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Representation theory for the Hubbard model

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Abstract

The space of electronic states in a lattice, with fixed occupation and spin quantum numbers, is identified with the space of holomorphic cross sections of an irreducible homogeneous line bundle. The Hubbard Hamiltonian, among others, is represented here by a right-invariant differential operator and the Schrödinger equation by a linear partial differential equation for which the associated wavefunction admits a recurrent series expansion.

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1. Introduction

The space of states relevant for the description of electrons in a lattice L with l sites proves to be finite-dimensional. From the general rules of quantum mechanics an electron is represented by a state in a $2l$ -dimensional Hilbert space $E \otimes \mathcal{C}^2$, where E contains the spatial part of the state and \mathcal{C}^2 describes the spin components. After the identification $E \otimes \mathcal{C}^2 \cong E \oplus E$ is taken into account, a set of electrons in that lattice, which is represented by a vector in the antisymmetric tensor product $\Lambda(E \otimes \mathcal{C}^2)$, can be equally expressed as a point of

$$\mathcal{H} = \Lambda(E \oplus E) = \Lambda(E) \otimes \Lambda(E).$$

A basis of orthonormal spinless one-particle states $\{x_1, x_2, \dots, x_l\}$ generates the 4^l localized states $x^\alpha \otimes x^\beta$, $x^\alpha = x_1^{\alpha_1} x_2^{\alpha_2} \dots x_l^{\alpha_l}$, $\alpha_a = 0, 1$, which form an orthonormal basis of the Fock space \mathcal{H} . An equivalent description, treated in [1, 2], of these electronic states is furnished by the identification of \mathcal{H} with the isomorphic space

$$\mathcal{H} = \Lambda(E \oplus E) \cong \Lambda(E) \otimes \Lambda(E)^*$$

the complex Clifford algebra $C(l)$ of E , that allows us to describe simultaneously two aspects of the electronic problem in the lattice: its fermionic and bosonic character. Both aspects are displayed by two basis states in this Clifford algebra with given values for spins up and down or the number of pairs and holes in the lattice L , respectively.

In both instances, \mathcal{H} as a representation space for the unitary group U_l splits as a sum of irreducible subspaces labelled by two quantum numbers: the total spin s and the number

of particles N . There is a Hilbert space decomposition which gives \mathcal{H} as a direct sum of irreducible subspaces \mathcal{H}_{AB} with $N = l + A - B$ particles and total spin $s = (l - A - B)/2$:

$$\mathcal{H} = \bigoplus_{A+B \leq l} (1 + S_+)^{l-(A+B)} (\mathcal{H}_{AB} \oplus \mathcal{H}_{BA}).$$

Thus, the diagonalization problem for the Hubbard Hamiltonian, as for any Hamiltonian defined by an element in the enveloping algebra of the Lie algebra u_l , reduces to a corresponding series of spectral problems in the highest weight modules \mathcal{H}_{AB} indexed by the spin and occupation numbers s and N . They are irreducible subspaces for the action of the unitary group U_l , of highest weight $\lambda = (1, \dots, 1, 0, \dots, 0, -1, \dots, -1)$ with the first A components equal to 1 and the last B equal to -1 . As an abstract representation space for U_l , \mathcal{H}_{AB} , from now on denoted by \mathcal{H}_λ , admits two realizations in the Clifford algebra with generators $\{x_1, \dots, x_l, \partial_1, \dots, \partial_l\}$ where we denote by $\partial_a = \partial/\partial x_a$ the adjoint operator of the multiplication operator x_a (for details see [1, 2]). The first of these realizations is as a fermionic space of up and down spins. The dominant vector $x_1 \dots x_A \Omega^+ x_1 \dots x_{l-B}$ containing A spins up and $l - B$ spins down is written here in terms of a fixed volume form $\Omega^+ = \partial_1 \partial_2 \dots \partial_l$. But \mathcal{H}_λ can also be viewed, in the second realization, as a bosonic space with a defined number of pairs and holes for the basic states in the orbit of the dominant vector $x_1, \dots, x_A \partial_{l+1-B} \dots \partial_l$ with A pairs and B holes. In both cases the action of the S_+ spin operator should be considered to account for the distinct values of the S_z component of the spin in the space \mathcal{H} . Adding ones to each component of λ produces a highest weight for an irreducible subspace of $\Lambda(E) \otimes \Lambda(E)$, which corresponds to the dominant vector $x_1, \dots, x_A \otimes x_1, \dots, x_{l-B}$ with A spins up and $l - B$ spins down.

As we said before, the Hamiltonian is an element of the enveloping algebra of the unitary group which acts in any of its representations. With the notation conventions of [1, 2] we write

$$H\psi = -i[iK, \psi] + V(in_1, \dots, in_l)\psi \tag{1.1}$$

for ψ in $C(l)$; the potential V in the simplest version of the model is given by

$$V(in_1, \dots, in_l) = \frac{U}{2} \left(\sum_{a=1}^l [in_a, [in_a, \psi]] - \frac{l}{2} \psi \right) \tag{1.2}$$

but any polynomial in the number operators n_a can also be considered.

The present formulation for the Hubbard model, based on representation theory for Lie algebras, readily extends to most of the models of interacting electrons in a lattice. Let us examine some examples. Choosing now the space $\Lambda(E \oplus E)$ as the representation space for the system, spin up and down states for a single electron in the lattice are furnished by the set of anticommuting variables $x_1, x_2, \dots, x_l, y_1, y_2, \dots, y_l$. In terms of these, the procedure followed in [1] to translate the Hubbard Hamiltonian into the language of representation theory applies equally, for instance, to the Hamiltonian [3]

$$\begin{aligned} H = & -t \sum_{\langle ij \rangle, \sigma} (c_{i,\sigma}^+ c_{j,\sigma} + c_{j,\sigma}^+ c_{i,\sigma}) \\ & + V \sum_{\langle ij \rangle} (n_i - 1)(n_j - 1) + J \sum_{\langle ij \rangle} (S_i^z S_j^z + \frac{1}{2} S_i^+ S_j + \frac{1}{2} S_j^+ S_i) \\ & + X \sum_{\langle ij \rangle, \sigma} (c_{i,\sigma}^+ c_{j,\sigma} + c_{j,\sigma}^+ c_{i,\sigma}) (n_{i,-\sigma} + n_{j,-\sigma}) \\ & + Y \sum_{\langle ij \rangle} (c_{i,1}^+ c_{i,-1}^+ c_{j,-1} c_{j,1} + c_{j,1}^+ c_{j,-1}^+ c_{i,-1} c_{i,1}) \\ & + U \sum_i (n_{i,1} - \frac{1}{2})(n_{i,-1} - \frac{1}{2}) \end{aligned}$$

where more types of interactions are present. One finds in this case the following operator in the enveloping algebra of $gl(l, \mathcal{C})$:

$$\begin{aligned} H = & -t \sum_{(ij)} (\xi_{ij} + \xi_{ji}) + V \sum_{(ij)} (n_i - 1)(n_j - 1) \\ & - \frac{1}{4} J \sum_{(ij)} [\xi_{ij} \xi_{ji} + \xi_{ji} \xi_{ij} + (n_i - 1)(n_j - 1) - 1] \\ & + X \sum_{(ij)} (\xi_{ij} n_i + n_i \xi_{ji} + \xi_{ji} n_j + n_j \xi_{ij}) \\ & + \frac{1}{2} Y \sum_{(ij)} (\xi_{ij}^2 + \xi_{ji}^2) + \frac{U}{2} \sum_i (n_i - 1)^2. \end{aligned}$$

Here $\xi_{ij} = x_i \partial / \partial x_j + y_i \partial / \partial y_j$ is the operator that represents the elementary matrix E_{ij} with one in place (i, j) and zeros elsewhere; the electron number operators are $n_i = x_i \partial / \partial x_i + y_i \partial / \partial y_i$.

Analogous reasoning, when applied to the supersymmetric $U(2|2)$ Hamiltonian $H^0 = \sum_{(jk)} H_{jk}^0$ of [4], with

$$\begin{aligned} H_{jk}^0 = & (c_{k,1}^+ c_{j,1} + c_{j,1}^+ c_{k,1}) (1 - n_{j,-1} - n_{k,-1}) \\ & + (c_{k,-1}^+ c_{j,-1} + c_{j,-1}^+ c_{k,-1}) (1 - n_{j,1} - n_{k,1}) \\ & + \frac{1}{2} (n_j - 1)(n_k - 1) + c_{j,1}^+ c_{j,-1}^+ c_{k,-1} c_{k,1} + c_{j,-1} c_{j,1} c_{k,1}^+ c_{k,-1}^+ \\ & - \frac{1}{2} (n_{j,1} - n_{j,-1})(n_{k,1} - n_{k,-1}) - c_{j,-1}^+ c_{j,1} c_{k,1}^+ c_{k,-1} - c_{j,1}^+ c_{j,-1} c_{k,-1}^+ c_{k,1} \\ & + (n_{j,1} - \frac{1}{2})(n_{j,-1} - \frac{1}{2}) + (n_{k,1} - \frac{1}{2})(n_{k,-1} - \frac{1}{2}) \end{aligned}$$

leads to the operator

$$H^0 = \sum_{(jk)} [(1 - n_k) \xi_{jk} (1 - n_j) + (1 - n_j) \xi_{kj} (1 - n_k) + \frac{1}{2} (\xi_{kj} \xi_{jk} + \xi_{jk} \xi_{kj}) + \frac{1}{4} n_j n_k].$$

Finally, we shall cite the Hamiltonian related to the $SO(5)$ symmetry [5] that unifies antiferromagnetism and superconductivity. This symmetry was earlier conjectured [6] to be an approximate symmetry for high- T_c cuprate compounds. The kinetic energy coincides with that of the $SO(4)$ Hubbard Hamiltonian considered before, but the interaction is now given by a potential of the form

$$V^s = U^s \sum_a (n_a^s)^2$$

with $n_a^s = \frac{1}{2}(n_a - n_a^d)$, where n_a still denotes the number operator in site a and n_a^d represents an element of the Lie algebra. The potential energy V^s is then manifestly an element of the enveloping algebra as in previous examples.

The remarkable fact that emerges from these considerations is that, although spin operators are not in the enveloping algebra and do not represent the action of vectors in $gl(l, \mathcal{C})$, they appear in the resulting Hamiltonian combined in such a way that they have a meaning in representation theory. This seems to be intimately related to the symmetry properties for the Hamiltonians in question that allow us to preserve the irreducible representation subspaces.

No doubt the majority of the exact results for strongly interacting many-fermion systems are drawn from symmetry considerations which lead to a class of solutions with varying degrees of completeness and interest. In that direction we can cite the Bethe ansatz for one-dimensional models in the collected papers of [7], the results of the spin of the ground state [8,9], interactions with magnetic fields [10], the η Yang's symmetry [11], the occurrence of ferromagnetic ground states [12] and the half-filled states and energies for periodic lattices of [2], among others.

In the present paper we pursue a logical development of the connection of representation theory with fermionic systems indicated in [1, 2]. This relationship is best understood in the unitary context in the realm of Borel–Weil theory whose importance as a part of the Bott–Borel–Weil theorem [13] can scarcely be exaggerated. The theory of functions on homogeneous manifolds for the action of a Lie group, to which the theorem applies, serves to describe systems of fermions in a lattice. This description is quite similar to that used in the construction of the Penrose transform for the solutions of linear field equations [14].

The Borel–Weil theorem provides us with a global definition of the states of the fermionic system as opposite to the point by point construction through tensor products of simpler states we saw before. For states with fixed spin and occupation numbers this is achieved through the space of holomorphic cross sections of an homogeneous bundle for the unitary group where the Hamiltonian acts as a right-invariant differential operator. In this formulation the Schrödinger equation becomes a differential equation that describes the system in a way that resembles the duality between the matrix mechanics of Heisenberg and the wavefunction of Schrödinger in early quantum mechanics. A more recent parallel to this construction can be found in the reformulation of quantum field theory in the language of statistical mechanics that allows for the replacement of noncommuting variables in favour of ordinary functions [15].

Besides this unified approach, the present formulation yields a procedure for solving the Schrödinger equation. When written in terms of a coordinate system for the group manifold one obtains a partial differential equation for which the physical solutions admit a series expansion that leads to recurrent formulae for the coefficients of this wavefunction. The main result of the present work is thus the formulation of the algebraic system as a recurrent system for the coefficients of the Taylor series of the wavefunction.

The organization and content of the paper are as follows. In section 2 we associate the space of holomorphic cross sections of an irreducible homogeneous line bundle to the set of states with fixed values of the spin and number of particles. This identification follows from the Borel–Weil theorem in representation theory that we briefly recall. The Hamiltonian acts on this space by a right-invariant differential operator and the Schrödinger equation results in a differential equation which can be exactly solved, for example, in a two-point lattice.

Section 3 is devoted to the analysis of the differential equation which is conveniently written in a local coordinate system adapted to the Hubbard Hamiltonian. There we introduce the notion of a relative differential which proves to be useful for the treatment of this problem. Finally, in section 4 we obtain a recurrent description for the terms of the series expansion of the solutions and compare the approximate and exact solutions for the lattice with two sites.

2. Abstract fermions and the Borel–Weil theorem

Much of our understanding of the Hubbard problem in the present paper follows from the construction of the irreducible representations of the unitary group in terms of its homogeneous spaces as given by the Borel–Weil theorem. In this context the Hilbert space of states with fixed number of electrons and spin will be given by a subspace of $L^2(U_l)$ where the Hamiltonian acts as a right-invariant differential operator.

If T denotes the maximal torus in the unitary group $G = U_l$ given by the subgroup of diagonal matrices, every homomorphism $\lambda : T \rightarrow S^1$, where S^1 denotes the circle group, extends [16] to a holomorphic homomorphism $\lambda : B \rightarrow C^\times$, where B is the Borel subgroup of upper triangular matrices containing T . With such homomorphism λ we can define a homogeneous holomorphic line bundle

$$L_\lambda = G_C \times_B C_\lambda$$

on $G_C/B \cong G/T$, where L_λ is the quotient $(G_C \times C_\lambda)/B$.

The space of holomorphic cross sections of the bundle L_λ can be identified with the space of functions on G satisfying

$$f(g g_0) = \lambda(g_0^{-1}) f(g) \quad (2.1)$$

The Borel–Weil theorem [13, 14, 16] affirms that L_λ has no non-zero holomorphic sections unless λ is a dominant weight and in that case the space of holomorphic sections Γ_λ is an irreducible representation of G with highest weight λ .

As we previously observed, electronic states with fixed quantum numbers are a representation space for the unitary group G that, in the light of the Borel–Weil theorem, can be identified with the space of sections Γ_λ ; the holomorphic functions on G satisfying condition (2.1). The scalar product that makes it a Hilbert space is furnished by the restriction of the scalar product in $L^2(G)$ to Γ_λ :

$$(f_1, f_2) = \int_G \overline{f_1(g)} f_2(g) \, dg$$

where dg denotes the Haar measure on G . The correspondence between both spaces can be made more explicit as follows. Let ψ_1, ψ_2 be states in the algebraic space \mathcal{H}_λ of the previous section for which we define the scalar product [1]

$$(\psi_1, \psi_2) = \text{tr}(\psi_1^+ \psi_2)$$

in accordance with the interpretation of $\mathcal{H} = C(l)$ as the space of linear transformations of $\Lambda(E)$. We denote by $g \cdot v_\lambda$ the orbit of the dominant vector $v_\lambda = x^\alpha \partial^\beta$ if $\lambda = \alpha - \beta$ as in section 1. Such an orbit comes simply from the replacement in v_λ of the vectors x_a and ∂_b by their images for the action of G on E and E^* , respectively. Let ψ be a state in \mathcal{H} for which we define the function on G

$$f(g) = (g \cdot v_\lambda, \psi) \quad (2.2)$$

which satisfies condition (2.2) and hence belongs to Γ_λ . This gives the desired connection. Looking now at the scalar products one has the relation [17]

$$\int_G (g \cdot v_1, \psi_1)(\psi_2, g \cdot v_2) \, dg = \frac{1}{\dim \mathcal{H}_\lambda} (v_1, v_2)(\psi_2, \psi_1)$$

that, for $v_1 = v_2 = v_\lambda$ and $f_i(g) = (g \cdot v_\lambda, \psi_i)$, $i = 1, 2$, is

$$\int_G \overline{f_1(g)} f_2(g) \, dg = \frac{\|v_\lambda\|^2}{\dim \mathcal{H}_\lambda} (\psi_1, \psi_2)$$

which is the formula we were looking for. Besides the correspondence between states and sections of a bundle we should determine the action of the elements of the enveloping algebra in that bundle. They are conveniently described in terms of right-invariant differential operators acting on functions over the group G [18]. So for the kinetic energy operator one finds the expression

$$(Tf)(g) = i \frac{d}{dt} \Big|_{t=0} f(e^{iKt} g) \quad (2.3)$$

that describes the action of the vector field associated with the flow in G given by the one-parameter subgroup $\{\exp iKt\}$ and which corresponds to the action in \mathcal{H}_λ through formula (1.1), but notice that there K represents an action in $C(l)$. The complete Hubbard Hamiltonian is now

$$(Hf)(g) = \left[i \frac{d}{dt} + V \left(i \frac{\partial}{\partial \theta_1}, \dots, i \frac{\partial}{\partial \theta_l} \right) \right]_0 f(e^{iKt+i(\theta,n)} g) \quad (2.4)$$

where the subscript 0 means evaluation at $t = \theta_1 = \dots = \theta_l = 0$ and we have set $(\theta, n) = \theta_1 n_1 + \dots + \theta_l n_l$ in terms of the elementary diagonal matrices n_a . It is easy to see that the usual Hubbard Hamiltonian defined by the potential energy (1.2) is given by the Schrödinger operator

$$\left(i \frac{\partial}{\partial t} - \frac{U}{2} \Delta_\theta \right)_0 f(e^{iKt+i(\theta,n)} g)$$

neglecting the constant term.

An explicit solution of the associated Schrödinger differential equation can be obtained in the simplest cases. To see that, consider, for instance, the problem for a lattice with two sites. Let us parametrize the element g in U_2 by the angular coordinates θ, s, ϕ , in terms of which we write

$$g = h_\theta u_s k_\phi \tag{2.5}$$

where

$$h_\theta = \begin{pmatrix} e^{i\theta_1} & 0 \\ 0 & e^{i\theta_2} \end{pmatrix} \quad u_s = e^{i\frac{s}{2}\sigma_1} = \begin{pmatrix} \cos \frac{s}{2} & i \sin \frac{s}{2} \\ i \sin \frac{s}{2} & \cos \frac{s}{2} \end{pmatrix}$$

and

$$k_\phi = e^{i\frac{\phi}{2}\sigma_3} = \begin{pmatrix} e^{i\frac{\phi}{2}} & 0 \\ 0 & e^{-i\frac{\phi}{2}} \end{pmatrix}.$$

Let $F(\theta, s, \phi) = f(h_\theta u_s k_\phi)$ be the local expression for f in these coordinates and let the kinetic energy be defined by the hopping matrix

$$K = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

for which we obtain the operator

$$i \frac{d}{dt} \Big|_{t=0} f(e^{iKt} g) = i(\dot{\theta}, \nabla_\theta F) + i\dot{s} \frac{\partial F}{\partial s} + i\dot{\phi} \frac{\partial F}{\partial \phi}.$$

To compute the derivatives of the coordinates at $t = 0$, $\dot{\theta}$, \dot{s} and $\dot{\phi}$, we consider the curve $m(t)$ in G :

$$m(t) = e^{iKt} g = h_{\theta(t)} u_{s(t)} k_{\phi(t)}$$

where we take the right derivative

$$\frac{dm}{dt} m^{-1}$$

at $t = 0$ to get the formula

$$iK = \begin{pmatrix} i\dot{\theta}_1 & 0 \\ 0 & i\dot{\theta}_2 \end{pmatrix} + \frac{\dot{s}}{2} \begin{pmatrix} 0 & ie^{i(\theta_1-\theta_2)} \\ ie^{-i(\theta_1-\theta_2)} & 0 \end{pmatrix} + \frac{\dot{\phi}}{2} \begin{pmatrix} i \cos s & e^{i(\theta_1-\theta_2)} \sin s \\ -e^{-i(\theta_1-\theta_2)} \sin s & i \cos s \end{pmatrix}$$

from which we deduce the expression for the kinetic energy

$$i \frac{d}{dt} \Big|_{t=0} f(e^{iKt} g) = i \sin(\theta_1 - \theta_2) \cot s \left(\frac{\partial F}{\partial \theta_2} - \frac{\partial F}{\partial \theta_1} \right) + 2i \cos(\theta_1 - \theta_2) \frac{\partial F}{\partial s} + 2i \frac{\sin(\theta_1 - \theta_2)}{\sin s} \frac{\partial F}{\partial \phi}.$$

With our choice of coordinates the potential energy is simply

$$-\frac{U}{2} (\Delta_\xi + 1) \Big|_{\xi=0} f(e^{i(\xi,n)} g) = -\frac{U}{2} (\Delta_\theta + 1) F(\theta, s, \phi)$$

and the Schrödinger equation is now

$$-\frac{U}{2} \Delta_\theta F + i \sin(\theta_1 - \theta_2) \cot s \left(\frac{\partial F}{\partial \theta_2} - \frac{\partial F}{\partial \theta_1} \right) + 2i \cos(\theta_1 - \theta_2) \frac{\partial F}{\partial s} + 2i \frac{\sin(\theta_1 - \theta_2)}{\sin s} \frac{\partial F}{\partial \phi} = \left(E + \frac{U}{2} \right) F.$$

The highest weight $\lambda = (1, -1)$ defines the subspace of half-occupied states with spin zero which, in accordance with the properties stated for F , are described by a function of the following type:

$$F(\theta, s, \phi) = e^{-i\phi} [a(s)e^{i(\theta_1 - \theta_2)} + b(s)e^{-i(\theta_1 - \theta_2)} + c(s)].$$

The system of first-order ordinary differential equations for the functions a, b, c determines the energy levels and states, one finds at $E = U/2$ the solution

$$F(\theta, s, \phi) = e^{-i\phi} (e^{i(\theta_1 - \theta_2)} \sin^2 s/2 + e^{-i(\theta_1 - \theta_2)} \cos^2 s/2) \quad (2.6)$$

and for the levels $E^2 = 4 + U^2/4$ the corresponding solution is now

$$F(\theta, s, \phi) = e^{-i\phi} \left[e^{i(\theta_1 - \theta_2)} \sin^2 s/2 - e^{-i(\theta_1 - \theta_2)} \cos^2 s/2 + \frac{i}{2} \left(E - \frac{U}{2} \right) \sin s \right] \quad (2.7)$$

which show in each case the pair and holes content of the states prescribed by the weight μ appearing in $\exp -i(\mu, \theta)$. The weight $\mu = (1, -1)$ indicates a pair in site 1 and a hole in site 2, the same for $\mu = (-1, 1)$ but exchanging pairs and holes, and $\mu = (0, 0)$ represents a state without pairs and holes.

3. The differential equation

In general, for a lattice with arbitrary many points, there is not a simple explicit expression for the differential operator associated with the Hamiltonian. We shall see, however, that it can be written in a form that will prove useful for computations. Let g be in U_l and define the right-invariant differential form

$$\omega = dg g^{-1}$$

with values in the Lie algebra u_l . The coefficients of ω in a given basis of u_l span the cotangent bundle of U_l at the identity. The usual realization of u_l by the space of skew-Hermitian complex $l \times l$ matrices, with the trace scalar product defined by $(A, B) = \text{tr}(A^+ B)$, allows one to represent the differential of a function $f(g)$ in the form

$$df = (\omega, \Phi). \quad (3.1)$$

For a fixed coordinate system of U_l at the identity, the relative differential Φ of f is a matrix given in terms of the partial derivatives of f with respect to the chosen coordinates. Let us prove that, for a section f in Γ_λ , the corresponding Φ belongs to the space $\Gamma_\lambda \otimes gl_l(C)$. This can be seen by considering the representation (2.2) for f from which the differential is

$$df(g) = ([L(\omega), v_\lambda(g)], \psi)_{C(l)}$$

where $L(\omega)$ represents the form ω and $v_\lambda(g) = g \cdot v_\lambda$ is the orbit of v_λ . Due to the invariance of the scalar product we can write

$$df(g) = (L(\omega), [v_\lambda^+(g), \psi])_{C(l)}$$

from which, after we identify $gl_l(C)$ with the subspace $C\{x_a \frac{\partial}{\partial x_b}\} \subset C(l)$, one deduces that Φ corresponds to the gl_l component of $[v_\lambda^+(g), \psi]$, the subspace in $C(l)$ that contains $L(\omega)$.

Such a matrix Φ has the announced properties because the vector function $v_\lambda^+(g)$ transforms under a right translation by a diagonal element g_0 of the maximal torus T according to

$$v_\lambda^+(g g_0) = \lambda(g_0^{-1}) v_\lambda^+(g).$$

The matrix Φ allows one to write the kinetic energy in very simple terms. Since the kinetic energy operator (2.3) is given by the vector field ∂_K in U_l issued from the vector iK at the identity, we deduce from the contraction of equation (3.1) with ∂_K the formula

$$(Tf)(g) = i(iK, \Phi(g)) = (K, \Phi(g))$$

which implies the identification of the kinetic energy with the component of $\Phi(g)$ on K .

As before, we let $\theta = (\theta_1, \dots, \theta_l)$ be the angular coordinates of the torus T and denote by Z a skew-Hermitian matrix, $Z + Z^+ = 0$, with zero diagonal part. The local coordinates (θ, Z) allow one to write $g = \exp i\theta \exp Z$ and with this choice of coordinates the potential energy becomes

$$V \left(i \frac{\partial}{\partial \xi_1}, \dots, i \frac{\partial}{\partial \xi_l} \right) \Big|_{\xi=0} f(e^{i\xi} e^{i\theta} e^Z) = V \left(i \frac{\partial}{\partial \theta_1}, \dots, i \frac{\partial}{\partial \theta_l} \right) f(e^{i\theta} e^Z)$$

since $\exp i\xi \exp i\theta = \exp i(\xi + \theta)$.

The preceding formulae imply the equivalence of the Schrödinger equation $(H - E)f = 0$ for the Hamiltonian (2.4) with the pair of equations

$$dF = (\omega, \Phi) \tag{3.2}$$

$$(K, \Phi) + VF = EF. \tag{3.3}$$

The differential form ω in the present coordinates adopts the expression

$$\omega = dg g^{-1} = i d\theta + e^{i\theta} (de^Z e^{-Z}) e^{-i\theta}$$

and $F(\theta, Z) = f(e^{i\theta} e^Z)$.

The meaning of these equations is that they define Φ through (3.2) to give a differential equation for F upon substitution of Φ in (3.3). Although it will not be used in what follows, it seems of interest to see how this can be done. So we let $\{K/\|K\|, Q_\gamma\}$ be an orthonormal basis of u_l and write (3.2) in the form

$$dF = \frac{1}{\|K\|^2} (\omega, K)(K, \Phi) + \sum_\gamma (\omega, Q_\gamma)(Q_\gamma, \Phi)$$

as follows from the representation of ω in the fixed basis. Substitution of (K, Φ) as given by (3.3) in the expression above results in

$$dF = \frac{1}{\|K\|^2} (\omega, K)[E - V]F + \sum_\gamma (\omega, Q_\gamma)(Q_\gamma, \Phi)$$

from which we can eliminate Φ if we take the product of this equation with the $(l^2 - 1)$ differential form $\prod (\omega, Q_\gamma) = \chi'$. This is the case since each coefficient containing Φ in the expression for dF vanishes after multiplication with χ' because all the 1-forms (ω, Q_γ) are present in χ' . Denote by $\chi = \|K\|^{-1} \chi' \wedge (\omega, K)$ the invariant volume element for U_l . Then we have the equation for F :

$$\chi' \wedge dF = \frac{1}{\|K\|} \chi [E - V]F.$$

But this form of the Schrödinger equation appears to be more involved than the system (3.2) and (3.3) where the restrictions on F , as an element of Γ_λ , are explicitly taken into account through the relation (3.2).

4. Recurrence relations for the wavefunction

The analysis of the Schrödinger equation in the form (3.2) and (3.3) permits us to derive some conclusions about the state F . Because all objects F , Φ , ω appearing in these equations are analytic they admit a Taylor expansion in the local coordinates Z around $Z = 0$. This is the case for the differential form ω defined as

$$\omega = dg g^{-1} = i d\theta + \zeta^\theta$$

where we denote $\zeta^\theta = e^{i\theta} \zeta e^{-i\theta}$ and

$$\zeta = de^Z e^{-Z} = dZ + \frac{1}{2}[Z, dZ] + \frac{1}{3!}[Z, Z, dZ] + \dots$$

We thus have a series

$$\omega = \omega_0 + \omega_1 + \dots$$

with ω_m of degree m in the coordinates Z :

$$\omega_0 = i d\theta \quad \omega_1 = e^{i\theta} dZ e^{-i\theta}, \dots$$

For F and Φ we have analogous expansions

$$\begin{aligned} F(\theta, Z) &= F_0(\theta, Z) + F_1(\theta, Z) + \dots \\ \Phi(\theta, Z) &= \Phi_0(\theta, Z) + \Phi_1(\theta, Z) + \dots \end{aligned}$$

where $F_m(\theta, Z)$, $\Phi_m(\theta, Z)$ are defined by homogeneous polynomials, in the Z coordinates, of degree m . Both F and Φ satisfy the functional relations (2.1)

$$F(\theta, Z) = e^{-i(\lambda, \theta)} F(0, Z^\theta) \quad \Phi(\theta, Z) = e^{-i(\lambda, \theta)} \Phi(0, Z^\theta)$$

as local representatives of a section and a matrix of sections, respectively, of the line bundle L_λ , due to the fact that $e^{i\theta}$ belongs to T . Thus we see that F and Φ are determined by their dependence on Z . To proceed further, we substitute the analytic objects appearing in equations (3.2) and (3.3) by their foregoing expansions to obtain the recurrence relations for the homogeneous parts of F . In doing so one gets the set of conditions

$$dF_m = (\omega_0, \Phi_m) + (\omega_1, \Phi_{m-1}) + \dots + (\omega_m, \Phi_0) \quad (4.1)$$

$$(K, \Phi_m) = (E - V)F_m \quad (4.2)$$

for $m = 0, 1, 2, \dots$. Since ω_0 is diagonal while ω_1 is nondiagonal, we deduce from (4.1) at each step m the expression for the diagonal part of Φ_m and the nondiagonal components of Φ_{m-1} in terms of F_m and the preceding $\Phi_0, \Phi_1, \dots, \Phi_{m-2}$. Assume we have computed $\Phi_0, \Phi_1, \dots, \Phi_{m-1}$; then, setting together diagonal and nondiagonal parts we obtain for Φ_m the recurrent formula

$$\begin{aligned} \Phi_m &= i \nabla_\theta F_m + e^{i\theta} \nabla_Z F_{m+1} e^{-i\theta} + \frac{1}{2}[Z^\theta, \Phi_{m-1}]' \\ &\quad - \frac{1}{3!}[Z^\theta, Z^\theta, \Phi_{m-2}]' + \dots + \frac{(-1)^{m+1}}{(m+1)!}[Z^\theta, \dots, Z^\theta, \Phi_0]'. \end{aligned} \quad (4.3)$$

In this expression $[Z^\theta, Z^\theta, \Phi_{m-2}]'$, for instance, means the nondiagonal part of the matrix commutator

$$(\text{ad } Z^\theta)^2 \Phi_{m-2} = [Z^\theta, [Z^\theta, \Phi_{m-2}]]$$

with $Z^\theta = e^{i\theta} Z e^{-i\theta}$. The notation $\nabla_\theta F_m, \nabla_Z F_{m+1}$ is used to represent the differential dF_m in terms of the scalar product of these symbols with the matrix differentials of

$$\theta = \theta_1 n_1 + \dots + \theta_l n_l$$

and

$$Z = \sum_{\alpha>0} (z_\alpha e_\alpha - \bar{z}_\alpha f_\alpha)$$

in each case. Accordingly we write

$$dF = (d\theta, \nabla_\theta F) + (dZ, \nabla_Z F)$$

from which we deduce the relations

$$\nabla_\theta F = \sum_a n_a \frac{\partial F}{\partial \theta_a} \quad \nabla_Z F = \sum_\alpha e_\alpha \frac{\partial F}{\partial \bar{z}_\alpha} - f_\alpha \frac{\partial F}{\partial z_\alpha}.$$

As usual, $\{e_\alpha, f_\alpha\}$ represent the root vectors corresponding to the diagonal subalgebra with positive roots α . After substitution of Φ_m , as given by (4.3) in (4.2), we get the desired recurrence formula for the homogeneous components F_m of the wavefunction F :

$$(K^{-\theta}, \nabla_Z) F_{m+1} = (E - V) F_m - \frac{1}{2} (K, [Z^\theta, \Phi_{m-1}]) + \dots + \frac{(-1)^m}{(m+1)!} (K, [Z^\theta, \dots, Z^\theta, \Phi_0]) \tag{4.4}$$

where $\Phi_0, \Phi_1, \dots, \Phi_{m-1}$ are expressed in terms of F_0, F_1, \dots, F_m as prescribed by equation (4.3). Thus, formulae (4.3) and (4.4) give the desired recurrent relations for the analytic objects. Next, let us examine what these equations become when the functional relations in the space Γ_λ are taken into account.

The dependence in θ of the wavefunction F and the matrix Φ is determined by the Fourier expansions in the space of sections Γ_λ according to the formulae prescribed by the representation (2.2). One has

$$F(\theta, Z) = \sum_{\mu \leq \lambda} F_\mu(Z) e^{-i(\mu, \theta)}$$

$$\Phi(\theta, Z) = \sum_{\mu \leq \lambda} \Phi_\mu(Z) e^{-i(\mu, \theta)}$$

where the summation extends over all admissible weights μ for which $\lambda - \mu$ is a sum of positive roots. This set is the weight system Π_λ with highest weight λ [16]. Each Fourier component F_μ of the wavefunction F is proportional to the probability amplitude of having a number of pairs and holes in such a state fixed by the weight μ . The recurrence formulae (4.4) for F are further strengthened upon substitution of the previous Fourier expansions and they become

$$(K, \Phi_{m\mu}) = [E - V(\mu)] F_{m\mu} \tag{4.5}$$

besides the expressions for $\Phi_{m\mu}$ that follow from (4.3). To get a more detailed description of these equations we shall proceed as follows.

At $m = 0$ one has

$$F_0 = F_{0\lambda} e^{-i(\lambda, \theta)}$$

with $F_{0\lambda} = \text{const}$ as follows, for instance, from (2.2). For Φ_0 we deduce from equation (4.3) the formula

$$\Phi_0 = i \nabla_\theta F_0 + e^{i\theta} \nabla_Z F_1 e^{-i\theta}$$

$$= F_{0\lambda} e^{-i(\lambda, \theta)} n_\lambda + \sum_{\alpha, \mu} \left(e_\alpha \frac{\partial F_{1\mu}}{\partial \bar{z}_\alpha} e^{-i(\mu - \alpha, \theta)} - f_\alpha \frac{\partial F_{1\mu}}{\partial z_\alpha} e^{-i(\mu + \alpha, \theta)} \right)$$

where $n_\lambda = \lambda_1 n_1 + \lambda_2 n_2 + \dots + \lambda_l n_l$ is the diagonal matrix defined by the weight λ . Because the matrix Φ_0 is of the form

$$\Phi_0 = \Phi_{0\lambda} e^{-i(\lambda, \theta)}$$

we get, by direct substitution in the previous formula, the relation

$$\Phi_{0\lambda} = F_{0\lambda} n_\lambda - \sum_{\lambda-\alpha \in \Pi_\lambda} f_\alpha \frac{\partial F_{1\lambda-\alpha}}{\partial z_\alpha}$$

where the sum extends to those positive roots α for which $\lambda - \alpha$ is a weight. Besides the formula for Φ_0 one gets for F_1 the set of conditions

$$\partial F_1 / \partial \bar{z}_\alpha = 0 \quad (4.6)$$

for every α , and

$$\partial F_1 / \partial z_\alpha = 0 \quad (4.7)$$

if $\lambda - \alpha \notin \Pi_\lambda$ as follows from the definitions of Φ_0 and F_1 .

At degree zero the Schrödinger equation (4.5) is

$$(K, \Phi_{0\lambda}) = [E - V(\lambda)] F_{0\lambda}$$

that, after substitution of $\Phi_{0\lambda}$, results in a condition for the coefficients $\partial F_{1\lambda-\alpha} / \partial z_\alpha$ of the linear function F_1 :

$$- \sum_{\lambda-\alpha \in \Pi_\lambda} k_\alpha \frac{\partial F_{1\lambda-\alpha}}{\partial z_\alpha} = [E - V(\lambda)] F_{0\lambda}. \quad (4.8)$$

Along these lines one should continue with the case $m = 1$ for which the differential (4.3) takes the form

$$\Phi_1 = i \nabla_\theta F_1 + e^{i\theta} \nabla_Z F_2 e^{-i\theta} + \frac{1}{2} [Z^\theta, \Phi_0]' \quad (4.9)$$

with the corresponding Fourier expansion given by

$$\begin{aligned} \sum_\mu \Phi_{1\mu} e^{-i(\mu, \theta)} &= \sum_\mu F_{1\mu} e^{-i(\mu, \theta)} n_\mu \\ &+ \sum_{\alpha, \nu} \left(e_\alpha \frac{\partial F_{2\nu}}{\partial \bar{z}_\alpha} e^{-i(\nu-\alpha, \theta)} - f_\alpha \frac{\partial F_{2\nu}}{\partial z_\alpha} e^{-i(\nu+\alpha, \theta)} \right) \\ &+ \frac{1}{2} \sum_\alpha z_\alpha e^{-i(\lambda-\alpha, \theta)} [e_\alpha, \Phi_{0\lambda}]' \\ &- \frac{1}{2} \sum_\alpha \bar{z}_\alpha e^{-i(\lambda+\alpha, \theta)} [f_\alpha, \Phi_{0\lambda}]' \end{aligned} \quad (4.10)$$

where n_μ is the diagonal matrix defined by the weight μ and the sum over μ goes through Π_λ while $\alpha \in \Delta_+$, the system of positive roots for the Lie algebra.

The general procedure to analyse this type of expression, that one encounters at all orders m , is the following. As one easily realizes, each of the matrix elements (e_α, Φ) , (f_α, Φ) belongs to the space of sections Γ_λ and, at order m , satisfies the conditions previously found for F_m as a homogeneous part of the section given by F . These conditions will imply new relations for F_{m+1} and simultaneously allow for the construction of Φ_m . So, when applied to Φ_1 , we deduce from (4.10), considering the e_α component of this equation and equations (4.6) and (4.7), that

$$\frac{\partial^2 F_{2\nu}}{\partial \bar{z}_\alpha \partial \bar{z}_\beta} = 0 \quad (4.11)$$

and the expression

$$\frac{\partial}{\partial z_\beta} (e_\alpha, \Phi_{1\lambda-\beta}) = -([e_\alpha, f_\beta], \Phi_{0\lambda}) \quad (4.12)$$

which one deduces after some computation.

Analogous considerations for the f_α component give the formulae

$$\frac{\partial^2 F_{2\nu}}{\partial z_\alpha \partial \bar{z}_\beta} = \frac{1}{2} \delta_{\nu, \lambda - (\alpha - \beta)} ([f_\alpha, e_\beta], \Phi_{0\lambda}) \quad (4.13)$$

and

$$\frac{\partial}{\partial z_\beta} (f_\alpha, \Phi_{1\lambda - \beta}) = -\frac{\partial^2 F_{2\lambda - \alpha - \beta}}{\partial z_\alpha \partial z_\beta} - \frac{1}{2} ([f_\alpha, f_\beta], \Phi_{0\lambda}). \quad (4.14)$$

Notice that from (4.9) one finds that the diagonal part of Φ_1 is $i\nabla_\theta F_1$. Combining this diagonal part with (4.12) and (4.14) one obtains Φ_1 . In addition there appear in (4.14) a number of restrictions on F_2 inherited from the structure of the weight system.

The Schrödinger equation (4.5) at $m = 1$ becomes

$$\sum_\beta \bar{k}_\beta \frac{\partial F_{2\lambda - (\alpha - \beta)}}{\partial \bar{z}_\beta} - \sum_\beta k_\beta \frac{\partial F_{2\lambda - \alpha - \beta}}{\partial z_\beta} + \frac{1}{2} z_\alpha (K, [e_\alpha, \Phi_{0\lambda}]) = [E - V(\lambda - \alpha)] F_{1\lambda - \alpha}$$

for each α . This is nothing other than an algebraic system on the coefficients of F_2 which are located in the $z_\alpha z_\beta$ terms. Taking into account equation (4.13) one finds for these coefficients $\partial^2 F_{2\lambda - \alpha - \beta} / \partial z_\alpha \partial z_\beta$ the set of conditions

$$\begin{aligned} & \sum_\beta k_\beta \frac{\partial^2 F_{2\lambda - \alpha - \beta}}{\partial z_\alpha \partial z_\beta} + \sum_\beta \frac{k_\beta}{2} ([f_\alpha, f_\beta], f_{\alpha + \beta}) \frac{\partial F_{1\lambda - \alpha - \beta}}{\partial z_{\alpha + \beta}} \\ &= - \sum_\beta \bar{k}_\beta ([f_\alpha, e_\beta], f_{\alpha - \beta}) \frac{\partial F_{1\lambda - (\alpha - \beta)}}{\partial z_{\alpha - \beta}} \\ & \quad - [E - V(\lambda - \alpha)] \frac{\partial F_{1\lambda - \alpha}}{\partial z_\alpha} + \bar{k}_\alpha ([f_\alpha, e_\alpha], n_\lambda) F_{0\lambda}. \end{aligned}$$

The same arguments yield for the terms of higher degree $m = 3, 4, \dots, M$ the equations for the coefficients of the polynomials $F_{m\mu}(Z)$. If M is the highest degree for the terms containing the variables z_α alone, the equations for the spectrum are brought by the conditions

$$\partial^{M+1} F_{M+1} / \partial z_{\alpha_1} \partial z_{\alpha_2} \dots \partial z_{\alpha_{M+1}} = 0$$

in the Schrödinger equation at level M . We have thus obtained a graded structure for the system of equations determining the states and spectrum of the Hubbard Hamiltonian. Even the trivial case $l = 3, \lambda = (1, 0, 0)$, essentially the diagonalization of the matrix K , shows the main features of the preceding equations.

We shall illustrate the foregoing construction in the particular case $l = 2$ with $\lambda = (1, -1)$ already considered in section 2. In that case the set of weights is $\Pi_\lambda = \{0, \pm\lambda\}$ and the matrix $Z = ze - \bar{z}f$. The kinetic energy is defined by $K = e + f$ so that one finds for F , in accordance with the previous formulae, the expression

$$\begin{aligned} F(\theta, Z) &= (1 - |z|^2) e^{-i(\theta_1 - \theta_2)} - [E - V(\lambda)] z \\ & \quad - (1 - \frac{1}{2} [E - V(0)] [E - V(\lambda)]) z^2 e^{i(\theta_1 - \theta_2)} + \dots \end{aligned} \quad (4.15)$$

neglecting higher-order terms and setting $F_{0\lambda} = 1$. For the present case this approximation is enough to completely determine the state. The corresponding energy levels arise upon consideration of cubic terms in Z , from which one encounters the equation

$$[E - V(\lambda)] + [E - V(-\lambda)] \{1 - \frac{1}{2} [E - V(0)] [E - V(\lambda)]\} = 0. \quad (4.16)$$

It is now time to compare formulae (4.15) and (4.16) with the results of section 2. We first identify the old coordinates (θ, s, ϕ) with those of (4.15), which we now denote by $(\tilde{\theta}, Z)$,

writing for g in (2.5)

$$\begin{aligned} g &= h_\theta u_s k_\phi \\ &= (h_\theta k_\phi) k_\phi^{-1} u_s k_\phi \\ &= h_{\tilde{\theta}} \exp i \frac{s}{2} \begin{pmatrix} 0 & e^{-i\phi} \\ e^{i\phi} & 0 \end{pmatrix} \end{aligned}$$

from which we deduce

$$\tilde{\theta}_1 = i(\theta_1 + \phi/2) \quad \tilde{\theta}_2 = i(\theta_2 - \phi/2)$$

with

$$z = i \frac{s}{2} e^{-i\phi}$$

and the identification $f(g) = F(\theta, s, \phi) = \tilde{F}(\tilde{\theta}, Z)$, letting \tilde{F} denote the expression for the wavefunction in (4.15). The potential energy for the present case is

$$V(\lambda) = \frac{U}{2} (\|\lambda\|^2 - 1) = \frac{U}{2}$$

from which we get upon substitution in (4.16)

$$\left(E - \frac{U}{2}\right) \left(E^2 - \frac{U^2}{4} - 4\right) = 0$$

in full agreement with the results of section 2 for the energy levels.

At $E = U/2$ we obtain from (2.6) the formula for the second-order approximation in s :

$$F(\theta, s, \phi) = e^{-i\phi} \left\{ \frac{s^2}{4} e^{i(\theta_1 - \theta_2)} + \left(1 - \frac{s^2}{4}\right) e^{-i(\theta_1 - \theta_2)} + \dots \right\}$$

whilst for the levels $E^2 = \frac{U^2}{4} + 4$ in (2.7) we have in the same approximation

$$F(\theta, s, \phi) = e^{-i\phi} \left\{ \frac{s^2}{4} e^{i(\theta_1 - \theta_2)} + \frac{i}{2} \left(E - \frac{U}{2}\right) s - \left(1 - \frac{s^2}{4}\right) e^{-i(\theta_1 - \theta_2)} + \dots \right\}$$

in accordance with formula (4.15).

To conclude, we observe that solution (4.15) is greatly simplified when $E = V(\lambda)$, which represents an eigenvalue in (4.16) provided that $V(\lambda) = V(-\lambda)$. Generalization of this type of symmetry argument would be of interest in connection with the problem of solving the differential equation in concrete situations.

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