The Origin of Degeneracies and Crossings in the 1d Hubbard Model

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Abstract

The paper is devoted to the connection between integrability of a finite quantum system and degeneracies of its energy levels. In particular, we analyze in detail the energy spectra of finite Hubbard chains. Heilmann and Lieb demonstrated that in these systems there are crossings of levels of the same parameter independent symmetry. We show that this apparent violation of the Wigner-von Neumann noncrossing rule follows directly from the existence of nontrivial conservation laws and is a characteristic signature of quantum integrability. The energy spectra of Hubbard chains display many instances of permanent (at all values of the coupling) twofold degeneracies that cannot be explained by parameter independent symmetries. We relate these degeneracies to the different transformation properties of the conserved currents under spatial reflections and the particle-hole transformation and estimate the fraction of doubly degenerate states. We also discuss multiply degenerate eigenstates of the Hubbard Hamiltonian. The wave functions of many of these states do not depend on the coupling, which suggests the existence of an additional parameter independent symmetry.

1 Introduction

The close connection between symmetry and degeneracy has been explored since the foundation of Quantum Mechanics. Famous examples include degeneracies of spectra in angular momentum in the Hydrogen atom (well known as the accidental degeneracy) [1] and the 3d harmonic oscillator [2]. In the present paper we focus on the implications of the rich symmetry structure for the spectrum of the 1d Hubbard model as well as for a general class of quantum integrable systems. We analyze in detail how degeneracies and other spectral properties of the Hubbard Hamiltonian reflect the symmetries of the model.

Here we restrict ourselves to the case of Hamiltonians that depend on a single real parameter, referred to as a coupling. In this case one can distinguish between two types of degeneracy. The first type, often called permanent degeneracy, refers to energy levels which remain degenerate for all values of the parameter. The appearance of permanent degeneracies suggests the existence of non–commuting symmetry operators (see e.g. [2]).

The second type of degeneracy is a crossing of energy levels that occurs at a particular value of the coupling. Multiple level crossings at a certain point indicate a higher symmetry of the system at this particular point as compared to other points. For example, the limits of zero or infinite coupling frequently have enhanced symmetry.

Simple pairwise crossings are also interesting from a different perspective. As is well known, in the absence of symmetries energy levels repel, or, equivalently, crossings of levels are prohibited unless the states have different symmetry. This *noncrossing rule* was suggested by Hund in 1927 [3], and justified by von Neumann and Wigner [4] two years latter. Since then the level repulsion phenomenon has been revisited and elaborated upon in various contexts, see for example [5, 6, 7] and references therein. Usually textbooks, e.g., [2, 8, 9], present a simplified version of the justification due to Teller [10].

The mathematical validity of the noncrossing rule depends crucially on the interpretation of the word symmetry, normally understood as a space (or internal space) symmetry. This was highlighted by an interesting example by Heilmann and Lieb in 1971 [11]. These authors pointed out that the noncrossing rule is apparently violated in the case of the 1d Hubbard Hamiltonian for the benzene molecule if only those symmetries that do not depend on the coupling constant are taken into account. Indeed, Fig. 1 illustrates that a substantial number of crossings can be found even within the subsets of levels characterized by the same set of quantum numbers. Based on this fact, Heilmann and Lieb concluded that "there must be a natural parameter dependent group" to account for these violations.

The 1d Hubbard model is solvable by Bethe's *Ansatz*, and usually the applicability of this *Ansatz* is understood to rest upon *Quantum Integrability* of the model, i.e the existence of an infinite number of mutually commuting operators. Such commuting operators are often alternately termed as "conserved currents ", or "dynamical conservation laws", or simply "dynamical symmetries", and are invariably associated with all known quantum integrable models. However, it was not until 1986 when the parameter dependent integrals of motion (conserved currents), were identified by Shastry [16, 17, 18], who constructed a transfer matrix that commuted with the Hubbard Hamiltonian.

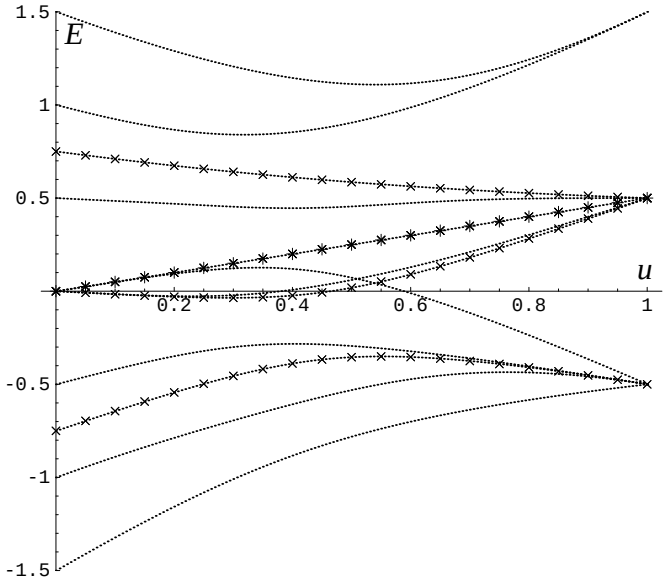

Figure 1: Energies for $(P, \sigma, I^{(o)}, S, L) = (3, 1, 1, 0, 1)$ in units of $U - 4T$ as functions of $u = U/(U - 4T)$. Levels marked with crosses are twofold degenerate. They also correspond to $(P, \sigma, I^{(o)}, S, L) = (3, -1, 1, 0, 1)$. Upside down the figure shows levels for the same set of quantum numbers with $S \leftrightarrow L$. ***** shows the seven fold degenerate level.

The Hubbard Hamiltonian to be considered consists of the kinetic term, which allows electrons

to hop between the nearest neighbors on a regular polygon (i.e. periodic boundary conditions are assumed) and the Coulomb interaction between electrons of opposite spin on the same site.

$$\hat{H} = T\sum_{j=1}^{N}\sum_{s=\uparrow\downarrow}(c_{js}^{\dagger}c_{j+1\,s} + c_{j+1\,s}^{\dagger}c_{js}) + U\sum_{j=1}^{N}\left(\hat{n}_{j\uparrow} - \frac{1}{2}\right)\left(\hat{n}_{j\downarrow} - \frac{1}{2}\right) \tag{1.1}$$

where $c_{js}^{\dagger}$ and c_{js} are the creation and annihilation operators for an electron of spin projection s on site j and $\hat{n}_{js} = c_{js}^{\dagger}c_{js}$ is the number operator. The goal of this paper is to study how the interplay between parameter dependent integrals of motion and ordinary (parameter independent) symmetries is manifested in permanent degeneracies and level crossings in the energy spectrum. The Hamiltonian (1.1) is chosen as a tutorial example of a many body system that has both parameter dependent and parameter independent symmetries.

The paper is organized as follows. Section 2 is devoted to parameter independent symmetries of the Hubbard model that are later used in Section 4 to diagonalize the Hamiltonian and assign symmetry quantum numbers such as the total momentum, spin, particle–hole symmetry etc. to all states. Section 3 discusses the structure and properties of parameter dependent conservation laws. Permanent degeneracies are treated in detail in Section 5. In the same section we consider the multiple permanent degeneracies and mention spectral properties of the dynamical conservation laws.

In Section 6 we formulate the noncrossing rule in the framework of adiabatic equations of motion for matrix elements of the Hamiltonian and higher currents. This language is useful for understanding the suppression of level repulsion in integrable models. Next, based on numerical analysis, we discuss a curious behavior of the transverse matrix element in the vicinity of crossings specific to the Hubbard Hamiltonian. Finally, to illustrate the connection between level crossings and integrability we consider in some detail a simple case of integrable 3×3 matrix systems (Section 6). In this case we conclude that there are no "accidental degeneracies", i.e. all degeneracies may be associated with dynamical conservation laws.

The majority of the results do not depend on the number of sites (N) or electrons (M). However, cases of even and odd N and M have to be treated differently, the latter case being substantially simpler because of less symmetry that needs to be taken into account. We therefore take for concreteness that both these numbers are even, $N = 2n$ and $M = 2m$ with an equal number of spin up and spin down electrons. Throughout the paper analytical results are illustrated by numerical computations for a special case of benzene ($m = n = 3$), and a few other choices of (m, n).

2 U–independent Symmetries

The starting point of our analysis of the spectral properties of the Hubbard Hamiltonian (1.1) is the list of its U–independent symmetries. We will follow closely the paper by Heilmann and Lieb [11] adopting in most cases their notation.

The role of the U–independent symmetries is twofold. First, they greatly simplify the diagonalization of the Hamiltonian and integrals of motion and provide a convenient labeling for various parts of the spectrum. Besides, for the purposes of studying specifically the effect of parameter dependent conservation laws all these symmetries have to be factored out anyway.

U–independent symmetries fall into three major categories – the symmetry of the polygon, the spin symmetry, and the particle-hole symmetry. Spatial symmetries can be generated by two operators:

operator $\hat{C}_{2n}$ that rotates the polygon by π/n, and operator $\hat{\sigma}$ that reflects it in a line through vertices n and $2n$ (see Fig. 2). These operators can be expressed in terms of on site creation and annihilation operators as

$$\hat{C}_{2n} = \hat{\sigma}\hat{\sigma}' \quad \hat{\sigma} = \prod_{s=\uparrow,\downarrow}\prod_{k=1}^{n-1} \hat{\mathbf{J}}_{ks;-ks} \quad \hat{\sigma}' = \prod_{s=\uparrow,\downarrow}\prod_{k=1}^{n} \hat{\mathbf{J}}_{k-1,s;2n-k,s} \tag{2.2}$$

where $\hat{\mathbf{J}}_{js,j's'}$ interchanges the orbitals (js) and $(j's')$

$$\hat{\mathbf{J}}_{js,j's'} = 1 - \hat{n}_{js} - \hat{n}_{j's'} + c^\dagger_{js}c_{j's'} + c^\dagger_{j's'}c_{js} \tag{2.3}$$

Eigenvalues of $\hat{C}_{2n}$ are $e^{i\pi P/n}$, where P is an integer $0 \leq P \leq 2n-1$ that represents the total momentum of the state. The reflection operator $\hat{\sigma}$ has eigenvalues ± 1.

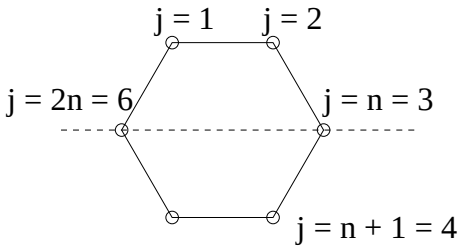

Figure 2: Regular hexagon ($n = 3$). $\hat{C}_6$ rotates by $\pi/3$. $\hat{\sigma}$ reflects in a line through vertices 3 and 6.

The spin symmetry can be generated by $\hat{\mathbf{S}}^2$ and $\hat{S}_z$

$$\hat{S}_z = \frac{\hat{\mathbf{n}}_\uparrow - \hat{\mathbf{n}}_\downarrow}{2} \quad \hat{S}_+ = (\hat{S}_-)^\dagger = \sum_{j=1}^{2n} c^\dagger_{j\uparrow}c_{j\downarrow} \tag{2.4}$$

$$\hat{\mathbf{S}}^2 = \frac{\hat{S}_-\hat{S}_+ + \hat{S}_+\hat{S}_-}{2} + \hat{S}_z^2 \tag{2.5}$$

where

$$\hat{\mathbf{n}}_s = \sum_{j=1}^{2n} \hat{n}_{js} \tag{2.6}$$

To describe the particle-hole symmetry we first define operators $\hat{J}^{(o)}_s$ and $\hat{J}^{(h)}_s$. The operator $\hat{J}^{(o)}_s$ changes the sign of the wave-function each time there is a spin s electron on an odd site, while the operator $\hat{J}^{(h)}_s$ interchanges holes and particles for a spin direction s.

$$\hat{J}^{(o)}_s = \prod_{j=0}^{n-1}(1 - 2\hat{n}_{2j+1,s}) \quad \hat{J}^{(h)}_s = \prod_{j=1}^{2n}(c^\dagger_{js} + c_{js}) \tag{2.7}$$

It is convenient to introduce the following combinations of these operators:

$$\hat{J}^{(o)} = \hat{J}^{(o)}_\uparrow \hat{J}^{(o)}_\downarrow \quad \hat{J}^{(h)} = \hat{J}^{(h)}_\uparrow \hat{J}^{(h)}_\downarrow \quad \hat{I}^{(o)} = \hat{J}^{(o)}\hat{J}^{(h)} \quad \hat{Z}_\uparrow = \hat{J}^{(o)}_\uparrow \hat{J}^{(h)}_\downarrow \tag{2.8}$$

Note the action of various symmetries on the creation and annihilation operators

$$\hat{Z}^\dagger_\uparrow c_{j\uparrow}\hat{Z}_\uparrow = (-1)^j c_{j\uparrow} \quad \hat{Z}^\dagger_\uparrow c_{j\downarrow}\hat{Z}_\uparrow = -c^\dagger_{j\downarrow} \tag{2.9}$$

$$\hat{I}^{(o)} c_{js} \hat{I}^{(o)} = (-1)^{j+1} c_{js}^{\dagger} \tag{2.10}$$

$$\hat{\sigma} c_{js} \hat{\sigma} = c_{-j,s} \tag{2.11}$$

$$\hat{J}^{(o)} c_{js} \hat{J}^{(o)} = (-1)^{j} c_{js} \tag{2.12}$$

It follows from equations (2.9) and (2.10) that

$$\hat{Z}_{\uparrow} |m_{\uparrow}, m_{\downarrow}\rangle = |m_{\uparrow}, 2n - m_{\downarrow}\rangle \tag{2.13}$$

and

$$\hat{I}^{(o)} |m_{\uparrow}, m_{\downarrow}\rangle = |2n - m_{\uparrow}, 2n - m_{\downarrow}\rangle \tag{2.14}$$

where $|m_{\uparrow}, m_{\downarrow}\rangle$ is a state with $m_{\uparrow}$ spin up electrons and $m_{\downarrow}$ spin down electrons, and $2n$ is the number of sites. Thus, operators $\hat{I}^{(o)}$ and $\hat{Z}_{\uparrow}$ conserve the number of particles only at a half filling with an equal number of up and down electrons.

Equations (2.9) and (2.10) are used to evaluate various commutation relations for $\hat{I}^{(o)}$ and $\hat{Z}_{\uparrow}$.

$$\{\hat{Z}_{\uparrow}, \hat{H}\} = 0 \quad [\hat{\sigma}, \hat{H}] = 0 \tag{2.15}$$

$$[\hat{I}^{(o)}, \hat{H}] = \{\hat{J}^{(o)}, \hat{T}\} = \{\hat{I}^{(o)}, \hat{S}_z\} = [\hat{I}^{(o)}, \hat{\mathbf{S}}^2] = 0 \tag{2.16}$$

$$\hat{I}^{(o)} \hat{C}_{2n} - \hat{C}_{2n} \hat{I}^{(o)} (-1)^{\hat{\mathbf{n}}} = \hat{Z}_{\uparrow} \hat{C}_{2n} + \hat{C}_{2n} \hat{Z}_{\uparrow} (-1)^{\hat{\mathbf{n}}_{\downarrow}} = \hat{Z}_{\uparrow} \hat{\sigma} - (-1)^{n-1} \hat{\sigma} \hat{Z}_{\uparrow} = 0 \tag{2.17}$$

where $\{\hat{A}, \hat{B}\} \equiv \hat{A}\hat{B} + \hat{B}\hat{A}$, $\hat{\mathbf{n}} = \hat{\mathbf{n}}_{\uparrow} + \hat{\mathbf{n}}_{\downarrow}$, and $\hat{T}$ is the kinetic energy operator

$$\hat{T} = T \sum_{j=1}^{N} \sum_{s=\uparrow\downarrow} (c_{js}^{\dagger} c_{j+1\,s} + c_{j+1\,s}^{\dagger} c_{js})$$

$\hat{Z}_{\uparrow}$ is a unitary operator that anticommutes with the Hamiltonian. Therefore it defines a mapping from the set of operators that commute with the Hamiltonian onto itself, i.e. $[\hat{A}, \hat{H}] = 0$ implies $[\hat{Z}_{\uparrow}^{\dagger} \hat{A} \hat{Z}_{\uparrow}, \hat{H}] = 0$. Using this transformation, we can construct a new $su(2)$ algebra (η-pairing $su(2)$) from the spin $su(2)$ (2.4) [12, 13, 14, 15].

$$\hat{L}_z = \frac{\hat{\mathbf{n}}_{\uparrow} + \hat{\mathbf{n}}_{\downarrow}}{2} - n \quad \hat{L}_{-} = \sum_{j=1}^{2n} (-1)^{j} c_{j\uparrow} c_{j\downarrow} \quad \hat{L}_{+} = (\hat{L}_{-})^{\dagger} \tag{2.18}$$

The Casimir operator of this new $su(2)$

$$\hat{\mathbf{L}}^2 = \hat{Z}_{\uparrow}^{\dagger} \hat{\mathbf{S}}^2 \hat{Z}_{\uparrow} \tag{2.19}$$

preserves the number of particles and therefore its eigenvalues $L(L+1)$ can be included in the set of quantum numbers used to label the eigenstates. The combination $SU(2) \times SU(2)/\mathbf{Z}_2$ yields the complete $SO(4)$ symmetry of the Hubbard Hamiltonian [12, 13, 14, 15].

3 Conserved Currents

Now let us turn to the parameter dependent integrals of motion. In principle, an infinite number of these integrals can be obtained by methods outlined in [16, 17, 18]. Clearly, on a finite lattice only a finite number of these integrals are independent (see Section 6 for more details). The general form of the rth conserved current is

$$\hat{I}_r(U,T) = \sum_{k=0}^{l} U^k T^{l-k} \hat{I}_r^k$$

where $\hat{I}_r^k$ are parameter independent operators. The U–independent part of $\hat{I}_r$ has a simple form

$$\hat{I}_r(U=0) = T^l \hat{I}_r^0 = \pm(i)^{r+1} T^l \sum_{j=1}^{N} \sum_{s=\uparrow\downarrow} (c_{j+r,s}^\dagger c_{js} - (-1)^r c_{js}^\dagger c_{j+r,s}) \tag{3.20}$$

As far as permanent degeneracies are concerned, an important feature of the currents is that odd ($r = 2k+1$) and even ($r = 2k$) currents transform differently (equations (3.23)–(3.26)) under spatial reflections ($\hat{\sigma}$) and partial particle-hole transformation ($\hat{Z}_\uparrow$). Odd currents are in many respects similar to the Hamiltonian, while properties of even currents are essentially different.

First few nontrivial currents were derived explicitly in [17, 19, 20, 21]. (See also [21] and [22] for a discussion on the derivation and the structure of the higher conserved currents.) To analyze the benzene example we will need the explicit form of only the first two nontrivial integrals of motion. Since $\hat{I}_1 \equiv \hat{H}$, these two are

$$\hat{I}_2 = -iT \sum_{j=1}^{N} \sum_{s=\uparrow\downarrow} (c_{j+2s}^\dagger c_{js} - c_{js}^\dagger c_{j+2s}) - iU \sum_{j=1}^{N} \sum_{s=\uparrow\downarrow} (c_{j+1s}^\dagger c_{js} - c_{js}^\dagger c_{j+1s})(\hat{n}_{j+1,-s} + \hat{n}_{j,-s} - 1) \tag{3.21}$$

$$\begin{aligned}
\hat{I}_3 \;=\; & T^3 \sum_{j=1}^{N} \sum_{s=\uparrow\downarrow} \left(c_{j+3s}^\dagger c_{js} + c_{js}^\dagger c_{j+3s}\right) + T^2 U \sum_{j=1}^{N} \sum_{s=\uparrow\downarrow} \left\{ \left(c_{j+1s}^\dagger c_{j-1s} + c_{j-1s}^\dagger c_{j+1s}\right) \right. \\
& \left. \left(\hat{n}_{j+1,-s} + \hat{n}_{j,-s} + \hat{n}_{j-1,-s} - \frac{3}{2}\right) + \left(c_{j+1s}^\dagger c_{js} - c_{js}^\dagger c_{j+1s}\right) \left(c_{j,-s}^\dagger c_{j-1,-s} - c_{j-1,-s}^\dagger c_{j,-s}\right) - \right. \\
& \left. \left(\hat{n}_{j+1s} - \frac{1}{2}\right) \left(\hat{n}_{j,-s} - \frac{1}{2}\right) \right\} + T^2 U \sum_{j=1}^{N} \left\{ \left(c_{j+1\uparrow}^\dagger c_{j\uparrow} - c_{j\uparrow}^\dagger c_{j+1\uparrow}\right) \left(c_{j+1\downarrow}^\dagger c_{j\downarrow} - c_{j\downarrow}^\dagger c_{j+1\downarrow}\right) \right. \\
& \left. - \left(\hat{n}_{j\uparrow} - \frac{1}{2}\right) \left(\hat{n}_{j\downarrow} - \frac{1}{2}\right) \right\} - TU^2 \sum_{j=1}^{N} \sum_{s=\uparrow\downarrow} \left(c_{j+1s}^\dagger c_{js} + c_{js}^\dagger c_{j+1s}\right) \left(\hat{n}_{j+1,-s} - \frac{1}{2}\right) \left(\hat{n}_{j,-s} - \frac{1}{2}\right) \\
& - U^3/4 \sum_{j=1}^{N} \left(\hat{n}_{j\uparrow} - \frac{1}{2}\right) \left(\hat{n}_{j\downarrow} - \frac{1}{2}\right)
\end{aligned} \tag{3.22}$$

Odd currents have the same U–independent symmetry as the Hubbard Hamiltonian, i.e. in all commutation relations of Section 2 the Hamiltonian can be replaced with any other odd current. For

even currents two of the commutation relations are different. Namely, for odd currents one can show that

$$[\hat{\sigma}, \hat{I}_{2k+1}] = 0 \tag{3.23}$$

$$\{\hat{Z}_{\uparrow}, \hat{I}_{2k+1}\} = 0 \tag{3.24}$$

while for even currents

$$\{\hat{\sigma}, \hat{I}_{2k}\} = 0 \tag{3.25}$$

$$[\hat{Z}_{\uparrow}, \hat{I}_{2k}] = 0 \tag{3.26}$$

In other words, equations (3.23–3.26) mean that even and odd currents have different $\hat{\sigma}$ and $\hat{Z}_{\uparrow}$ parities. For $k = 1$ equations (3.23–3.26) have been derived in [20]. Note also that since both $\hat{\sigma}$ and $\hat{Z}_{\uparrow}$ are unitary and I_r is Hermitian, equations (3.25) and (3.24) imply

$$Tr\hat{I}_r = 0 \tag{3.27}$$

Another property of conserved currents which we will use bellow is

$$\hat{J}^{(o)}\hat{I}_r(T,U)\hat{J}^{(o)} = (-1)^{r+1}\hat{I}_r(-T,U) \tag{3.28}$$

Equations (3.23)–(3.26) and (3.28) for I_2 and I_3 can be verified by inspection. For higher currents they can be derived by establishing the transformation properties of the transfer matrix obtained in [16, 17, 18].

Finally, let us measure U, T and all other energies in units of $U - 4T$. This is equivalent to the replacement

$$U - 4T = 1 \quad U = u \quad T = (u-1)/4 \tag{3.29}$$

We see from (3.28) that the spectrum and the eigenfunctions of $\hat{I}_r$ for $T \leq 0$ and $T \geq 0$ are related via a simple transformation and it is therefore sufficient to consider $T \leq 0$. Thus, we have to compute the spectra only for $0 \leq u \leq 1$.

4 Diagonalization

In this section we outline a method that we use for detailed numerical study of the spectra of the Hamiltonian and conserved currents. In subsequent sections we will compare the computer generated results for benzene ($m = n = 3$) and several other values of m and n to general predictions based on symmetry.

From the results of Section 2 it follows that the set of quantum numbers that label the eigenstates of the Hamiltonian and integrals of motion is $\{P, \sigma, I^{(o)}, S, L\}$. However, there are certain restrictions on this set since not all symmetries and integrals of motion mutually commute. The quantum number $I^{(o)}$ can be assigned only when $m = n$ and σ can be used only when $P = 0$ or $P = n$ (see (2.14) and (4.34)). Also, since $\hat{\sigma}$ changes P to $2n - P$ without affecting the energy and other quantum numbers, the spectrum for $2n > P > n$ is the exact copy of that for $n > P > 0$. Therefore, it is sufficient to diagonalize the Hamiltonian and the currents for P ranging from 0 to n. Finally, since even currents anticommute with $\hat{\sigma}$, their eigenvalues cannot be specified whenever σ is specified.

To utilize the conservation of momentum, we introduce in the usual way the momentum space creation and annihilation operators $d^\dagger_{ps}$ and d_{ps}

$$d^\dagger_{ps} = \frac{1}{\sqrt{2n}} \sum_{j=1}^{2n} e^{i\pi pj/n} c^\dagger_{js} \quad d_{ps} = \frac{1}{\sqrt{2n}} \sum_{j=1}^{2n} e^{-i\pi pj/n} c_{js} \tag{4.30}$$

where $p = 0, 1, \ldots, 2n-1$.

Next, we choose a basis for $2m$-electron wave functions with m spin up and m spin down electrons.

$$|\mathbf{r}\rangle = |\mathbf{p};\mathbf{q}\rangle = d^\dagger_{p_1\uparrow} \ldots d^\dagger_{p_m\uparrow} d^\dagger_{q_1\downarrow} \ldots d^\dagger_{q_m\downarrow} |0\rangle \tag{4.31}$$

with the following ordering convention

$$\begin{array}{l} p_1 < p_2 < \ldots < p_m \\ q_1 < q_2 < \ldots < q_m \end{array} \tag{4.32}$$

Components of $|\mathbf{r}\rangle$ that are not in the interval $[0, 2n-1]$ have to be reduced modulo $2n$ into this interval. If the components of a vector are not in the order (4.32) they have to be permuted to obtain these ordering and the wave function should be multiplied by (-1) if the permutation is odd. The total momentum of the state is

$$P = \sum_{k=1}^{2m} \mathbf{r}_k \qquad (\text{modulo } 2n) \tag{4.33}$$

From (2.9–2.11) and (4.30) we identify the action of operators of U–independent symmetry on basic states (4.31)

$$\hat{\sigma}|\mathbf{r}\rangle = |-\mathbf{r}\rangle \tag{4.34}$$

$$\hat{I}^{(o)}|\mathbf{r}\rangle = (-1)^{2m+P} |-\overline{(\mathbf{r}+\mathbf{ne})}\rangle \tag{4.35}$$

$$\hat{Z}_\uparrow |\mathbf{p};\mathbf{q}\rangle = (-1)^{(m+Q)} |(\mathbf{p}+\mathbf{ne}); -\overline{\mathbf{q}}\rangle \tag{4.36}$$

where $Q = \sum_{k=1}^m q_k$ is the total momentum of spin down electrons, $\overline{\mathbf{r}}$ denotes taking the complement of the set $\mathcal{R} \equiv \{r_k\}$ in the set of integers from 0 to $2n-1$. Finally, $+\mathbf{ne}$ stands for adding n to each component of a vector.

The rotation operator $\hat{C}_{2n}$ commutes with the Hamiltonian, conserved currents, $\hat{I}^{(o)}$, $\hat{\mathbf{S}}^2$, and $\hat{\mathbf{L}}^2$. Therefore, these operators split into blocks corresponding to different values of P. This significantly reduces the size of the matrices to be diagonalized. To generate the blocks for each value of P we need to derive the matrix elements of the Hamiltonian, integrals of motion, and symmetry operators in the basis (4.31). Equations (4.34) and (4.35) allow to write down $\hat{\sigma}$, $\hat{I}^{(o)}$, and $\hat{Z}_\uparrow$ in the matrix notation. Matrix elements of the Hamiltonian, and the operators $\hat{\mathbf{S}}^2$, $\hat{I}_2$, and $\hat{I}_3$ are summarized in Appendix B.

Now we have all ingredients needed to produce a computer program (e.g. on *Mathematica*) that generates exact blocks of the Hamiltonian, symmetry operators, and first two currents for any value of the total momentum P.

After the value of the total momentum P is chosen, the program picks one of the remaining U–independent symmetries, say $\hat{\sigma}$, and finds a unitary transformation that makes it diagonal. The columns of the matrix of this transformation are the eigenvectors of $\hat{\sigma}$. Since we know the eigenvalues

of $\hat{\sigma}$ exactly (± 1), determining the eigenvectors for each eigenvalue reduces to a set of linear equations which can be solved analytically.

In this way, step by step, we diagonalize all parameter independent symmetries and split the Hamiltonian and conserved currents into smaller blocks. If the system is not too large, this can be done analytically using *Mathematica*. For example, the complete Hamiltonian for benzene is a 400×400 matrix, while individual blocks range in size from 1×1 to 16×16.

Finally, when all U–independent symmetry is exhausted, we get exact blocks of the Hamiltonian and conserved currents with all U–independent symmetry quantum numbers assigned to each block. Each block is then diagonalized individually at different values of u ranging from 0 to 1 (see (3.29)). Often, the small size of a block allows for analytical diagonalization.

5 Permanent Degeneracies and Other Spectral Properties

As soon as the Hamiltonian (1.1) is diagonalized, we discover numerous cases of permanent degeneracy, see e.g. Table 1 and Fig. 1, 3, and 5. We make the following observations. The majority of degeneracies are twofold degeneracies with respect to $\sigma = \pm 1$. However, there are also several multiply degenerate levels. The characteristic feature of these states is that the energies are linear in U.

P	n	m	(degree of degeneracy, number of levels)
0	3	2	(1, 12); (2, 12)
3	3	2	(1, 15); (2, 7); (3, 1); (7, 1)
0	3	3	(1, 32); (2, 18)
3	3	3	(1, 30); (2, 12); (7, 2)
0	4	2	(1, 28); (2, 31); (3, 1); (7, 1)
4	4	2	(1, 15); (2, 41); (3, 1)
0	4	3	(1, 70); (2, 150); (3, 2); (8, 2)
4	4	3	(1, 56); (2, 155); (3, 1); (7, 1); (8, 2)
0	4	4	(1, 126); (2, 229); (3, 1), (7, 1); (12, 2)
4	4	4	(1, 126); (2, 229); (3, 1); (7, 1); (12, 2)

Table 1: Degrees of degeneracy in the sectors $P = \{0, n\}$ for $n = \{3, 4\}$

First, we analyze the twofold degeneracies. Let $\psi(E, I_{2k+1}, \sigma, S, L)$, where E is the energy, be an eigenstate of the Hamiltonian as well as all other *odd* currents and operators $\hat{\sigma}$, $\hat{\mathbf{S}}^2$, and $\hat{\mathbf{L}}^2$. Being an eigenstate of $\hat{\sigma}$, the state ψ cannot be an eigenstate of any even current since $\hat{I}_{2k}$ and $\hat{\sigma}$ anticommute. Let $\phi(E, I_{2k}, P, S, L, I_{2k+1})$ denote an eigenstate of all even and odd currents. On the other hand $\phi \equiv \psi$ when σ is not assigned, i.e. when $P \neq \{0, n\}$. We note that equation (3.25) means that either the state ψ is annihilated by the operator $\hat{I}_{2k}$, $\hat{I}_{2k}\psi = 0$ for all U, or

$$\hat{I}_{2k}\psi(E, I_{2k+1}, \sigma, S, L) = \psi(E, I_{2k+1}, -\sigma, S, L) \tag{5.37}$$

Equations (3.26) and (3.25) imply

$$\hat{Z}_{\uparrow}\psi_n(E, I_{2k+1}, S, L) = \psi_n(-E, -I_{2k+1}, L, S) \tag{5.38}$$

$$\hat{Z}_{\uparrow}\phi_n(E, I_{2k}, S, L, I_{2k+1}) = \phi_n(-E, I_{2k}, L, S, -I_{2k+1}) \tag{5.39}$$

$$\hat{\sigma}\phi_n(E, I_{2k}, P, S, L, I_{2k+1}) = \phi_n(E, -I_{2k}, -P, S, L, I_{2k+1}) \tag{5.40}$$

It follows from equation (5.38) that for each state of energy E and eigenvalues of odd currents $\{I_{2k+1}\}$ there is a state with the energy $-E$ and eigenvalues $\{-I_{2k+1}\}$. According to equation (2.13) these two states have the same number of particles only if $m = n$. Equation (5.39) implies that eigenstates of I_{2k} are doubly degenerate. Finally, from (5.37) we conclude that any state in the sector $P = \{0, n\}$ that is not annihilated by *all* $\hat{I}_{2k}$ is at least twofold permanently degenerate. This applies to all values of m and n. In other words, all energy levels in the sector $P = \{0, n\}$ that are not in the kernel of $\hat{I}_{2k}$ for all U and k are doubly degenerate (see also [20]). Consequently, all nondegenerate states should be annihilated by any even current.

A twofold degeneracy is explained on symmetry grounds as soon as we identify an even current that maps the two degenerate states into each other. Unfortunately, we do not yet know how to prove for arbitrary m and n that for any twofold degeneracy there exists such an even current. For benzene we checked numerically that all doubly degenerate states are maped into each other by $\hat{I}_2$ and therefore no other even currents are needed to explain twofold degeneracies.

Since nondegenerate states are annihilated by any even current, nondegenerate states exist only if all even currents have nontrivial kernels. Let us show that this necessary condition is met when m is odd or $m \neq n$. Indeed, since $\hat{I}_{2k}$ maps the subspace $\sigma = +1$ into the subspace $\sigma = -1$ (5.37), its kernel has to contain at least $|d_{+1} - d_{-1}|$ states, where $d_{\pm 1}$ are the dimensions of $\sigma = \pm 1$ subspaces. Since the eigenstates of $\sigma = \pm 1$ are $|\mathbf{r}\rangle \pm |-\mathbf{r}\rangle$ (4.34), $d_{+1} - d_{-1}$ is the number of states such that $|\mathbf{r}\rangle = |-\mathbf{r}\rangle$ minus the number of states such that $|\mathbf{r}\rangle = -|-\mathbf{r}\rangle$. This is calculated to be

$$d_{+1} - d_{-1} = \left\{ \binom{n-1}{[\frac{m}{2}]} + (-1)^{m+1} \binom{n-1}{[\frac{m-1}{2}]} \right\}^2 \tag{5.41}$$

where $[x]$ is the integer part of x[1].

The evaluation of an upper bound on the fraction of the nondegenerate states (f) in the sector $P = \{0, n\}$ can be reduced to a combinatorial problem. We note that the number of such states cannot exceed the dimension of $ker I_2$ at $U = 0$ restricted to the subspace $P = \{0, n\}$. Let us denote this dimension by K. The kernel of I_2 at $U = 0$ consists of all states $|\mathbf{r}\rangle$ such that

$$\sum_{k=1}^{m} \Big[\sin \frac{2\pi p_k}{n} + \sin \frac{2\pi q_k}{n} \Big] = 0 \tag{5.42}$$

Thus we have $f \leq K/D \equiv g$, where D is the dimension of $P = \{0, n\}$ subspace. First, one can show by explicitly constructing a $P = 0$ state such that the left hand side of (5.42) is nonzero that $K < D$ for $2n - 2 \geq m \geq 2$ and $n \neq 2$. This means that twofold degenerate states exist for all values of m and n except $n = 2$ and $m = \{0, 1, 2n - 1, 2n\}$. Numerical values of g for the first few m and n are tabulated in Table 2. Since $g(m, n) = g(2n - m, n)$, only values for $m \leq n$ are shown.

We see from Table 1 that at small m and n a substantial fraction of levels are nondegenerate. Next, we consider the limit $n \gg m$. The exact value of D depends on the greatest common divider

[1]The high degeneracy of the zero eigenvalue of even integrals of motion suggests that even conserved currents have an additional symmetry. An interesting open question is whether the corresponding eigenstates can be chosen to be independent of U (compare to the discussion on multiply degenerate levels of the Hamiltonian bellow).

$m \setminus n$	2	3	4	5	6
2	1.0	0.89	0.79	0.76	0.71
3	–	0.88	0.765	0.70	0.64
4	–	–	0.764	0.675	0.62
5	–	–	–	0.670	0.610
6	–	–	–	–	0.608

Table 2: Values of K/D. Note that the upper bound on the number of nondegenerate states monotonically decreases as m and n increase.

of m and n. However, this is not essential for large n, since we can always decrease or increase n by a small number so that m and n become mutually prime, in which case the dimension of $P = \{0, n\}$ subspace is $1/n$ of the total dimension of the Hilbert space.

$$D = \frac{1}{n}\binom{2n}{m}^2 \sim n^{2m-1} \quad \text{for } n \gg m \tag{5.43}$$

To analyze the behavior of K in the limit $n \gg m$, we note that there are two ways how a number of terms in (5.42) can cancel. The first option is the pairwise cancellation. Alternatively, r terms can cancel if their momenta correspond to the vertices of the regular r–gon. This can happen only if n is divisible by r. For a given p there are at most four other momenta with which it can cancel pairwise. Therefore, for $n \gg m$ the number of ways in which the sum (5.42) can cancel pairwise grows slower than n^m, while the number of non-pairwise cancellations grows slower than n^{m-1}. We conclude that

$$f \leq \frac{\text{const}}{n^{m-1}} \quad \text{for } n \gg m \tag{5.44}$$

This asymptotics combined with numerical values from Table 2 suggests that almost all states in the sector $P = \{0, n\}$ are at least twofold degenerate in the thermodynamical limit.

As for the multiply degenerate states the first observation is that, at least for benzene, all of their eigenvalues are linear in the coupling parameter u. This seems to suggest that these states are simultaneous eigenstates of the kinetic ($\hat{T}$) and the potential ($\hat{U}$) energy operators (3.29). Indeed, this turns out to be the case for the majority of the multiply degenerate levels for benzene. However, the benzene Hamiltonian also has two eigenstates with $E = \pm u/2$ and $P = 3$ that are not simultaneous eigenstates of $\hat{T}$ and $\hat{U}$.

Some of the multiply degenerate states can be obtained using the prescription of [13]. The idea is the following. We take a state $|\mathbf{r}\rangle$ that has only one species of electrons, say $2l$ ($l \leq n$) spin down electrons, and no spin up electrons

$$|\mathbf{r}\rangle = |0; \mathbf{q}\rangle = |0; q_1, \ldots q_{2l}\rangle \tag{5.45}$$

Clearly, $|\mathbf{r}\rangle$ is an eigenstate of both $\hat{T}$ and $\hat{U}$.

$$\hat{T}|\mathbf{r}\rangle = \frac{u-1}{2}\sum_{k=1}^{2l} \cos\frac{\pi q_k}{n}|\mathbf{r}\rangle \quad \hat{U}|\mathbf{r}\rangle = u(n/2 - l)|\mathbf{r}\rangle \tag{5.46}$$

On the other hand, $|\mathbf{r}\rangle$ is a lowest weight state in the $so(4)$ algebra constructed from $\mathbf{S}$ and $\mathbf{L}$

$$\begin{aligned} S_z|\mathbf{r}\rangle &= -l|\mathbf{r}\rangle \quad S = l \\ \hat{L}_z|\mathbf{r}\rangle &= (l-n)|\mathbf{r}\rangle \quad L = n - l \end{aligned} \tag{5.47}$$

The energy according to (5.46) is

$$E(u) = \frac{u-1}{2}\sum_{k=1}^{2l}\cos\frac{\pi q_k}{n} + u(n/2 - l) \tag{5.48}$$

If $m \geq l$, we can get an eigenstate $|\tilde{\mathbf{r}}\rangle$ with m spin up and m spin down electrons, by applying the raising operators of the $so(4)$ algebra

$$|\tilde{\mathbf{r}}\rangle = \hat{S}_+^l \hat{L}_+^{m-l}|\mathbf{r}\rangle \tag{5.49}$$

The total number of states that can be obtained in this way is

$$M = \sum_{l=0}^{m}\binom{2n}{2l} \tag{5.50}$$

while the number of states that have the same energy (5.48) cannot exceed $\binom{2n}{2l}$. For $m = n = 3$ the allowed choices for l are $l = \{0, 1, 2, 3\}$. The choice $l = 1$ yields 15 eigenstates of which 3 states have the total momentum $P = 3$ and are degenerate with the energy $E = u/2$. By partial particle-hole symmetry (5.38) the choice $l = 2$ also gives 3 states with $P = 3$ and the energy $E = -u/2$. The actual number of states of energy $u/2$ and $P = 3$ is 7 (Table 1). Wave functions of 6 of these states are independent of U.

We arrive at the conclusion that contrary to what was conjectured in [13], not all U–independent eigenstates can be obtained using the above prescription. The six U–independent eigenstates together with the corresponding states that have lowest weight in $so(4)$ are given in Appendix A.

Clearly, the multiple degeneracies discussed above mean that there is an additional U–independent symmetry of the Hubbard Hamiltonian that have been overlooked in Section 2. This symmetry seems to be related to the high degeneracy of the spectra of the potential and kinetic energy operators. However, currently we do not know what is the algebra of generators of this additional symmetry and how its representations are to be classified.

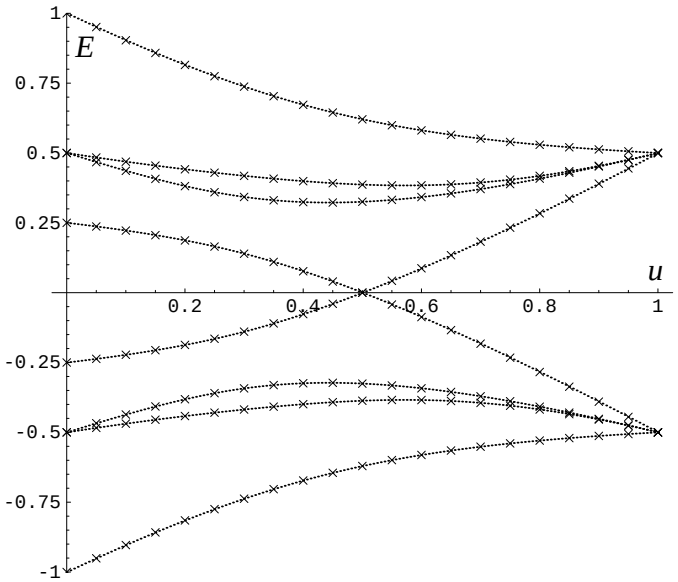

Figure 3: Energies for $(P, \sigma, I^{(o)}, S, L) = (0, 1, 1, 1, 1)$ (cf. Fig 4) in units of $U - 4T$ as functions of $u = U/(U - 4T)$. Levels marked with crosses are twofold degenerate with respect to $\sigma = \pm 1$. They also correspond to $(P, \sigma, I^{(o)}, S, L) = (0, -1, 1, 1, 1)$ (equation (5.37)). Note that since $S = L$ the spectrum is symmetric under the reflection $E \to -E$ (equation (5.38)).

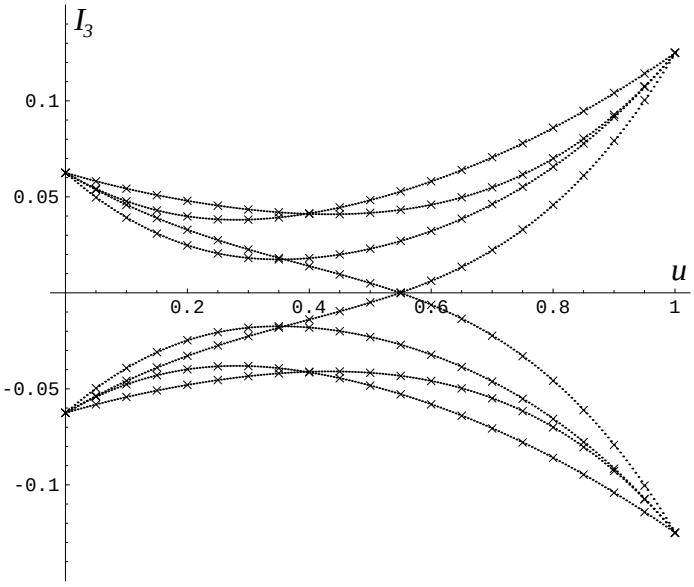

Figure 4: Eigenvalues of $\hat{I}_3$ for $(P, \sigma, I^{(o)}, S, L) = (0, 1, 1, 1, 1)$ (cf. Fig. 3) in units of $U - 4T$ as functions of $u = U/(U - 4T)$. All eigenvalues are twofold degenerate with respect to $\sigma = \pm 1$. They also correspond to $(P, \sigma, I^{(o)}, S, L) = (0, -1, 1, 1, 1)$ (equation (5.37)). The spectrum is symmetric under the reflection $I_3 \to -I_3$ (equation (5.38)). Note however that crossings of $\hat{I}_3$ and $\hat{H}$ occur at different values of u except $u = \{0, 1\}$.

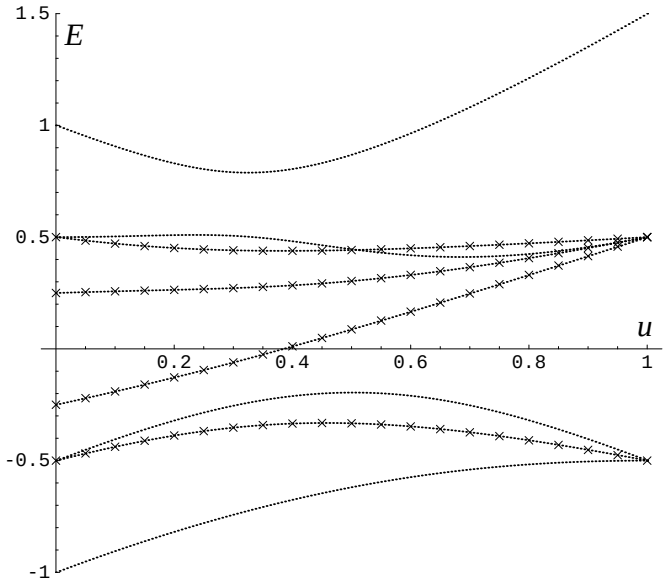

Figure 5: Energies for $(P, \sigma, I^{(o)}, S, L) = (0, -1, -1, 0, 1)$ (cf. Fig. 6 and 7) in units of $U - 4T$ as functions of $u = U/(U - 4T)$. Levels marked with crosses are twofold degenerate with respect to $\sigma = \pm 1$. They also correspond to $(P, \sigma, I^{(o)}, S, L) = (0, 1, -1, 0, 1)$ (equation (5.37)). Upside down the figure shows levels for the same set of quantum numbers with $S \leftrightarrow L$ (equation (5.38)). Note the nondegenerate levels.

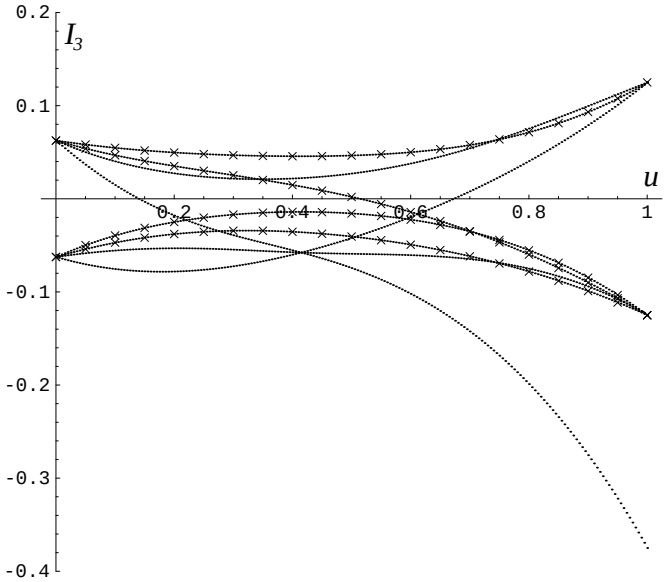

Figure 6: Eigenvalues of $\hat{I}_3$ for $(P, \sigma, I^{(o)}, S, L) = (0, -1, -1, 0, 1)$ (cf. Fig. 5 and 7) in units of $U - 4T$ as functions of $u = U/(U - 4T)$. Levels marked with crosses are twofold degenerate with respect to $\sigma = \pm 1$. They also correspond to $(P, \sigma, I^{(o)}, S, L) = (0, 1, -1, 0, 1)$ (equation (5.37)). Upside down the figure shows levels for the same set of quantum numbers with $S \leftrightarrow L$ (equation (5.38)).

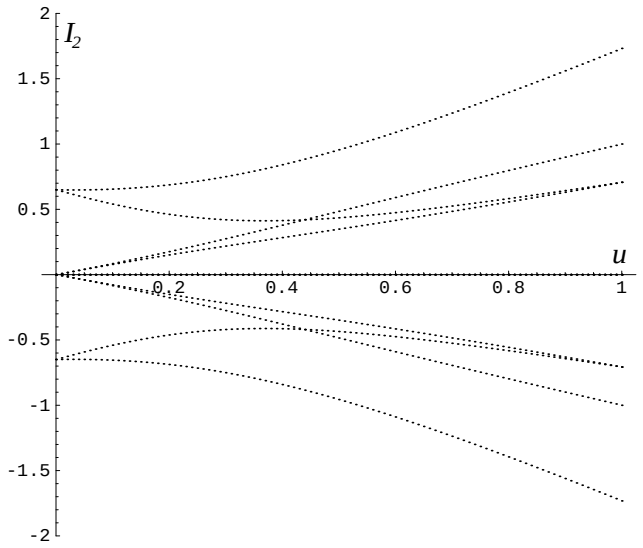

Figure 7: Eigenvalues of $\hat{I}_2$ for $(P, I^{(o)}, S, L) = (0, -1, 0, 1)$ in units of $U - 4T$ as functions of $u = U/(U - 4T)$. Note the difference as compared to Fig. 5 and 6 The quantum number σ cannot be assigned since $\hat{I}_2$ anticommutes with $\hat{\sigma}$ (3.25). All eigenvalues are twofold degenerate with respect to $S \leftrightarrow L$ and $E \to -E$ (equation (5.39)). Since $P = -P = 0$ the spectrum is symmetric under the reflection (equation (5.40)).

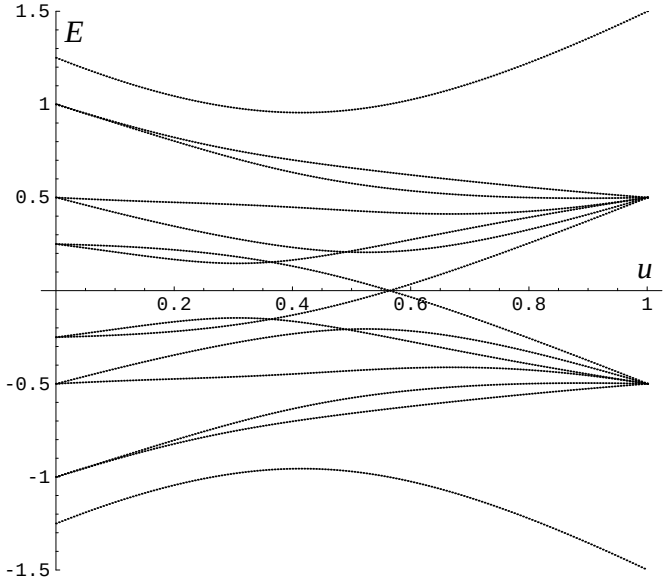

Figure 8: Energies for $(P, I^{(o)}, S, L) = (2, 1, 0, 0)$ (cf. Fig 9 and 10) in units of $U-4T$ as functions of $u = U/(U-4T)$. Since $S = L$ the spectrum is symmetric under the reflection $E \to -E$ (equation (5.38)). Note the level crossings.

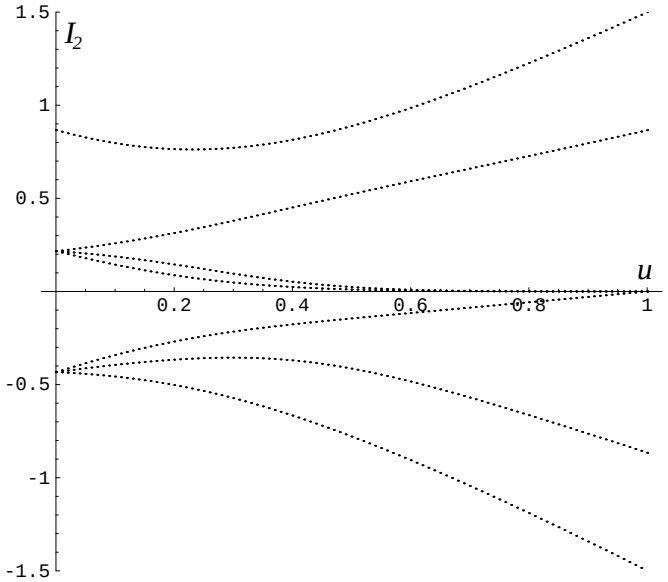

Figure 9: Eigenvalues of $\hat{I}_2$ for $(P, I^{(o)}, S, L) = (2, 1, 0, 0)$ in units of $U - 4T$ as functions of $u = U/(U - 4T)$. All eigenvalues are twofold degenerate with respect to $E \leftrightarrow -E$ (equation 5.39). Note that unlike Fig 8 and 10 there is no reflection symmetry since $P \neq -P$ (equation (5.40)).

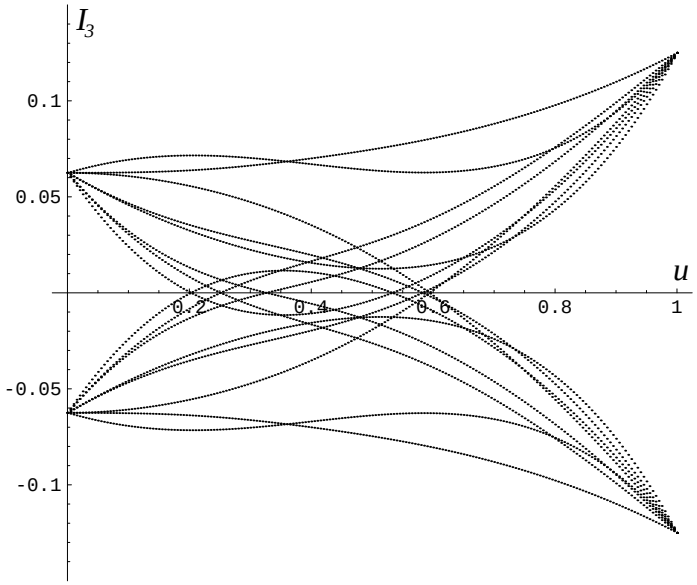

Figure 10: Eigenvalues of $\hat{I}_3$ for $(P, I^{(o)}, S, L) = (2, 1, 1, 1)$ (cf. Fig 8 and 9) in units of $U - 4T$ as functions of $u = U/(U - 4T)$. Since $S = L$ the spectrum is symmetric under the reflection $E \to -E$ (equation (5.38)).

6 Level Crossings

The spectra of the Hamiltonian and conserved currents display numerous cases of crossings of levels that have the same U–independent symmetry quantum numbers. In this section we argue that this type of behavior is in fact expected in integrable models.

Let us first clarify the notion of a nontrivial integral of motion for a quantum system on a finite lattice. Let $H(u) = H_0 + uV$ be a Hamiltonian that, in a certain basis, can be represented by an $s \times s$ matrix. For example, $H(u)$ can be one of the blocks of the Hubbard Hamiltonian. Clearly, any matrix M that is an analytical function of $H(u)$ and u, $M = f(u, H(u))$, commutes with H. Obviously, M is not an independent conserved quantity. Therefore, we say that $J(u)$ is a nontrivial integral of motion if $J(u)$ is hermitian, $[J(u), H(u)] = 0$ and at the same time $J(u)$ cannot be written as an analytical function of $H(u)$ and u.

Now let us show that the existence of a nontrivial integral of motion implies at least one level crossing. Since $J(u)$ and $H(u)$ commute, there is a basis where both these operators are diagonal. Let $E_1(u), \ldots, E_s(u)$ and $J_1(u), \ldots, J_s(u)$ be the eigenvalues of $H(u)$ and $J(u)$ respectively. Consider the following set of algebraic equations:

$$\begin{array}{rcl} a_1 E_1^{s-1}(u) + \ldots + a_{s-1} E_1(u) + a_s &=& J_1(u) \\ \vdots & & \vdots \\ a_1 E_s^{s-1}(u) + \ldots + a_{s-1} E_1(u) + a_s &=& J_s(u) \end{array} \tag{6.51}$$

If equations (6.51) have a solution, $J(u)$ and $H(u)$ are not independent. Namely, $J(u) = a_1 H^{s-1} + \ldots + a_s$. The system (6.51) has no solutions if and only if $E_i(u^*) = E_j(u^*)$ and $J_i(u^*) \neq J_j(u^*)$ for some i, j, and u^*. Thus, the Hamiltonian can have a nontrivial integral of motion only if it has a level crossing.

Let us analyze the suppression of level repulsion in integrable models in more detail. Here we consider only real Hamiltonians that depend linearly on the coupling constant $H(u) = H_0 + uV$. We assume that there is a value of $u = \tilde{u}$ at which all eigenvalues of $H(\tilde{u})$ are nondegenerate. This is true for instance for blocks of the Hubbard Hamiltonian for benzene. In general, since all integrals of motion mutually commute, permanent degeneracies occur only with respect to quantum numbers of parameter independent symmetries. Therefore, after all these symmetries are factored out, at a certain value of u all states in a given block are nondegenerate. Hence, we can use the nondegenerate perturbation theory to write down the variation of the eigenvalues and the matrix elements of the perturbation with u in the vicinity of $\tilde{u}$.

$$\frac{dE_n(u)}{du} = V_{nn}(u) \tag{6.52}$$

$$\frac{dV_{nn}(u)}{du} = 2 \sum_{j \neq n} \frac{V_{nj}^2(u)}{E_n(u) - E_j(u)} \tag{6.53}$$

$$\frac{dV_{nm}(u)}{du} = \sum_{j \neq n} \frac{V_{nj}(u) V_{mj}(u)}{E_n(u) - E_j(u)} + \sum_{j \neq m} \frac{V_{nj}(u) V_{mj}(u)}{E_m(u) - E_j(u)} \tag{6.54}$$

where all matrix elements are evaluated in the running basis

$$\begin{array}{l} H\psi_n(u) = E_n(u)\psi_n(u) \\ V_{ij}(u) \equiv \langle \psi_i(u) | V | \psi_j(u) \rangle \end{array}$$

Equations (6.52)–(6.54) were used in [23] to derive the distribution of energy eigenvalues of the irregular spectrum in the semiclassical limit. Note in particular that these equations are not model specific. The model itself is defined by the initial conditions – the values of $V_{ij}(\tilde{u})$ and $E_i(\tilde{u})$. If the initial conditions in any block are slightly perturbed[2], the integrability is lost and the majority of crossings are converted into anticrossings (see e.g. Fig. 11 and 12). At the same time, since the perturbation has the block diagonal structure of the original Hamiltonian, the perturbed Hamiltonian still has the same U–independent symmetries.

Now consider a pair of levels that get close at $u = u_0$, i.e. we assume that the absolute value of the energy difference between these two levels $\Delta(u) = E_1(u) - E_2(u)$ is much smaller than the energy distance to the remaining levels. Then, from (6.52) and (6.53) we obtain the following equations for $\Delta(u)$:

$$\frac{d\Delta}{du} = V_{11} - V_{22} \tag{6.55}$$

$$\frac{d^2\Delta}{du} = \frac{4V_{12}^2}{\Delta} + F(u) \tag{6.56}$$

where

$$F(u) = 2\sum_{j\neq 1,2}\Big[\frac{V_{1j}^2(u)}{E_1(u) - E_j(u)} - \frac{V_{2j}^2(u)}{E_2(u) - E_j(u)}\Big]$$

We can interpret E_1 and E_2 as coordinates of two one dimensional particles. Particles move with a relative velocity $(V_{11} - V_{22})$ and interact with a force $4V_{12}^2/\Delta + F(u)$. If $V_{12} \not\to 0$ as $\Delta \to 0$, an infinite repulsion prevents the particles from colliding. On the other hand, if levels 1 and 2 have different U–independent symmetry, $V_{12}(u)$ is identically zero and levels are permitted to cross. These arguments constitute the essence of the noncrossing rule.

Let us incorporate conservation laws into the picture. Let the corresponding block of the conserved current be $J(u^*) = J(u) + (u^* - u)W + (u^* - u)^2W' + \ldots$ Since $J(u^*)$ commutes with $H(u^*)$ to all orders in $(u - u^*)$, we get

$$[H(u^*), J(u^*)] = 0 \Rightarrow [H(u), W] + [V, J(u)] = 0 \tag{6.57}$$

Evaluating the matrix element of the above equation between states 1 and 2, we find

$$V_{12}(u) = W_{12}(u)\frac{E_1(u) - E_2(u)}{J_1(u) - J_2(u)} \tag{6.58}$$

Therefore, unless $J_1(u) = J_2(u)$ in the vicinity of $u = u_0$, $V_{12} \approx \text{const}\,\Delta \to 0$ as $\Delta \to 0$ and levels are allowed to cross.

We have checked for benzene that the eigenvalues of the Hamiltonian, $\hat{I}_2$, and $\hat{I}_3$ are never degenerate at the same value of u except at two points of special symmetry $u = 0$ and $u = 1$. Because $\hat{I}_2$ also connects all doubly degenerate states, we conclude that $\hat{I}_2$ and $\hat{I}_3$ together with U–independent symmetries explain all cases of level crossings and permanent degeneracies in the spectrum of the Hubbard Hamiltonian for benzene.

[2]e.g. by adding small random numbers to $E_i(\tilde{u})$ and $V_{ij}(\tilde{u})$.

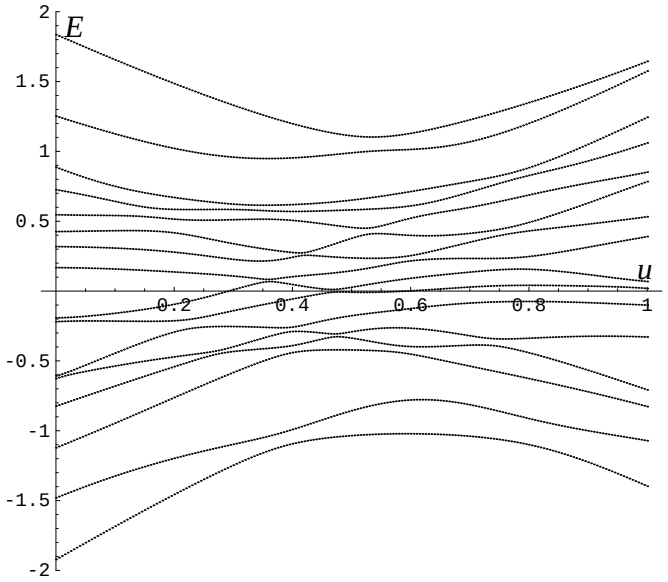

Figure 11: The block for $(P, I^{(o)}, S, L) = (1, 1, 0, 1)$ has been perturbed by adding small random numbers to $V_{ij}(\tilde{u})$ and $E_i(\tilde{u})$ at $\tilde{u} = 0.6$. Energies at other values of u are determined according to (6.52)–(6.54) and plotted in units of $U - 4T$ as functions of $u = U/(U - 4T)$.

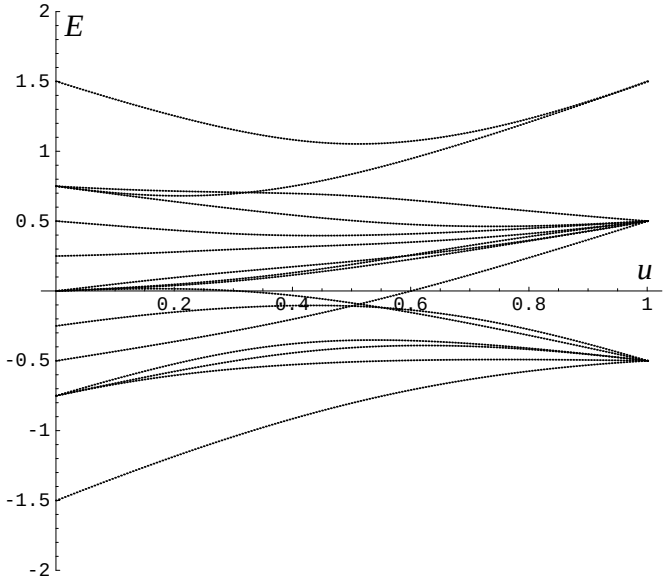

Figure 12: Unperturbed energies for $(P, I^{(o)}, S, L) = (1, 1, 0, 1)$ in units of $U - 4T$ as functions of $u = U/(U - 4T)$.

In the vicinity of a crossing at $u = u^*$ the transverse matrix element $V_{12}(u)$ can be expanded in series in the energy difference $\Delta(u)$.

$$V_{12}(\Delta) = a_1\Delta + a_2\Delta^2 + \dots \tag{6.59}$$

The coefficient at the linear term can be derived using the degenerate perturbation theory.

$$a_1 = \sum_{j\neq 1,2} \frac{V_{1j}(u^*)V_{2j}(u^*)}{E_1(u^*) - E_j(u^*)} \tag{6.60}$$

Here the basis at $u = u^*$ has to be chosen so that $V_{12}(u^*) = 0$ (see e.g. Chapter 4 in [2]).

The surprising feature of the Hubbard Hamiltonian is that, at least for benzene, the linear term vanishes for all crossings at $u \neq \{0, 1\}$, while individual terms in the summation (6.60) do not. At this point, we do not have an explanation for this seemingly puzzling phenomenon.

To see that this is not a mere consequence of integrability, we study a simple example of 3×3 Hamiltonians. This example also illustrates the connection between crossings and integrability and is therefore interesting on its own right.

Let

$$H = H_0 + uV \quad I = I_0 + uW \tag{6.61}$$

be two 3×3 real symmetric matrices. We call a pair (H, I) integrable if these two matrices commute

$$[H, I] = 0 \tag{6.62}$$

Since we can always add multiples of the identity matrix to H and I without affecting integrability (6.62) or any of the level crossings, with no loss of generality, we can assume that both H and I are traceless

$$TrH = TrI = 0$$

Further, we say that a pair (H, I) is trivial if the u dependence can be eliminated from either H or I by a u–independent unitary transformation (change of basis) and (or) by taking linear combinations of H and I.

First we demonstrate that if (H, I) is a nontrivial integrable pair, both $H(u)$ and $I(u)$ have a single level crossing. Indeed, one can check that by changing the basis and taking linear combinations any nontrivial integrable pair can be brought to the following "canonical" form:

$$H = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{bmatrix} + u \begin{bmatrix} v_{11} & 0 & v_{13} \\ 0 & v_{22} & v_{23} \\ v_{13} & v_{23} & -v_{11} - v_{22} \end{bmatrix} \tag{6.63}$$

$$I = \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{bmatrix} + u \begin{bmatrix} w_{11} & w_{12} & w_{13} \\ w_{12} & w_{22} & w_{23} \\ w_{13} & w_{23} & -w_{11} - w_{22} \end{bmatrix} \tag{6.64}$$

Matrix elements of W can be written in terms of v_{ij}'s using (6.62).

$$w_{11} = \frac{5v_{11}^2 - v_{11}v_{22} + 2v_{13}^2 - 4v_{22}^2 - 4v_{23}^2}{9(v_{11} - v_{22})} \tag{6.65}$$

$$w_{12} = \frac{2v_{13}v_{23}}{3(v_{11}-v_{22})} \quad w_{13} = v_{13}/3 \tag{6.66}$$

$$w_{22} = -\frac{4v_{11}^2 + 4v_{13}^2 + v_{11}v_{22} - 5v_{22}^2 - 2v_{23}^2}{9(v_{11}-v_{22})} \tag{6.67}$$

$$w_{23} = -v_{23}/3 \quad w_{33} = -w_{11} - w_{22} \tag{6.68}$$

Since W has five independent matrix elements, while V has only four, w_{ij}'s are constrained by

$$w_{33} + \frac{w_{13}}{3w_{23}} + \frac{w_{23}}{3w_{13}} - \frac{2}{3}w_{13}w_{23} = 0 \tag{6.69}$$

$H(u)$ has an apparent crossing at $u = 0$. Further, it turns out that the matrix $I(u)$ has a crossing if and only if the constraint (6.69) is met! This can be verified either directly or using [24], where, among other things, degeneracies of real symmetric 3×3 matrices are analyzed in detail. The crossing of I is at

$$2/u^* = (w_{22} - w_{11}) + w_{12}(w_{13}/w_{23} - w_{23}/w_{13}) \tag{6.70}$$

Similarly, it can be shown that linear combinations of H and I always have crossings too. Therefore, if (H, I) is a nontrivial integrable pair, both $H(u)$ and $I(u)$ have a single level crossing.

Now let us show that the converse is also true, i.e. that any real symmetric 3×3 matrix that has a pairwise crossing is also integrable. We start with a real symmetric 3×3 matrix $H = H_0 + uV$ that has a pairwise crossing at $u = u^*$. By redefining the parameter $u \to u - u^*$ and a suitable choice of basis we can write H in the form (6.63). Therefore, there exists a matrix I of the form (6.64) such that $[I, H] = 0$. In view of this explicit construction of a "dynamical conservation law", we may say that there are no accidental degeneracies in the case of 3×3 real matrices.

Finally, we note that the linear term in expansion (6.59) is non zero for both H and I unless specially arranged.

7 Conclusion

7.1 Summary

We have shown that for all m and n except $m = \{0, 1, 2n-1, 2n\}$ and $n = 2$ there are twofold permanent degeneracies for the values of the total momentum $P = 0$ and $P = n$. These degeneracies are a consequence of different transformation properties of even and odd currents with respect to spatial reflections ($\hat{\sigma}$) and partial particle-hole transformation ($\hat{Z}_\uparrow$) (equations (3.23–3.26)). We have argued that in the thermodynamical limit the fraction of doubly degenerate states in the sector $P = \{0, n\}$ approaches one. For benzene ($m = n = 3$) we have checked that all doubly degenerate states are maped into each other by the first even current $\hat{I}_2$. We have also seen that some states can be nondegenerate since all even currents have nontrivial kernels.

We have learned from the benzene example that there is a number of multiply degenerate states that are simultaneous eigenstates of the potential and kinetic energy operators. The wave functions of these states do not depend on the coupling U. This suggests the existence of an additional U–independent symmetry. However, as we have seen in Section 5 and Appendix A some of these states

cannot be obtained by applying the raising (lowering) operators of the $so(4)$ algebra to states that have only one species of electrons.

Further, we have demonstrated how the constraints of the noncrossing rule are lifted in integrable models. In fact, we have argued that in integrable models crossings of levels with the same parameter independent symmetry quantum numbers are expected. This was also illustrated by a simple example of 3×3 matrix models where there is a one to one correspondence between crossings and integrability. We have seen that for $m = n = 3$ the first two nontrivial conserved currents are sufficient to explain all cases of level crossings. We have shown numerically that in the case of benzene the transverse matrix element is quadratic in energy difference in the vicinity of all pairwise level crossings.

7.2 Open Questions

1. What is the symmetry responsible for the multiply (more than twofold) degenerate levels in the spectrum of the Hubbard Hamiltonian? Are energies of multiply degenerate states always linear in the coupling parameter? How one can count the degrees of degeneracy and the number of multiply degenerate states for arbitrary m and n?

2. What is the symmetry responsible for the high degeneracy of the zero eigenvalue of even integrals of motion?

3. For given m and n what is the exact number of states such that $\hat{I}_{2k}\psi = 0$ for all k and U? What is the exact number of twofold degenerate states with $P = \{0, n\}$?

4. Is the transverse matrix element always quadratic in energy difference in the vicinity of all pairwise level crossings in the Hubbard model? What is the explanation of this phenomenon?

8 Appendix A

Here we write down U–independent eigenstates that have $E = u/2$. See Section 4 for notations.

$$\begin{aligned} |\mathbf{r}_1\rangle &= -|0,1,2;1,2,3\rangle - 1/2|0,1,3;0,2,3\rangle + 1/2|0,3,4;0,3,5\rangle + \\ &\quad |0,4,5;3,4,5\rangle - 1/2|1,2,4;1,2,5\rangle + 1/2|1,4,5;2,4,5\rangle + (\uparrow\leftrightarrow\downarrow) \end{aligned} \qquad \begin{array}{cc} S=0 & L=2 \\ S_z=0 & L_z=0 \end{array} \tag{8.71}$$

$$\begin{aligned} |\mathbf{r}_2\rangle &= |0,2,5;1,3,4\rangle + |0,3,4;1,2,5\rangle + |0,3,5;1,2,4\rangle \\ &\quad -|1,4,5;0,2,3\rangle - |2,3,5;0,1,4\rangle - |2,4,5;0,1,3\rangle + (\uparrow\leftrightarrow\downarrow) \end{aligned} \qquad \begin{array}{cc} S=0 & L=1 \\ S_z=0 & L_z=0 \end{array} \tag{8.72}$$

$$|\mathbf{r}_3\rangle = -|0,2,5;1,3,4\rangle + 1/2|0,3,4;0,3,5\rangle + 1/2|1,2,4;1,2,5\rangle$$
$$1/2|1,4,5;2,4,5\rangle + 1/2|0,1,3;0,2,3\rangle + |0,1,4;2,3,5\rangle - (\uparrow\leftrightarrow\downarrow) \qquad \begin{matrix} S=1 & L=2 \\ S_z=0 & L_z=0 \end{matrix} \tag{8.73}$$

$$|\mathbf{r}_4\rangle = -|0,1,3;0,2,3\rangle - |0,3,4;0,3,5\rangle +$$
$$|1,2,4;1,2,5\rangle + |1,4,5;2,4,5\rangle + (\uparrow\leftrightarrow\downarrow) \qquad \begin{matrix} S=0 & L=2 \\ S_z=0 & L_z=0 \end{matrix} \tag{8.74}$$

$$|\mathbf{r}_5\rangle = |0,1,2;1,2,3\rangle + |0,1,4;2,3,5\rangle|0,1,5;2,3,4\rangle +$$
$$|0,2,4;1,3,5\rangle + |0,2,5;1,3,4\rangle + |0,4,5;3,4,5\rangle - (\uparrow\leftrightarrow\downarrow) \qquad \begin{matrix} S=1 & L=2 \\ S_z=0 & L_z=0 \end{matrix} \tag{8.75}$$

$$|\mathbf{r}_6\rangle = 1/2|0,1,3;0,2,3\rangle + |0,1,5;2,3,4\rangle - |0,2,4;1,3,5\rangle -$$
$$1/2|0,3,4;0,3,5\rangle - 1/2|1,2,4;1,2,5\rangle + 1/2|1,4,5;2,4,5\rangle - (\uparrow\leftrightarrow\downarrow) \qquad \begin{matrix} S=1 & L=2 \\ S_z=0 & L_z=0 \end{matrix} \tag{8.76}$$

The corresponding lowest weight eigenstates of the Hamiltonian are

$$|\tilde{\mathbf{r}}_1\rangle = -|1;2\rangle - |2;1\rangle + |4;5\rangle + |5;4\rangle \quad S_z=0 \quad L_z=-2 \tag{8.77}$$

$$|\tilde{\mathbf{r}}_2\rangle = |0,1;2,3\rangle - |0,2;1,3\rangle - 2|0,3;1,2\rangle - 2|0,3;4,5\rangle - |0,4;3,5\rangle + |0,5;3,4\rangle$$
$$-2|1,2;0,3\rangle - |1,3;0,2\rangle + |2,3;0,1\rangle + |3,4;0,5\rangle - |3,5;0,4\rangle - 2|4,5;0,3\rangle \qquad \begin{matrix} S_z=0 \\ L_z=-1 \end{matrix} \tag{8.78}$$

$$|\tilde{\mathbf{r}}_3\rangle = |;1,2\rangle + |;4,5\rangle \quad S_z=-1 \quad L_z=-2 \tag{8.79}$$

$$|\tilde{\mathbf{r}}_4\rangle = -2|0;3\rangle - 2|3;0\rangle + |1;2\rangle + |2;1\rangle + |4;5\rangle + |5;4\rangle \quad S_z=0 \quad L_z=-2 \tag{8.80}$$

$$|\tilde{\mathbf{r}}_5\rangle = |;0,3\rangle \quad S_z=-1 \quad L_z=-2 \tag{8.81}$$

$$|\tilde{\mathbf{r}}_6\rangle = |;1,2\rangle - |;4,5\rangle \quad S_z=-1 \quad L_z=-2 \tag{8.82}$$

States $|\tilde{\mathbf{r}}_3\rangle$, $|\tilde{\mathbf{r}}_5\rangle$, and $|\tilde{\mathbf{r}}_6\rangle$ describe one species of electrons (spin down). The remaining states cannot be obtained by the prescription detailed in the end of Section 5.

9 Appendix B

In this section we collect the expressions for the matrix elements of the Hamiltonian, $\hat{I}_2$, $\hat{I}_3$ and $\hat{\mathbf{S}}^2$. Let $\tilde{p}_1 < \ldots < \tilde{p}_t$ be the momenta of spin up electrons that are in $\mathcal{P} = \{p_k\}$ but not in $\mathcal{P}' = \{p'_k\}$, $\tilde{p}_{t+1} < \ldots < \tilde{p}_{2t}$ be the momenta that are in $\mathcal{P}'$ but not in $\mathcal{P}$. Similarly, we can define $\mathcal{Q} = \{q_k\}$, $\tilde{q}_1 < \ldots < \tilde{q}_u$, and $\tilde{q}_{u+1} < \ldots < \tilde{q}_{2u}$. The number of elements in the intersection of $\mathcal{P}$ with $\mathcal{P}'$ and $\mathcal{Q}$ with $\mathcal{Q}'$ is therefore $L(\mathcal{P} \cap \mathcal{P}') = m - t$ and $L(\mathcal{Q} \cap \mathcal{Q}') = m - u$. We also define

$$\epsilon(\mathbf{r}', \mathbf{r}) = \langle \mathbf{r}' | d^\dagger_{\tilde{p}_{t+1}\uparrow} d_{\tilde{p}_1\uparrow} \ldots d^\dagger_{\tilde{p}_{2t}\uparrow} d_{\tilde{p}_t\uparrow} d^\dagger_{\tilde{q}_{u+1}\downarrow} d_{\tilde{q}_1\downarrow} \ldots d^\dagger_{\tilde{q}_{2u}\downarrow} d_{\tilde{q}_u\downarrow} | \mathbf{r} \rangle = \pm 1 \tag{9.83}$$

In this notation the matrix elements of $\mathbf{S}^2$, H, $\hat{I}_2$ and $\hat{I}_3$ take the following form:

$$\begin{aligned} \langle \mathbf{r}' | \mathbf{S}^2 | \mathbf{r} \rangle &= n - L(\mathcal{P} \cap \mathcal{Q}) && \text{if } |\mathbf{r}\rangle = |\mathbf{r}'\rangle \\ &= \epsilon(\mathbf{r}', \mathbf{r}) && \text{if } \mathcal{R} = \mathcal{R}' \text{ and } u = t = 1 \\ &= 0 && \text{otherwise} \end{aligned} \tag{9.84}$$

$$\langle \mathbf{r}' | H | \mathbf{r} \rangle = \frac{u-1}{2} \sum_{k=1}^{2m} \cos\frac{\pi r_k}{n} \delta_{\mathbf{r}',\mathbf{r}} - \frac{u}{2n} \epsilon(\mathbf{r}', \mathbf{r}) \delta_{u1} \delta_{t1} \delta_{PP'} \tag{9.85}$$

$$\langle \mathbf{r}' | \hat{I}_2 | \mathbf{r} \rangle = \frac{u-1}{4} \sum_{k=1}^{2m} \sin\frac{2\pi r_k}{n} \delta_{\mathbf{r}',\mathbf{r}} - \frac{u}{2n} \epsilon(\mathbf{r}', \mathbf{r}) \delta_{u1} \delta_{t1} \delta_{PP'} \tag{9.86}$$

$$\begin{aligned} \langle \mathbf{r}' | \hat{I}_3 | \mathbf{r} \rangle &= \frac{(u-1)^3}{128} \sum_{k=1}^{2m} \sin\frac{3\pi r_k}{n} \delta_{\mathbf{r}',\mathbf{r}} - \frac{u^2(u-1)}{8n^2} \Big[\sum_{k,j,l=1}^{m} \cos\frac{\pi p_k}{n} \cos\frac{\pi(q_j - q_l)}{n} \delta_{\mathbf{r}',\mathbf{r}} + p \leftrightarrow q \Big] - \\ &\frac{u(u-1)^2}{8} \sum_{k=1}^{m} \sin\frac{\pi p_k}{n} \cos\frac{\pi q_k}{n} \delta_{\mathbf{r}',\mathbf{r}} + \epsilon(\mathbf{r}', \mathbf{r}) \frac{u^2(u-1)}{8n^2} \sum_{k=1}^{m} \Big[\cos\frac{\pi(\tilde{p}_2 + \tilde{q}_2 - p'_k)}{n} + \\ &\cos\frac{\pi(\tilde{p}_2 - \tilde{q}_1 - p'_k)}{n} + p \leftrightarrow q \Big] \delta_{u1} \delta_{t1} \delta_{PP'} + \epsilon(\mathbf{r}', \mathbf{r}) \frac{u^2(u-1)}{4n^2} \Big[(\cos\frac{\pi(\tilde{q}_4 - \tilde{q}_2)}{n} - \\ &\cos\frac{\pi(\tilde{q}_4 - \tilde{q}_1)}{n} \Big] \delta_{PP'} \sum_{k=1}^{m} \cos\frac{\pi p'_k}{n} \delta_{u2} \delta_{t0} + (p \leftrightarrow q, u \leftrightarrow t)] + \\ &\epsilon(\mathbf{r}', \mathbf{r}) \frac{u^2(u-1)}{8n^2} \Big[\Big(\cos\frac{\pi(\tilde{q}_4 - \tilde{q}_2 - \tilde{p}_1)}{n} + \cos\frac{\pi(\tilde{q}_4 - \tilde{q}_2 - \tilde{p}_2)}{n} + \cos\frac{\pi(\tilde{q}_3 - \tilde{q}_2 - \tilde{p}_1)}{n} + \\ &\cos\frac{\pi(\tilde{q}_3 - \tilde{q}_2 + \tilde{p}_2)}{n} \Big) \delta_{u1} \delta_{t2} + (p \leftrightarrow q, u \leftrightarrow t) \Big] \delta_{PP'} - \\ &\epsilon(\mathbf{r}', \mathbf{r}) \frac{u(u-1)^2}{16n} \Big[\cos\frac{\pi(\tilde{p}_1 + \tilde{p}_2)}{n} (2\cos\frac{\pi(\tilde{q}_1 - \tilde{q}_2)}{n} + 1) + \cos\frac{\pi(\tilde{p}_1 + \tilde{q}_2)}{n} + p \leftrightarrow q - \\ &\cos\frac{\pi(\tilde{p}_1 - \tilde{q}_1)}{n} - \cos\frac{\pi(\tilde{p}_2 - \tilde{q}_2)}{n} - \cos\frac{\pi(\tilde{p}_2 - \tilde{p}_1)}{n} + \cos\frac{\pi(\tilde{p}_1 + \tilde{q}_1)}{n} - \\ &\cos\frac{\pi(\tilde{p}_2 - \tilde{q}_1)}{n} - 1/2 \Big] \delta_{u1} \delta_{t1} \delta_{PP'} \end{aligned} \tag{9.87}$$

References

[1] Pauli W., 1926 *Z. Phys* **36** 336
Fock V. A., 1935 *Zs. f. Physik* **98** 145

[2] Landau L. D. and Lifshitz E. M. 1958 *Quantum Mechanics* (London)

[3] Hund F. 1927 *Phys.* **40** 742

[4] v. Neumann J. and Wigner E. 1929 *Phys. Zeit.* **30** 467

[5] Beenakker C. W. J., 1997 *Rev. Mod. Phys.* **69** 731

[6] Berry M. V., 1985 *in Chaotic behavior in quantum systems* ed.Giulio Casatil, Plenum, New York, 123-140.

[7] Arnold V. I., 1972 *Funct. Anal. Appl.* **6** 94
Arnold V. I., 1989 *Mathematical Methods of Classical Mechanics* (Springer-Verlag: New York) Appendix J

[8] Merzbacher E., 1961 *Quantum Mechanics* (New York) 407

[9] Davydov A. S. 1965 *Quantum Mechanics* (New York) 175

[10] Teller E., 1937 *J. Phys. Chem* **41** 109

[11] Heilmann O. J. and Lieb E. H., 1971 *Ann. N. Acad. Sci.* **172** 583

[12] Yang C.N., 1989 *Phys. Rev. Lett.* **63** 2144

[13] Yang C.N. and Zhang S., 1990 *Mod. Phys. Lett.* **B4** 759

[14] Affleck I., 1990 *Physics, Geometry and Topology* ed. H. C. Lee (New York: Plenum Press) p.1

[15] Pernici M., 1990 *Europhys. Lett.* **12** 75.

[16] Shastry B. S. 1986 *Phys. Rev. Lett.* **56** 1529

[17] Shastry B. S. 1986 *Phys. Rev. Lett.* **56** 2453

[18] Shastry B. S. 1988 *J. Stat. Phys.* **50** 57

[19] Lüscher M., 1976 *Nucl. Phys.* **B117** 475

[20] Grosse H., 1989 *Lett. Math. Phys.* **18** 151

[21] Grabowski M. P. and Mathieu P. 1995 *Ann. Phys* **243** 213

[22] Shiroishi M., Ujino H. and Wadati M. `cond-mat/9708064`

[23] Pechukas P. 1983 *Phys. Rev. Lett.* **51** 943

[24] Stepanov V.V. and Muller G. `chao-dyn/9806021`