{-1} \tag{5}$$

and noting that $\text{card}\{\sigma_d\} = 2^{N/d}$ and that for a correct counting of the diagonal elements the condition $\gcd(l, d) = 1$ must be imposed in the summations over l in (3), (4) and (5) the trace reads

$$\text{Tr } R(z) = N^{-1} \sum_{\alpha=0}^{N} \sum_{\beta=0}^{N-1} A_\beta(N, 2) \left[z + 2t \cos 2\pi \left(\frac{\alpha}{N+1} + \frac{\beta}{N} \right) \right]^{-1} \tag{6}$$

in terms of the arithmetical polynomials [10]

$$A_\beta(N, x) = \sum_{d|N} c(\beta, d) x^{N/d}$$

whose coefficients $c(\beta, d) = \sum_{1 \leq l \leq d, \gcd(l,d)=1} \omega_d^{\beta l}$ are Ramanujan sums [11].

The eigenspectrum follows from the properties of $R(z)$ whose poles are the $N(N+1)$ energy eigenvalues

$$E_{\alpha\beta} = -2t \cos 2\pi \left(\frac{\alpha}{N+1} + \frac{\beta}{N} \right) \qquad \alpha = 0, 1, \ldots, N \quad \beta = 0, 1, \ldots, N-1 \tag{7}$$

that increase as $(\alpha, \beta) = (0, 0), (1, 0), (0, 1), (2, 0), (1, 1), (0, 2), \ldots$. There are $(N+1)2^N$ eigenstates $\Phi^{\alpha\beta,k}$, $k = 1, 2, \ldots, m_{\alpha\beta}$ and the degeneracy of an eigenenergy $E_{\alpha\beta}$ is given by the multiplicity

$$m_{\alpha\beta} = \text{Tr Res } R(E_{\alpha\beta}) = N^{-1} A_\beta(N, 2) \tag{8}$$

which is, as required, an integer by generalisation of Fermat's Little Theorem [10].

Let us now define a 'density' of eigenstates per configuration

$$n_{\sigma_d}(E) = -\pi^{-1} \text{ Im} \langle i\sigma_d | R(E + i0) | i\sigma_d \rangle = \sum_{\alpha=0}^{N} \sum_{\beta=0}^{N-1} a_{\sigma_d}^{\alpha\beta} \delta(E - E_{\alpha\beta}) \tag{9}$$

where the weight that the eigenstates of energy $E_{\alpha\beta}$ have on a given configuration σ_d is

$$a_{\sigma_d}^{\alpha\beta} = \sum_{k=1}^{m_{\alpha\beta}} |\Phi_{i\sigma_d}^{\alpha\beta,k}|^2 = \mathrm{Res}\langle i\sigma_d|R(E_{\alpha\beta})|i\sigma_d\rangle = N^{-1}(N+1)^{-1}\sum_{l=1}^{d}\omega_d^{\beta l}$$

$$= \begin{cases} 0 & \text{if } d \nmid \beta \text{ and } \beta \neq 0 \\ d/[N(N+1)] & \text{if } d|\beta \text{ or } \beta = 0 \end{cases} . \tag{10}$$

Discussion. The exact N-particle energies $E_{\alpha\beta}$ given by (7) are $m_{\alpha\beta}$-fold degenerate, and from (8) and (10) it appears that both multiplicity and 'density' of states per configuration are ruled by the factorisation of the integer N, which thereby controls the thermodynamic behaviour and the collective motion of the N electrons.

If N is prime, its only divisors are 1 and N, whence $m_{\alpha\beta} = N^{-1}[2^N + 2c(\beta, N)]$; the $\beta = 0$ levels are the most degenerate with $m_{\alpha 0} = N^{-1}(2^N - 2N - 2)$, whereas $m_{\alpha 1} = N^{-1}(2^N - 2), \ldots$. The ferromagnetic configurations of weight $a_{\sigma_N} = (N+1)^{-1}\delta(\beta)$ are only allowed for $\beta = 0$ eigenstates (notably the ground state), where they overcome the other configurations of weight $a_{\sigma_1} = N^{-1}(N+1)^{-1}$.

If N is composite, the degeneracy (8) of the $\beta = 0$ states are given by the arithmetical polynomial $A_0(N, 2)$ whose coefficients are the Euler functions $\phi(d)$, i.e. the number of integers not greater than and prime to d. For $\beta = 1$, the coefficients of the arithmetical polynomial $A_1(N, 2)$ are merely Mobius functions [11] $\mu(d)$ and the multiplicity of those eigenstates depends mainly upon the presence of squared factors in the prime decomposition of d. For example, if $N = p^r$ with p prime, we have simply $m_{\alpha 1} = N^{-1}(2^N - 2^{N/p})$. From (10) we infer that for $\beta = 0$ eigenstates all configurations σ_d are allowed, the N electrons tend to propagate in d packets having the same spin configuration with greater probability weight for larger d and the ferromagnetic configuration has the maximum weight $a_{\sigma_N}^{\alpha 0} = (N+1)^{-1}$. Concerning $\beta \neq 0$ eigenstates, the necessary and sufficient condition for packets of N/d electrons to propagate is that $d|N$ and $d|\beta$, so the size of the predominating packet is $N/\gcd(N, \beta)$. Notice that the ferromagnetic configurations are forbidden for those excited states.

So by an analytic calculation of the Green function and spectrum, we have elucidated the spin configuration dependence of the kinetic energy of a simple hole in a strongly correlated one-dimensional Hubbard model and shown that electrons tend to move forming identical and consecutive packets. The different allowed correlated spin motions compete obeying strict rules with probability weights fixed by the arithmetical properties of the number of electrons; so that in this packing scheme ferromagnetically correlated states appears to be only special cases not always present nor even favoured in every energy eigenstates. Moreover, eigenstates have degeneracies that can also be taken into account correctly in the derivation of thermodynamic properties, which thus obey arithmetic rules just as well; those results will be reported elsewhere. In any case, difficult questions remain unanswered concerning how those subtle features of the model carry over to weaker-coupling regions and higher dimensions.

References

[1] Nagaoka Y 1966 *Phys. Rev.* **147** 392
[2] Lieb E H and Wu F Y 1968 *Phys. Rev. Lett.* **20** 1445
[3] Lieb E H 1988 *Phys. Rev. Lett.* **62** 1201
[4] Brickmann W F and Rice T M 1970 *Phys. Rev.* B **2** 1324

[5] Joynt R 1988 *Phys. Rev.* **37** 7979
[6] Shastry B S 1986 *Phys. Rev. Lett.* **56** 2453
[7] Carmelo J and Baeriswyl D 1987 *Phys. Rev.* B **37** 7541
[8] de Vega H J and Woynarowich F 1985 *Nucl. Phys.* B **251** 439
[9] Zaanen J, Paxton A T, Jepsen O and Andersen O K 1988 *Phys. Rev. Lett.* **60** 2685
[10] Audit Ph 1989 *J. Phys. A: Math. Gen.* **22** L1085
[11] Hardy G H and Wright E M 1938 *An Introduction to the Theory of Numbers* (Oxford: Oxford Science Publishing)