Exactly Soluble Model of Interacting Electrons*

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We diagonalize a many-fermion Hamiltonian consisting of terms quadratic as well as quartic in the field operators. A dual spectrum of eigenstates is an interesting result. We also derive a formula for obtaining the free energy at finite temperature.

I. INTRODUCTION

The Hubbard model of interacting electrons on a linear chain,

$$\mathcal{H}_{\text{Hub}} = -\epsilon \sum_{\substack{j=1 \\ \sigma=\pm 1/2}}^{N-1} (c_{j\sigma}^* c_{j+1\sigma} + c_{j+1\sigma}^* c_{j\sigma}) + U \sum_{j=1}^{N} (n_{j\uparrow} - \tfrac{1}{2})(n_{j\downarrow} - \tfrac{1}{2}), \quad \text{where } n_{j\sigma} = c_{j\sigma}^* c_{j\sigma}, \tag{1}$$

was given an ingenious solution by Lieb and Wu[1] who obtained the ground state, and later by others[2] who found the elementary excitations. The complete set of eigenstates has not yet been determined nor has the statistical mechanics, although numerical calculations[3,4] on finite systems ($N = 6$) has revealed many interesting features such as level crossings and dual excitation spectra. These are totally absent in the approximate RPA solution of (1), and such structure is lacking in the exactly soluble, relativistic model of interacting electrons.[5] It is therefore of interest to discuss the predictions of a new model, a modification of (1), which we have been able to solve exactly for arbitrary N, ϵ, and U. We obtain and classify the eigenstates and eigenvalues, and reduce the calculation of the free energy to the solution of an implicit equation. One of our results is a two-fold degeneracy of the ground state, which is antiferromagnetically ordered. A dual excitation spectrum is also a feature of this model.

II. MODEL HAMILTONIAN

Like (1), the exactly soluble Hamiltonian is a combination of quadratic and quartic terms:

$$\mathcal{H} = \frac{\epsilon}{4} \sum_{\substack{j=1 \\ \sigma=\pm}}^{N-1} (c_{j\sigma} - c_{j\sigma}^*)(c_{j+1\sigma} + c_{j+1\sigma}^*) + U \sum_{j=1}^{N} (n_{j\uparrow} - \tfrac{1}{2})(n_{j\downarrow} - \tfrac{1}{2}). \tag{2}$$

The c's are a complete set of anticommuting operators.

An important (and anomalous) operator in the above is

$$\sum (c_{j\sigma} c_{j+1\sigma} - c_{j\sigma}^* c_{j+1\sigma}^*), \tag{3}$$

which causes charges to be created or destroyed in pairs (as in the BCS theory of superconductivity). It

is evident that the current density operator $\mathbf{j}$ has to be suitably modified to take this into account in order to satisfy an equation of continuity. These considerations have also suggested to us that one should seek an analogous modification of the current operator in the BCS theory, as we discuss elsewhere.[6] In the present work the anomalous terms (3) are introduced merely as a convenience to allow a solution of the problem. This device first proved useful in the exact solution of one and two "magnetic" impurity atoms in a three-dimensional nonmagnetic metal host,[7] although the subsequent calculations and results, in these problems, have little in common with the present work.

Our first step in the manipulation of $\mathcal{H}$ is a Jordan–Wigner transformation to pseudospin matrices T_i and S_i, defined via

$$S_j^- = c_{j\uparrow} e^{\pi i \sum_{m<j} n_{m\uparrow}}, \quad T_j^- = c_{j\downarrow} e^{\pi i \left(\sum_{\text{all } m} n_{m\uparrow} + \sum_{m<j} n_{m\downarrow} \right)}, \tag{4}$$

with similar equations relating S^+ and T^+ to the c^*'s. Insertion into (2) yields

$$\mathcal{H} = -\epsilon \sum_j (S_j^x S_{j+1}^x + T_j^x T_{j+1}^x) + U \sum_j S_j^z T_j^z. \tag{5}$$

It is now advantageous to introduce a new set of spin matrices, the P_j^α and J_j^α, in terms of which the original spin vectors are

$$\begin{aligned} (S_j^x, S_j^y, S_j^z) &= (J_j^x, 2J_j^y P_j^x, 2J_j^z P_j^x), \\ (T_j^x, T_j^y, T_j^z) &= (-2P_j^z J_j^x, 2P_j^y J_j^x, P_j^x). \end{aligned} \tag{6a}$$

The inverse of these relations is useful to record:

$$\begin{aligned} (J_j^x, J_j^y, J_j^z) &= (S_j^x, 2S_j^y T_j^z, 2S_j^z T_j^z), \\ (P_j^x, P_j^y, P_j^z) &= (T_j^z, 2S_j^x T_j^y, -2S_j^x T_j^x). \end{aligned} \tag{6b}$$

[Note that our matrices are all normalized to spin $\frac{1}{2}$, such that, e.g., $(P_j^x)^2 = \frac{1}{4}$.] When this is substituted into $\mathcal{H}$, there results

$$\mathcal{H} = -\epsilon \sum_j J_j^x J_{j+1}^x (4P_j^z P_{j+1}^z + 1) + \tfrac{1}{2} U \sum_j J_j^z. \tag{7}$$

III. EIGENVALUES

Now we note that the P_j^z are the constants of the motion and can therefore each be taken to be either $+\frac{1}{2}$ or $-\frac{1}{2}$. We denote this the "P-eigenvalue."

Inspection of (7) shows that if neighboring sites have opposite P-eigenvalues, the connection via the $J_j^x J_{j+1}^x$ bond becomes broken. Conversely, if they have similar P-eigenvalues, the bond strength is

$$-2\epsilon J_j^x J_{j+1}^x$$

regardless of whether the P-eigenvalue is $\pm\frac{1}{2}$. Thus in any eigenstate the chain of N atoms is partioned into a number of noninteracting "molecules" of alternating P-eigenvalue. The number of such molecules can be as small as 1, which is indeed the case of the ground state, consisting of a single molecule of N atoms all of which belong to a common eigenvalue of P_j^z. As, however, this eigenvalue can be $\pm\frac{1}{2}$, the ground state is a doublet regardless of the relative magnitudes of ϵ and U. At the opposite extreme, the largest number of molecules is N, each consisting of a single site.

We now solve for the eigenvalue spectrum of any one such molecule, which, we shall assume, extends from a site A ($A \geq 1$) to a site B ($A < B \leq N$). The applicable part of $\mathcal{H}$ is

$$\mathcal{H}_{AB} = -2\epsilon \sum_A^{B+1} J_j^x J_{j+1}^x + \tfrac{1}{2} U \sum_A^B J_j^z. \tag{8}$$

The eigenvalues are symmetric in ϵ, therefore we restrict the following to $\epsilon \geq 0$. This $\mathcal{H}$ is reduced to quadrature by a transformation to fermions, the inverse of (4). Define the set of anticommuting operators a_j:

$$a_j = J_j^- e^{\pi i \sum_{i<j} J_i^+ J_i^-} \tag{9}$$

and similar Hermitian conjugates, such that

$$\mathcal{H}_{AB} = \tfrac{1}{2} \epsilon \sum_A^{B-1} (a_j - a_j^*)(a_{j+1} + a_{j+1}^*) + \tfrac{1}{2} U \sum_A^B (a_j^* a_j - \tfrac{1}{2}). \tag{10}$$

The diagonalization of precisely this quadratic form has been previously studied in connection with the "Heisenberg–Ising model",[8] and it is straightforward to "plagiarize" these old results:

The diagonal form of $\mathcal{H}_{AB}$ becomes

$$\mathcal{H}_{AB} = \sum_A \Lambda_k (a_k^* a_k - \tfrac{1}{2}), \tag{11}$$

where

$$\Lambda_k = [(U/2 - \epsilon)^2 + 2U\epsilon \sin^2 k/2]^{1/2} \tag{12a}$$

and the k's are the roots of

$$\sin k(B - A + 2)/\sin k(B - A + 1) = 2\epsilon/U, \tag{12b}$$

i.e.,

$$\Lambda_k = |\sin k/\sin k(B - A + 1)|(U/2). \tag{12c}$$

By (11), the ground-state energy is

$$E_{AB}^0 = -\tfrac{1}{2} \sum_k \Lambda_k. \tag{12d}$$

Because of obvious symmetry in $\mathcal{H}$, we have taken $\epsilon \geq 0$ in these relations without loss of generality. For $0 < \epsilon < U/2$ there are $B - A + 1$ real roots, exhausting the normal modes. For $\epsilon > U/2$, however, there are only $B - A$ real roots but, in addition, an imaginary one representing a "surface" state. Denoting it $k_0 \equiv iv$, one finds.[8]

$$\begin{aligned} &\sinh(B - A + 2)v/\sinh(B - A + 1)v = 2\epsilon/U, \\ &\Lambda_0 = |\sinh v/\sinh v(B - A + 1)|(U/2). \end{aligned} \tag{13}$$

It is interesting to note that when $B - A \to \infty$, $\Lambda_0 \to 0$ for all $U < 2|\epsilon|$.

IV. THERMODYNAMICS

The partition function of an ℓ-atom molecule is

$$z(\ell) = \prod_k 2 \cosh \tfrac{1}{2} \beta \Lambda_k, \quad \beta = 1/kT, \tag{14}$$

where the set of ℓ k's and Λ_k's are given in the preceding equations, with $\ell \equiv B - A + 1$. If we decompose the chain of N atoms into molecules of lengths

$\ell_1, \ell_2, \cdots$, subject to the constraint

$$\sum \ell_i = N, \tag{15}$$

then the grand partition function is $Z = \exp(-\beta F)$, where F = free energy. This is given in terms of the individual molecules as

$$Z = \sum \prod_i z(\ell_i). \tag{16}$$

The sum is over all possible decompositions. We now discuss a method for calculating this in the thermodynamic limit ($N \to \infty$).

Let

$$z(\ell) \equiv \lambda^\ell \, e^{\phi(\ell)}, \tag{17}$$

where λ includes the extensive contribution, and $\phi(\ell)$ the influence of finite ends, of a molecule ℓ units in length. Thus, we define λ by

$$\log\lambda = \lim_{\ell\to\infty} \ell^{-1} \log z(\ell) = \pi^{-1} \int_0^\pi d\theta \log \times \{2 \cosh \tfrac{1}{2}\beta[(U/2 - \epsilon)^2 + 2U\epsilon \sin^2\theta/2]^{1/2}\}. \tag{17'a}$$

We have

$$\phi(\ell) \equiv \log[z(\ell)\lambda^{-\ell}] \tag{17'b}$$

an intensive quantity, i.e.,

$$\lim_{\ell\to\infty} \ell^{-1}\phi(\ell) = 0. \tag{17'c}$$

The calculation of Z reduces to that of an auxiliary quantity G, defined via:

$$Z = \lambda^N \sum e^{\sum_i \phi(\ell_i)} \equiv \lambda^N G(N), \tag{18}$$

G obeys an iterative equation:

$$G(N) = e^{\phi(1)}G(N-1) + e^{\phi(2)}G(N-2) + \cdots. \tag{19}$$

In the thermodynamic limit ($N \to \infty$) we set $G(N) = g^{-N}$, with $g > 1$, and

$$1 = \sum_{\ell=1}^{\infty} e^{\phi(\ell)} g^{-\ell} \tag{20}$$

follows from (19), and is the implicit equation determining Z.

If $\phi(\ell)$ were constant for $\ell \geq 1$, then (20) is solved by

$$1 = e^\phi \sum_{\ell=1}^{\infty} g^{-\ell} = e^\phi/(g-1),$$

i.e.,

$$g = 1 + e^\phi. \tag{21a}$$

If $\phi(\ell) = \phi(1)$ for $\ell = 1$ and $\phi(2)$ for $\ell \geq 2$, then

$$1 = e^{\phi(1)}g^{-1} + e^{\phi(2)}g^{-1} \sum_{\ell=1}^{\infty} g^{-\ell}$$

$$= e^{\phi(1)}g^{-1} + e^{\phi(2)}/g(g-1),$$

i.e., $$g = \tfrac{1}{2}(1 + e^{\phi(1)}) + [\tfrac{1}{4}(1 + e^{\phi(1)})^2 + (e^{\phi(2)} - e^{\phi(1)})]^{1/2}. \tag{21b}$$

It is easy to see if $\phi(\ell)$ becomes constant after r steps, the solution of an rth degree equation yields g, and hence G and Z. If ϕ is not really constant at $\ell > r$, corrections may be obtained by iteration. It is believed that because the $\phi(\ell)$ are analytic functions of the temperature, the solution g and hence Z must be analytic as well, so that there is no phase transition at finite T.

V. ELEMENTARY EXCITATION

Assuming the ground state to be a single molecule of length N, belonging to either P-eigenvalue $\pm\frac{1}{2}$, the spectra of elementary excitations are twofold: (A) the set of internal excitations, of energy Λ_k, and (B) the (quite distinct) breaking up of the chain into smaller molecules which must, of course, belong to alternating P-eigenvalues. Both type excitations are counted in the calculation of Z in the previous chapter. They must be treated distinctly in a study of the dynamics of our model.

A. Internal Excitations

Consider Eqs. (11) and (12) with $B - A = N - 1 \to \infty$. We observe that for $|\epsilon| \leq \frac{1}{2}U$ the spectrum of elementary excitations represents the addition of a quasiparticle of energy:

$$\Lambda_k = [(U/2 - \epsilon)^2 + 2U\epsilon \sin^2 k/2]^{1/2} \tag{22}$$

with k ranging over closely spaced eigenvalues from 0 to π.

When $|\epsilon| > \frac{1}{2}U$ then is also a bound state of energy $\Lambda_0 = 0$.

B. External Excitations

For lack of a better name we denote "external excitations" the process of creating an additional molecule.

As we are principally concerned with excitations connecting to the ground state, the problem reduces to consideration of the energy to break up the original ground state molecule extending from (1 to N) into three: (1 to $A-1$), (A to B), and ($B+1$ to N). It may be assumed that A and $N - B$ both $\gg 1$ and that $B - A \equiv \ell - 1 \ll N$. We define the ground state energy of a molecule of length L to be $E_0(L)$, and the ground state of the same molecule with the two ends connected (periodic boundary conditions[9]) $E_{0p}(L)$, with $E_{0p}(L) \leq E_0(L)$ and $E_0(L) - E_{0p}(L) = O(1)$ for obvious reasons. Then the energy $\Delta(\ell)$ to break the initial molecule into 3 is calculable as follows:

$$\Delta(\ell) = E_0(\ell) + [E_{0p}(N-\ell) - E_{0p}(N)] + [E_0(N-\ell) - E_{0p}(N-\ell)], \tag{23}$$

where ($N \to \infty$),

$$E_{0p}(N-\ell) - E_{0p}(N) = (\ell/2\pi)\int_0^\pi d\theta \, \Lambda_\theta = (\ell/\pi)(U/2 + |\epsilon|)E(2U|\epsilon|/[U/2 + |\epsilon|]^2). \tag{24}$$

Here $E(x)$ is the complete elliptic integral. Also,

$$E_0(N-\ell) - E_{0p}(N-\ell) = \tfrac{1}{4}[|U/2 + |\epsilon|| - |U/2 - |\epsilon||] + (1/2\pi)\int_0^\pi d\theta \, \Phi(\theta)\frac{\partial \Lambda_\theta}{\partial \theta}, \tag{25}$$

where Φ is defined through $k = \theta + (1/L)\Phi(\theta)$, where k satisfied Eq. (12) with $B - A + 1 \equiv L$ and $\theta =$

$(\pi n/L)$, $(n = 0, 1, \cdots, L-1)$, and $L \to \infty$. Thus

$$\frac{\sin\left[\left(\theta + \frac{1}{L}\Phi\right)(L+1)\right]}{\sin\left[\left(\theta + \frac{1}{L}\Phi\right)L\right]} = \frac{\sin(\theta+\Phi)}{\sin\Phi} = \frac{2\epsilon}{U}, \quad (26)$$

which has the solution

$$\Phi(\theta) = \cot^{-1}[(2\epsilon/U - \cos\theta)/\sin\theta]. \quad (27)$$

In the special limit, $2\epsilon = U$, the $\Delta(\ell)$ becomes

$$\Delta(\ell) = U[\tfrac{1}{2} - 1/\pi - \tfrac{1}{4}(\csc x - 1/x)],$$

where $x = \pi/(4\ell + 2)$. For $2\epsilon > U$, using $\theta = \pi n/(L+1)$ in Eq. (2b), we get $\Phi(\theta)$ for Eq. (25) by replacing $2\epsilon/U$ by $U/2\epsilon$ in Eq. (27).

VI. MATRIX ELEMENTS AND CORRELATION FUNCTIONS

Here we are concerned with some typical ground state correlations and some matrix elements to excited states. The ground state of a linear chain (length $N \to \infty$) is at least twofold degenerate: Aside from the two choices of P-eigenvalue there exists, for $U < 2|\epsilon|$, the option of exciting or not exciting the surface state of Eq. (13) which has energy $\Lambda_0 = 0$. Let us label the set of possible ground states by $|\alpha\rangle$. Then

$$\langle\alpha|n_{j\uparrow}|\alpha\rangle = \tfrac{1}{2} + 2\langle\alpha|J_j^z P_j^x|\alpha\rangle = \tfrac{1}{2}$$
and
$$\langle\alpha|n_{j\downarrow}|\alpha\rangle = \tfrac{1}{2} + \langle\alpha|P_j^x|\alpha\rangle = \tfrac{1}{2}. \quad (28)$$

Thus $\sigma_j^z \sigma_{j+p}^z$ correlations are nonexistent for all $p \neq 0$:

$$\langle\alpha|(n_{j\uparrow} - n_{j\downarrow})(n_{j+p\uparrow} - n_{j+p\downarrow})|\alpha\rangle = 0. \quad (29)$$

However, the nearest-neighbor transverse correlations are

$$\begin{aligned}\langle\alpha|c_{j\uparrow}^* c_{j\downarrow} c_{j+1\downarrow}^* c_{j+1\uparrow}|\alpha\rangle &= -\langle\alpha|[(J_j^z - \tfrac{1}{2})(P_j^z + iP_j^y)] \\ &\quad \times [(J_{j+1}^z - \tfrac{1}{2})(P_{j+1}^z + iP_{j+1}^y)]|\alpha\rangle \\ &= -\tfrac{1}{4}\langle\alpha|(J_j^z - \tfrac{1}{2})(J_{j+1}^z - \tfrac{1}{2})|\alpha\rangle. \end{aligned} \quad (30)$$

This can easily be calculated by (9), (10) and a plane wave expansion related to use of periodic boundary conditions ($a_j = 1/N^{-1/2}\sum_k e^{ik\cdot R_j} c_k$). One can see that (30) is negative, and concludes that nearest-neighbor sites within a molecule are antiferromagnetically correlated.

This also allows us to estimate the spin correlation of adjacent ends of two molecules. If j is at the end of one molecule (has P-eigenvalue P_j^z) and $j+1$ at the beginning of the next P-eigenvalue $P_{j+1}^z = -P_j^z$), then the expectation value (30) becomes intrinsically positive. It is therefore tempting to interpret the molecules as antiferromagnetic domains, and the break in P-eigenvalue between j and $j+1$ as the domain wall. However, the true picture must be somewhat more complex than this, as we see when examining matrix elements to excited states. The fundamental charge density operator $n_{i\uparrow} + n_{i\downarrow}$ has matrix element:

$$\langle\gamma|n_{i\uparrow} + n_{i\downarrow}|\alpha\rangle = 2\langle\gamma|(J_i^z + \tfrac{1}{2})P_i^x|\alpha\rangle, \quad (31)$$

where $|\alpha\rangle$ is one of the ground states. This vanishes unless $\langle\gamma|$ is an "external" elementary excited state, having the same P-eigenvalue as $|\alpha\rangle$ for $j \neq i$ and opposite P-eigenvalue at i. The energy of such a state relative to the ground state, $\Delta(1)$, has already been calculated in a previous chapter.

Similarly, a magnetic field (in the z direction) involves matrix elements

$$\langle\gamma|n_{i\uparrow} - n_{i\downarrow}|\alpha\rangle = 2\langle\gamma|J_i^z - \tfrac{1}{2})P_i^x|\alpha\rangle \quad (32)$$

which connect to the same "external" excited states $\langle\gamma|$ as the above.

VII. CONCLUSION

We have reduced to quadrature a many-body problem of fermions with spin, constrained to a linear chain. The problem was first brought to the form, Eq. (7), in which the nonlinear terms (with P_j^z) could be characterized by quantum numbers $\pm\frac{1}{2}$. The remainder, Eq. (8), could be solved by transforming to a quadratic form in spinless fermions.

We found the ground state to be a single molecule. For $U > 2|\epsilon|$ the ground state is twofold degenerate, such as an antiferromagnetic Ising chain, and has two Néel ground states (differing by one atomic translation). However, when $U < 2|\epsilon|$ the ground state is fourfold degenerate. There is a "phase transition" for $T = 0$ at $U = 2|\epsilon|$. We obtain an implicit expression for the partition function and estimate for fixed U and ϵ, that there is no phase transition when the temperature T is varied.

Finally, we find that external perturbations (magnetic or electric fields) connect only to that part of the excitation spectrum we have labelled "external" excitations. Internal excitations (Λ_k), in which all P_j^z-eigenvalues are conserved, are therefore not accessible to probing by external forces even though they contribute to the thermodynamic properties. Thus at $U = 2|\epsilon|$ the model has an absorption threshold at finite energy, i.e., an "optical" gap, even though the continuous spectrum of internal elementary excitations extends down to $\Lambda_k = 0$.

The dual excitation spectrum suggests that a solution of the free energy equations (14)–(21) will yield *two* maxima in the specific heat, a feature which has already been discovered in numerical computation[4] of the properties of finite Hubbard-model chains ($N \leq 6$).

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