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A Symbolic Solution of the Hubbard Model for Small Clusters

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1 Introduction

The one-band Hubbard model [1] describes a system of spin one-half fermions on a lattice by the Hamiltonian

$$H = -t \sum_{\langle ij \rangle \sigma} \hat{a}_{i\sigma}^\dagger \hat{a}_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} + U N_e, \quad (1)$$

where $\hat{a}_{i\sigma}^\dagger$ and $\hat{a}_{i\sigma}$ are the Wannier fermionic creation and destruction operators creating and destroying an electron of spin σ at site i of the lattice. The physical meaning of each term comprising the Hubbard Hamiltonian is straightforward. The first term of Eq.(1). the kinetic energy, accounts for electron tunneling from site j to site i and thereby reduces the energy of the system by a factor t for each tunneling event. The site summation denoted by $\langle ij \rangle$ is over all bonds of the lattice. In our investigation we restrict ourselves to nearest-neighbor tunneling or “hopping”. The interaction part of the Hubbard Hamiltonian accounts for the Coulomb interaction between two electrons residing on the same site and therefore is a simplification of the full Coulomb interaction term

$$H^{int} = \int d^3r d^3r' \hat{\psi}^\dagger(r) \hat{\psi}(r) V(r-r') \hat{\psi}^\dagger(r') \hat{\psi}(r'), \quad (2)$$

where $\hat{\psi}(r)$ is the field operator at the space point r . The last two terms of Eq.(1) are obtained from Eq.(2) if one substitutes for the field operator a linear combination of Wannier states, denoted $\phi_{i\sigma}(r)$, as follows, $\hat{\psi}(r) = \sum_{i\sigma} \hat{a}_{i\sigma} \phi_{i\sigma}(r)$. U denotes the intra-site matrix elements of the Wannier states so that the significant “short-ranged” part of the Coulomb interaction is modeled. Eq.(2) reduces to

$$H^{int} = U \sum_{i\sigma\sigma'} n_{i\sigma} n_{i\sigma'} = U \sum_i n_{i\uparrow} n_{i\downarrow} + U \sum_{i\sigma} n_{i\sigma}^2. \quad (3)$$

The last term of Eq.(3) is a constant self-energy, $U N_e$, where N_e is the total number of electrons, because $n_{i\sigma}^2 = n_{i\sigma}$ for fermions [2]. Since this term only causes a constant energy shift of the spectrum we will choose to ignore it in any eigenvalue plots.

Obtaining exact analytic solutions of the Hubbard model is difficult. Exact solutions are possible for certain cases and limits, for example when $U/t = 0$ or U/t is large, the “strong-coupling” limit where doubly occupied sites are effectively prohibited. One theoretical approach involves altering the Hubbard Hamiltonian by a unitary transformation to re-express it in a t/U expansion [3]. The lowest order terms of this expansion are kept in the large- U limit. This is called t - J model and has recently received much attention[4].

Alternatively, numerical approaches to solve the Hubbard and t - J models on finite-size clusters abound. These include non-perturbative quantum Monte Carlo simulations on lattice sizes up to 8×8 [5] and exact diagonalization methods [7] usually using the Lanczos algorithm [6]. Falicov has pioneered the

use of group-theoretic techniques to simplify the exact diagonalization problem [8]. In addition to employing point group operations to block diagonalized the Hamiltonian matrix of elements he has focused on employing more general operations of the cluster-permutation group. These permutation operations are available only because of the small finite size of the cluster. The advantage of cluster-permutations is greatest for $N = 8$.

The approach we present for investigating the one-band Hubbard model is best classified as a symbolic method with application to small clusters. Unlike the theoretic approaches, the symbolic approach gives exact information for *all* values of the parameters. However, in contrast to numerical approaches, the symbolic approach suffers from a limitation imposed by the inherent computational overhead of symbolic manipulations. As a result, for the time being, we are limited to very small cluster calculations. In this paper we explore only up to the 2×2 cluster.

In the symbolic approach, we first define manipulation rules, herein termed production rules, for the Wannier creation and annihilation operators allowing these operators to act on any general state vector. Building upon these “elementary” production rules, we implement new production rules to affect more complex operations. This ability to form a hierarchy of operations is an advantage of the symbolic approach, giving flexibility to define any quantized operator. For example, we could have just as easily worked with the $t - J$ Hamiltonian in this investigation in place of the Hubbard Hamiltonian of Eq.(1). One of the more interesting operators we have implemented in this way is a “site-interchanger”, discussed in detail later.

Now here are a few words about organization. This paper is divided into two parts. Part I describes the formalism we have developed to symbolically solve the Hubbard Hamiltonian for small clusters. Part II presents a summary analysis of the data we have obtained for the triangular and square clusters. Following Part I and Part II are three appendices which are included for reference only. Our findings for these clusters are recorded in Appendices A and B, respectively. The purpose of Appendix A and Appendix B is to document the bases and the contents of the Hamiltonian’s smallest blocks which are identified by a definite symmetry and total-spin and, furthermore, to illustrate the structures involved in working with these clusters. Finally, Appendix C provides a complete listing of Mathematica code for the Hubbard package.

Part I

Formalism

Here we detail the theoretical formalism used to symbolically solve the Hubbard model for the triangular and square cluster. We first present an overall summary of the method of solution. We then discuss the implementation of operators used to block diagonalize the Hamiltonian by symmetry and total-spin. These are a fermionic site-interchange operator and the total-spin-squared operator, respectively. Finally, we discuss the implementation of the second quantized form of Wannier creation and annihilation operators in the number representation, which is the foundation of our formalism.

2 Method of Solution

The first step in solving the Hubbard model for small clusters, given a lattice of size N and number of electrons N_e , is to determine a set of basis states. Since the z-component of the spin commutes with the Hamiltonian, we have chosen to work with a set of basis states in the number representation with a given S_z . This is done for convenience since one can immediately determine S_z for any such state by inspection. Throughout this paper we shall denote an S_z basis by the symbol: $\{\phi_n\}$. As an example of the size of the basis, in the case of half-filling, where $N_e = N$, for the triangular and square clusters there are nine and 36 states, respectively. The triangular cluster possesses the C_{3v} point group symmetry and the square C_{4v} .

Table 1: C_3 and C_{3v} Character Table

C_3	E	C_3	C_3^2	C_{3v}	E	$2C_3$	$3\sigma_v$
A	1	1	1	A_1	1	1	1
E	1	ϵ	ϵ^*	A_2	1	1	-1
E	1	ϵ^*	ϵ	E	2	-1	0

Table 2: C_4 and C_{4v} Character Table

C_4	E	C_4	C_2	C_4^3	C_{4v}	E	$2C_4$	C_2	$2\sigma_v$	$2\sigma_d$
A	1	1	1	1	A_1	1	1	1	1	1
B	1	-1	1	-1	A_2	1	1	1	-1	-1
E	1	i	-1	$-i$	B_1	1	-1	1	1	-1
E^*	1	$-i$	-1	i	B_2	1	-1	1	-1	1
					E	2	0	-2	0	0

The second step is to determine matrices representing the point group oper-

ations in the basis $\{\phi_n\}$. This is accomplished by successively employing site-interchange operations, as detailed below, to rotate or reflect any particular state according to the appropriate group operation desired. Let us denote these various operations by the generic symbol R . The C_{3v} group has six group operations and three irreducible representations, and C_{4v} has eight and five, respectively. See Table(1) and Table(2). Let us denote the i th irreducible representations by Γ_i^R . Given that we have constructed a *reducible* matrix representation, denoted $\{M_{mn}^R\}$, of the symmetry group in our basis $\{\phi_n\}$, we then construct projection operators, denoted $P_{mn}^{\Gamma_i}$, for each of the irreducible representations of the group [8]. This is done as follows

$$P_{mn}^{\Gamma_i} = \sum_R tr(\Gamma_i^R) M_{mn}^R, \quad (4)$$

where $tr(\Gamma_i^R)$ is the character or trace listed in the i th row and R th column of the character tables. We can also determine the number of times the Γ_i^R irreducible representation occurs in M_{mn}^R by knowing the character, $tr(M_{mn}^R)$ [10]. In practice the useful quantity b_i is determined by

$$b_i = \sum_R tr(\Gamma_i^R) tr(M_{mn}^R), \quad (5)$$

giving the size of the i th block of the resulting block-diagonalized Hamiltonian matrix of elements.

The third step is to apply $P_{mn}^{\Gamma_i}$ onto the $\{\phi_n\}$ basis to find linear combinations that possess a definite symmetry

$$\psi_m^{\Gamma_i} = \sum_n P_{mn}^{\Gamma_i} \phi_n. \quad (6)$$

Throughout this paper we shall denote a ‘‘symmetry’’ basis by the symbol: $\{\psi_n^{\Gamma_i}\}$. Specifically, for the case of C_{3v} , we obtain four sets of states: $\{\psi_n^{A_1}\}$, $\{\psi_n^{A_2}\}$, $\{\psi_n^E\}$, and $\{(\psi_n^E)^*\}$. For the case of C_{4v} , we obtain six sets of states: $\{\psi_n^{A_1}\}$, $\{\psi_n^{B_1}\}$, $\{\psi_n^{A_2}\}$, $\{\psi_n^{B_2}\}$, $\{\psi_n^E\}$, and $\{(\psi_n^E)^*\}$. The E-representation always appears twice¹. In the $\{\psi_n\}$ basis the Hamiltonian therefore decouples into four diagonal blocks for the triangular cluster and six diagonal blocks for the square cluster. The group theory has helped in reducing the complexity of the problem.

The fourth step is to try to block diagonalize the Hamiltonian still further. This is done by calculating the matrix of elements of the total-spin-squared operator, SS , in each of the $\{\psi_m^{\Gamma_i}\}$ sub-basis and diagonalizing this matrix to determine linear combinations of the $\psi_m^{\Gamma_i}$ states which have a definite total-spin, that is, we find eigenvectors of SS . Let us denote these eigenvectors of SS as $\varphi_m^{\Gamma_i, S}$. Throughout this paper, we shall denote a ‘‘total-spin’’ basis by the symbol: $\varphi_m^{\Gamma_i, S}$. Since SS commutes with the Hamiltonian we thereby partition each symmetry block into smaller blocks, each having a definite total-spin.

¹An important point must be mentioned here. We have found using projection operators constructed from the C_3 and C_4 character tables breaks the size of the E -type blocks in two for the half-filling cases

The final step is to calculate the Hamiltonian matrix elements in the $\{\varphi_m^{\Gamma_i, S}\}$ bases, and analytically find, if possible, the eigenvalues and eigenvectors of each resulting “spin-and-symmetry” block and thereby complete the solution. In the case of the triangle, the largest $\varphi_m^{\Gamma_i, S}$ block is 3×3 and for the square it is 4×4 .

3 Pendleton’s Site-Interchange Operator

All symmetry operations of rotation or reflection are implemented by a particular successive application of Pendleton’s fermionic “site-interchanger”, which we denote by $\hat{\chi}_{ij}$ where the interchange of electrons occurs between sites i and j . The content of this section was originally produced by Pendleton [11]. We wish to construct $\hat{\chi}_{ij}$ from the Wannier creation and annihilation operators so as to correctly handle any necessary phase change due to the fermion anti-commutation relations. The simplest implementation of $\hat{\chi}_{ij}$ should involve only products of $\hat{a}_{i\sigma}$ and $\hat{a}_{i\sigma}^\dagger$:

We require that $\hat{\chi}_{ij}^2 = \mathbf{1}$, that the site-interchanger conserve the number of particles, $[\hat{\chi}_{ij}, \hat{N}] = 0$, that $\hat{\chi}_{ij}$ is hermitian, and that $\hat{\chi}_{ij}|0\rangle = |0\rangle$. Let us assume we have a one-particle state $\phi_{1e} = \hat{a}_{m\sigma}^\dagger|0\rangle$ where $m = i$ or j . A first guess at the form of a *spin-dependent* interchange operator between sites i and j would be

$$\hat{\chi}_{ij\sigma} = \hat{a}_{j\sigma}^\dagger \hat{a}_{i\sigma} + \hat{a}_{i\sigma}^\dagger \hat{a}_{j\sigma}. \quad (7)$$

This acts correctly on ϕ_{1e} . The problem with Eq.(7) is that its application on to the vacuum violates our requirement that $\hat{\chi}_{ij\sigma}|0\rangle = |0\rangle$. This is remedied easily enough by slightly modifying our first guess

$$\hat{\chi}_{ij\sigma} = \hat{a}_{j\sigma}^\dagger \hat{a}_{i\sigma} + \hat{a}_{i\sigma}^\dagger \hat{a}_{j\sigma} + \mathbf{1}. \quad (8)$$

Although Eq.(8) repairs the vacuum problem, now its application onto ϕ_{1e} would interchange the electron but incorrectly would also give back ϕ_{1e} , an extra unwanted electron. We administer the final remedy by including two more terms that have the effect of subtracting off the unwanted electron

$$\hat{\chi}_{ij\sigma} = \hat{a}_{j\sigma}^\dagger \hat{a}_{i\sigma} + \hat{a}_{i\sigma}^\dagger \hat{a}_{j\sigma} + \mathbf{1} - \hat{a}_{i\sigma}^\dagger \hat{a}_{i\sigma} - \hat{a}_{j\sigma}^\dagger \hat{a}_{j\sigma}. \quad (9)$$

Although we have constructed Eq.(9) by considering only a one-particle state, a remarkable fact is that $\hat{\chi}_{ij\sigma}$ works on any arbitrary state.

Let us investigate the properties of $\hat{\chi}_{ij\sigma}$ further. Let us rewrite Eq.(9) by factoring the creation operators,

$$\hat{\chi}_{ij\sigma} = \mathbf{1} + \hat{a}_{j\sigma}^\dagger (\hat{a}_{i\sigma} - \hat{a}_{j\sigma}) + \hat{a}_{i\sigma}^\dagger (\hat{a}_{j\sigma} - \hat{a}_{i\sigma}), \quad (10)$$

which leads one to write

$$\hat{\chi}_{ij\sigma} = \mathbf{1} - (\hat{a}_{j\sigma}^\dagger - \hat{a}_{i\sigma}^\dagger)(\hat{a}_{j\sigma} - \hat{a}_{i\sigma}). \quad (11)$$

Now of course, one is motivated to define the following unconventional creation, annihilation, and number operators

$$\hat{A}_{ij\sigma} = \sqrt{\frac{1}{2}}(\hat{a}_{j\sigma} - \hat{a}_{i\sigma}) \quad (12)$$

$$\hat{A}_{ij\sigma}^\dagger = \sqrt{\frac{1}{2}}(\hat{a}_{j\sigma}^\dagger - \hat{a}_{i\sigma}^\dagger) \quad (13)$$

$$\hat{N}_{ij\sigma}^A = \hat{A}_{ij\sigma}^\dagger \hat{A}_{ij\sigma} \quad (14)$$

so that Eq.(11) may be written as

$$\hat{\chi}_{ij\sigma} = \mathbf{1} - 2\hat{N}_{ij\sigma}^A. \quad (15)$$

Our new operators no longer work in the usual number representation and instead form mixed states

$$\hat{A}_{ij\sigma}^\dagger |0\rangle = \sqrt{\frac{1}{2}}(|j\sigma\rangle - |i\sigma\rangle) \equiv |\hat{A}_{ij\sigma}\rangle. \quad (16)$$

The number operator satisfies $(\hat{N}_{ij\sigma}^A)^2 = \hat{N}_{ij\sigma}^A$ and consequently we have

$$\hat{\chi}_{ij\sigma}^2 = (\mathbf{1} - 2\hat{N}_{ij\sigma}^A)^2 = \mathbf{1} - 4\hat{N}_{ij\sigma}^A + 4\hat{N}_{ij\sigma}^A{}^2 = \mathbf{1}, \quad (17)$$

satisfying another of our requirements.

Pendleton's interchanger can be written in exponential form

$$\hat{\chi}_{ij\sigma} = e^{z\hat{N}_{ij\sigma}^A} = \mathbf{1} + z\hat{N}_{ij\sigma}^A + \frac{z^2}{2!}\hat{N}_{ij\sigma}^A{}^2 + \dots = \mathbf{1} + \left(z + \frac{z^2}{2!} + \dots\right) \hat{N}_{ij\sigma}^A \quad (18)$$

or

$$\hat{\chi}_{ij\sigma} = \mathbf{1} + (e^z - 1)\hat{N}_{ij\sigma}^A. \quad (19)$$

Comparing Eq.(15) with Eq.(19), allows us to choose $z = \pi i$, so we have our site-interchanger,

$$\hat{\chi}_{ij\sigma} = \hat{\chi}_{ij\sigma} = e^{i\pi\hat{N}_{ij\sigma}^A}, \quad (20)$$

appearing as a rotation by 180° . To affect a complete site-interchange is straightforward

$$\hat{\chi}_{ij} \equiv \hat{\chi}_{ij\uparrow}\hat{\chi}_{ij\downarrow}. \quad (21)$$

In practice Eq.(9), Eq.(20), not is substituted into Eq.(21) to perform any calculation since we prefer to work in the usual number representation. For the triangular cluster, we implement the C_{3v} point operators as follows

$$\hat{R}^{C_3} = \hat{\chi}_{12}\hat{\chi}_{23} \quad (22)$$

$$\hat{R}^{C_3^2} = \hat{\chi}_{23}\hat{\chi}_{12} \quad (23)$$

$$\hat{R}_v^{\sigma(1)} = \hat{\chi}_{23} \quad (24)$$

$$\hat{R}_v^{\sigma(2)} = \hat{\chi}_{31} \quad (25)$$

$$\hat{R}_v^{\sigma(3)} = \hat{\chi}_{12}, \quad (26)$$

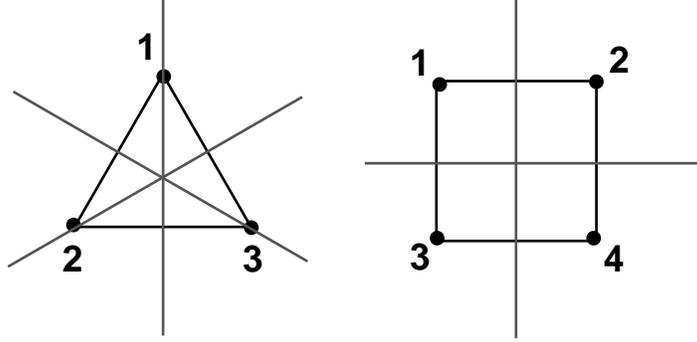


Figure 1: Symmetry axes for the triangular and square clusters.

which are 120° and 240° rotations, and reflections about sites 1, 2, and 3, respectively. For the square cluster, we implement the C_{4v} point group operators as follows

$$\hat{R}^{C_4} = \hat{\chi}_{34}\hat{\chi}_{23}\hat{\chi}_{12} \quad (27)$$

$$\hat{R}^{C_2} = \hat{\chi}_{23}\hat{\chi}_{12} \quad (28)$$

$$\hat{R}^{C_4^3} = \hat{\chi}_{12}\hat{\chi}_{23}\hat{\chi}_{34} \quad (29)$$

$$\hat{R}^{\sigma_v^{(13)}} = \hat{\chi}_{24} \quad (30)$$

$$\hat{R}^{\sigma_v^{(24)}} = \hat{\chi}_{13} \quad (31)$$

$$\hat{R}^{\sigma_d^{(13)}} = \hat{\chi}_{12}\hat{\chi}_{34} \quad (32)$$

$$\hat{R}^{\sigma_d^{(24)}} = \hat{\chi}_{14}\hat{\chi}_{23}, \quad (33)$$

which are 90° , 180° and 270° rotations, and reflections about two diagonals and the vertical and horizontal, respectively.

4 Implementation of the SS Operator

The site-specific total-spin operator is compactly written in terms of the Wannier creation and annihilation operators and the Pauli spin matrices as

$$\vec{S}_i = \frac{1}{2}\hat{a}_{i\alpha}^\dagger \vec{\sigma}_{\alpha\beta} \hat{a}_{i\beta}, \quad (34)$$

where $\hbar = 1$, $\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$, and

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

The components of Eq.(34) are then

$$\vec{S}_{ix} = \frac{1}{2}\hat{a}_{i\alpha}^\dagger \vec{\sigma}_{\alpha\beta}^x \hat{a}_{i\beta} = \frac{1}{2}(\hat{a}_{i\uparrow}^\dagger \hat{a}_{i\downarrow} + \hat{a}_{i\downarrow}^\dagger \hat{a}_{i\uparrow}) \quad (35)$$

$$\vec{S}_{iy} = \frac{i}{2}\hat{a}_{i\alpha}^\dagger \vec{\sigma}_{\alpha\beta}^y \hat{a}_{i\beta} = \frac{1}{2}(\hat{a}_{i\downarrow}^\dagger \hat{a}_{i\uparrow} - \hat{a}_{i\uparrow}^\dagger \hat{a}_{i\downarrow}) \quad (36)$$

$$\vec{S}_{iz} = \frac{1}{2}\hat{a}_{i\alpha}^\dagger \vec{\sigma}_{\alpha\beta}^z \hat{a}_{i\beta} = \frac{1}{2}(\hat{a}_{i\uparrow}^\dagger \hat{a}_{i\uparrow} - \hat{a}_{i\downarrow}^\dagger \hat{a}_{i\downarrow}). \quad (37)$$

With Eqs.(35) - (37) the square of the total spin operator is readily constructed

$$SS = \sum_{i=1}^N \sum_{j=1}^N \left(\vec{S}_{ix} \vec{S}_{jx} + \vec{S}_{iy} \vec{S}_{jy} + \vec{S}_{iz} \vec{S}_{jz} \right). \quad (38)$$

where $SS\varphi = S(S+1)\varphi$.

5 Production Rules for Second Quantization in the Number Representation

Let us denote the four possible states of a single site by the symbols: $p = \uparrow$, $m = \downarrow$, $d = \uparrow\downarrow$, and $e = \text{empty}$. The four basic site-dependent Wannier creation and annihilation operators can be defined by the following 20 production rules

$$\begin{aligned} a_p^\dagger[p] &= 0 & a_p[p] &= e & a_m^\dagger[p] &= d & a_m[p] &= 0 \\ a_p^\dagger[m] &= d & a_p[m] &= 0 & a_m^\dagger[m] &= 0 & a_m[m] &= e \\ a_p^\dagger[d] &= 0 & a_p[d] &= m & a_m^\dagger[d] &= 0 & a_m[d] &= p \\ a_p^\dagger[e] &= p & a_p[e] &= 0 & a_m^\dagger[e] &= m & a_m[e] &= 0 \\ a_p^\dagger[0] &= 0 & a_p[0] &= 0 & a_m^\dagger[0] &= 0 & a_m[0] &= 0 \end{aligned}$$

which embody the exclusion principle. A state is considered to be an ordered list of symbols, $\phi = |s_1, s_2, \dots, s_N\rangle$ where $s_i = p, m, d$, or e . The number of elements in the list equals the number of sites, N . The production rules for $\hat{a}_{i\sigma}^\dagger$ and $\hat{a}_{i\sigma}$ are

$$a^\dagger[\sigma, i, |s_1, s_2, \dots, s_N\rangle] = \begin{cases} \varepsilon |s_1, s_2, \dots, a_p^\dagger[s_i], \dots, s_N\rangle, & \text{if } \sigma = p \\ \varepsilon |s_1, s_2, \dots, a_m^\dagger[s_i], \dots, s_N\rangle, & \text{if } \sigma = m \end{cases} \quad (39)$$

$$a^\dagger[\sigma, i, 0] = 0. \quad (40)$$

$$a[\sigma, i, |s_1, s_2, \dots, s_N\rangle] = \begin{cases} \varepsilon |s_1, s_2, \dots, a_p[s_i], \dots, s_N\rangle, & \text{if } \sigma = p \\ \varepsilon |s_1, s_2, \dots, a_m[s_i], \dots, s_N\rangle, & \text{if } \sigma = m \end{cases} \quad (41)$$

$$a[\sigma, i, 0] = 0, \quad (42)$$

where $i = 1, \dots, N$ and $\varepsilon = \pm 1$ is a multiplicative phase determined by anti-commutation up to the indexed site. That is,

$$\varepsilon = \prod_{m=1}^i \delta[s_i], \quad (43)$$

where $\delta[p] = -1$, $\delta[m] = -1$, $\delta[d] = +1$, and $\delta[e] = +1$. Furthermore, to correctly implement the anti-commutation relations for fermions, ε must be multiplied by -1 in the following two cases: (1) when a down-spin is created on a site currently occupied by an up-spin; and (2), when a down-spin is destroyed on a site currently doubly occupied. These two rules are needed because our definition of a doubly occupied site, $d = \uparrow\downarrow$, implies a definite ordering of spins which must be preserved for the symbol d to be non-ambiguous.

Using the production rules Eqs.(39)-(42), we define rules for all other quantum operators of interest, such as $\hat{\chi}$, SS , \tilde{H} , and \hat{a}_k . Appendix C provides a full listing of all the source code for our symbolic approach.

Part II

Analysis

The purpose of this part is to analysis our findings for the triangular and square cluster recorded in Appendices A and B. We check our data for expected symmetries of the Hubbard Hamiltonian and find that our formalism is consistent. We check a theorem proved by Nagaoka concerning whether or not the ferromagnetic state above and below half-filling is the ground state. Then we compare spin-correlations of the ground states of the triangular and square clusters at half-filling. Finally we give some examples and interpretation of eigenvalue and photoemission energies as a function of U/t .

6 Double-Empty Symmetry Above and Below Half-Filling

It is well known that, energetically, the Hubbard Hamiltonian possesses a symmetry above and below half-filling. This symmetry ensures a one-to-one correspondence between states above half-filling with those below. The structure of the states, their exact symmetry and total-spin, above and below half-filling is identical provided that the respective \hat{S}_z bases, $\{\phi_n\}$, are labeled so that any state above half-filling with a particular doubly occupied site corresponds to a state below half-filling with no electrons on that site.

Lets consider the data presented in Part III for the triangular cluster and, further, consider the cases with $\hat{S}_z = 0$ above and below half-filling, Appendices A.2 and A.4. The first point to note is that $\{\psi_n^{N_e=4, S_z=0}\}$ can be mapped to $\{\psi_n^{N_e=2, S_z=0}\}$ by taking $d \rightarrow e$. The structure of the states are seen to be identical by comparing Eqs.(78-81) to Eqs. (85-88). Finally, the energies are also seen to be isomorphic by taking $t \rightarrow -t$ and if, above half-filling, we shift the energy down by $3U$. The origin of this shift is two-fold: (1) the second term of the Hubbard Hamiltonian, Eq.(1), causes a shift of U since $d \rightarrow e$; and (2), the third term of the Hamiltonian causes a shift of $2U$ in our case. The same symmetry is seen to exist for the cases with $\hat{S}_z = 1$, Appendices A.3 and A.5

For the case of the square cluster this symmetry is essentially the same, differing only in that the asymmetry in t is not present. The underlying reason for difference between the triangle and square arises from the freedom we have to divide the square into two sub-lattices such that for any lattice point has nearest-neighbors belonging to the co-lattice [12]. Then a phase difference of -1 between the wave function of the sub-lattices could account for a change in the sign of t .

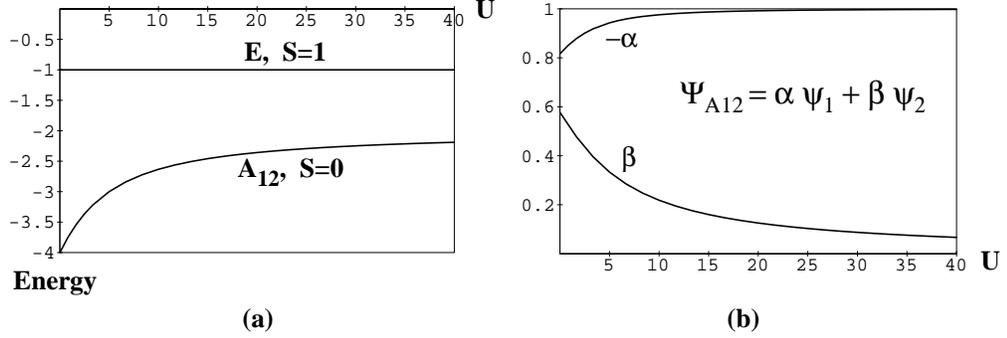


Figure 2: Below half-filling for the triangular cluster. Variation with U of: (a) lowest eigenvalues' for $S = 0$ and $S = 1$; and (b) coefficients of $\lambda_{A_{12}}^{N_e=2, S_z=0} = \alpha\psi_1 + \beta\psi_2$ eigenstate.

7 Check of Nagaoka's Theorem

Let us consider the triangular cluster below half-filling, $N_e = 2$. The ground state of this system could have either $S_z = 0$ or 1. In the $S_z = 0$ case, the lowest energy state has A_1 symmetry and total-spin $S = 0$. It is an eigenvector of the Hamiltonian block

$$\left. \begin{array}{l} \frac{1}{\sqrt{6}} (|emp\rangle - |pem\rangle + |mpe\rangle - |epm\rangle + |mep\rangle - |pme\rangle) \\ \frac{1}{\sqrt{3}} (|dee\rangle + |ede\rangle + |eed\rangle) \end{array} \right\} \rightarrow \langle H_{S=0}^{A_1} \rangle = \begin{pmatrix} -2t & \frac{4t}{\sqrt{2}} \\ \frac{4t}{\sqrt{2}} & U \end{pmatrix}. \quad (44)$$

In comparing Eq.(44) with the results presented in Appendix A, note that we have subtracted $2U$ from the diagonals of the matrix elements for simplicity. Diagonalizing Eq.(44), we find the lowest energy state to be

$$\Psi_{A_{12}}^{S_z=0, S=0} = \frac{\alpha}{\sqrt{6}} (|emp\rangle - |pem\rangle + |mpe\rangle - |epm\rangle + |mep\rangle - |pme\rangle) + \frac{\beta}{\sqrt{3}} (|dee\rangle + |ede\rangle + |eed\rangle), \quad (45)$$

where the coefficients α and β are plotted in Fig.(3:b).

In the $S_z = 1$ case, the lowest energy state, the ferromagnetic state, has E symmetry and total-spin $S = 1$

$$\Psi_E^{S_z=1, S=1} = (2|ep\rangle + |pe\rangle - |pp\rangle)/\sqrt{3} \rightarrow \langle H_{S=1}^E \rangle = (2U - t). \quad (46)$$

We see from Fig.(3:a), below half-filling the ferromagnetic state is not the ground state of the system for all values of U . Nagaoka has proven, in the limit $U \rightarrow \infty$, for an fcc or hcp lattice the ferromagnetic state with the maximum total-spin would not be the ground state of the system [12]. Our results are in agreement

with this statement, if we make an analogy between our triangular cluster and fcc or hcp.

Let us see in more detail why $\Psi_{A_{12}}^{S_z=0, S=0}$ is indeed the ground state of the system. Let us consider the $U = 0$ limit. Here the Hubbard Hamiltonian has only the kinetic energy term

$$H = -t \sum_{\langle ij \rangle \sigma} \hat{a}_{i\sigma}^\dagger \hat{a}_{j\sigma} \quad (47)$$

which we can transform to k -space to determine the band energy. To convert from Wannier states to Bloch states we use the discrete Fourier transform

$$\hat{a}_{i\sigma} = \frac{1}{\sqrt{N}} \sum_k e^{-ikR_i} \hat{a}_{k\sigma} \quad \hat{a}_{i\sigma}^\dagger = \frac{1}{\sqrt{N}} \sum_k e^{ikR_i} \hat{a}_{k\sigma}^\dagger, \quad (48)$$

and to do the inverse we use

$$\hat{a}_{k\sigma} = \sum_{\{R_i\}} e^{ikR_i} \hat{a}_{i\sigma} \quad \hat{a}_{k\sigma}^\dagger = \sum_{\{R_i\}} e^{-ikR_i} \hat{a}_{i\sigma}^\dagger, \quad (49)$$

where the possible momenta are $k = 2n\pi/Na$ and lattice vectors are $R_n = an$, $n = 0, 1, \dots, N-1$ and a is the cell-size. Substituting Eq.(48) into Eq.(47) gives

$$H = -\frac{t}{N} \sum_{\langle ij \rangle \sigma} \sum_k e^{ikR_i} \hat{a}_{k\sigma}^\dagger \sum_{k'} e^{-ik'R_j} \hat{a}_{k'\sigma} \quad (50)$$

$$= -\frac{t}{N} \sum_i \sum_\sigma \sum_{kk'} \hat{a}_{k\sigma}^\dagger \sum_{k'} \hat{a}_{k'\sigma} e^{ikR_i} \left(e^{-ik'(R_i+a)} + e^{-ik'(R_i-a)} \right) \quad (51)$$

where we have went from Eq.(50) to Eq.(51) by replacing the sum over the bonds, $\langle ij \rangle$, by a sum only over the lattice sites since for nearest-neighbor interactions, $R_j = R_i \pm a$ in the $\langle ij \rangle$ sum. We then have

$$H = \sum_{k\sigma} \epsilon_k \hat{a}_{k\sigma}^\dagger \hat{a}_{k\sigma} \quad (52)$$

where

$$\epsilon_k = -2t \cos ka \quad (53)$$

and where we have used

$$\frac{1}{N} \sum_{\langle ij \rangle \sigma} \sum_k e^{i(k-k')R_i} = \delta_{kk'}. \quad (54)$$

Referring to Fig.(3:a,b) clearly for $N_e = 2$ the $S_z = 0$ state has lower energy, $-4t$ with the $S_z = 1$ has energy $-t$. This agrees with Fig.(2:a). Let us write the Eq.(45) at $U = 0$. Here, expanding about $U = 0$, we have

$$\alpha = -\sqrt{\frac{2}{3}} - \frac{U}{9\sqrt{6}} + O(U^2) \quad (55)$$

$$\beta = \frac{1}{\sqrt{3}} - \frac{U}{9\sqrt{6}} + O(U^2) \quad (56)$$

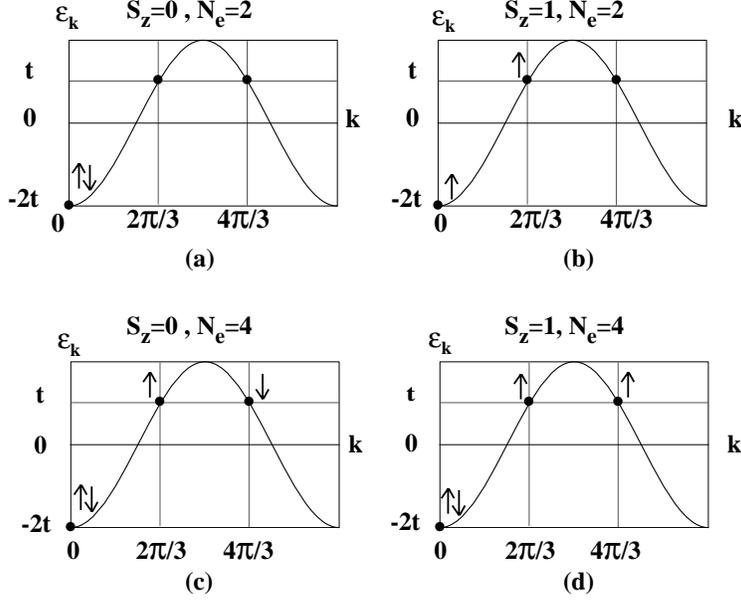


Figure 3: Lowest Energy Momentum States Above and Below Half-Filling for $S_z = 0, 1$.

so substituting Eqs.(55) and (56) into Eqs.(45) gives

$$\begin{aligned} \Psi_{A_{12}, U=0}^{S_z=0, S=0} \rightarrow & \quad (57) \\ & \frac{1}{\sqrt{9}} (|dee\rangle + |ede\rangle + |eed\rangle) - \\ & \sqrt{\frac{1}{9}} (|emp\rangle - |pem\rangle + |mpe\rangle - |epm\rangle + |mep\rangle - |pme\rangle). \end{aligned}$$

Alternatively, we can arrive at Eq.(57) by constructing the momentum states depicted in Fig.(3:a) using the Bloch creation operators, Eq.(49),

$$\begin{aligned} \hat{a}_{k=0\uparrow}^\dagger \hat{a}_{k=0\downarrow}^\dagger |0\rangle = & (\hat{a}_{1\uparrow}^\dagger + \hat{a}_{2\uparrow}^\dagger + \hat{a}_{3\uparrow}^\dagger)(\hat{a}_{1\downarrow}^\dagger + \hat{a}_{2\downarrow}^\dagger + \hat{a}_{3\downarrow}^\dagger) = & (58) \\ & |dee\rangle + |ede\rangle + |eed\rangle - \\ & |emp\rangle + |epm\rangle - |mep\rangle - |mpe\rangle + |pem\rangle + |pme\rangle. \end{aligned}$$

Normalizing this by $\sqrt{9}$, we see that Eq.(58) is indeed identical to Eq.(57).

Now let us consider the triangular cluster above half-filling, $N_e = 4$. Like the case just considered, the ground state of this system could have either $S_z = 0$ or 1. Remarkably, however, in the above half-filling case the ferromagnetic and non-ferromagnetic states are degenerate with eigenvalue $5U - 2t$, see Appendix A.2 and A.3. The reason for this degeneracy is depicted in Fig.(7:c,d). The degeneracy arises from the fact that $\epsilon_k = -2t \cos ka$ has the same value for $k = 2\pi/3$ and $k = 4\pi/3$, an effect our small cluster size.

8 Examples of Energy Plots

Here we give some examples illustrating the information one may obtain from energy plots. Let us see what information is contained in an eigenvalue plot such as Fig.(4). There we have plotted all the energies of the half-filled triangular cluster as a function of U . We have labeled each curve according to its symmetry. The A_1 and A_{22} energies are degenerate for all U . In Fig.(5) we have depicted

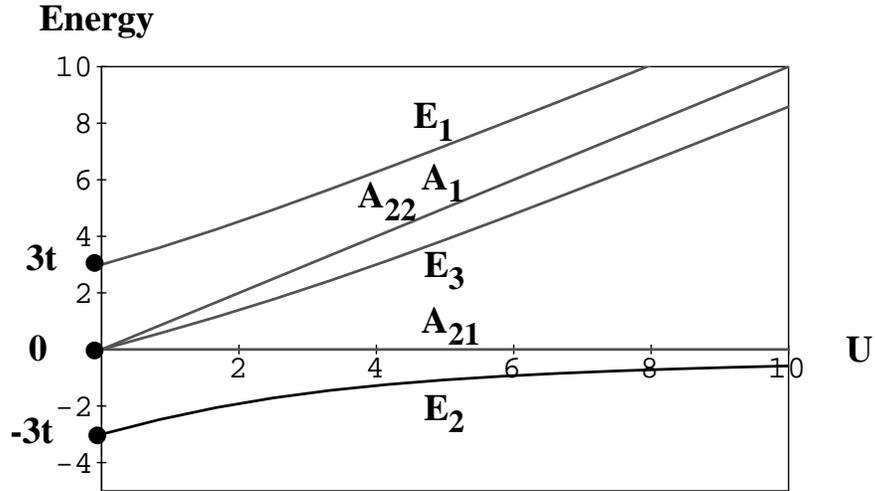


Figure 4: Eigenvalues for the triangular cluster at half-filling.

all the possible Bloch states for $N_e = 3$. There are five types of Bloch states we can possibly choose. These, in turn, correspond to the five non-degenerate energies for finite U plotted in Fig.(4). Consequently, we see why there are only three non-degenerate energies at $U = 0$ in Fig.(4): the Bloch states (1), (2), and (3) have the same energy at $U = 0$. It is possible to assign each Bloch state a given symmetry. Immediately, we assign (1) and (5) symmetries E_1 and E_2 , respectively, since they are the highest and lowest energy states. Then, we assign (2) with A_{21} symmetry since from Fig.(4) the energy of this state is independent of U and we know

$$\Psi_{A_{21}} = \frac{1}{\sqrt{3}} (|mpp\rangle + |mpm\rangle + |ppm\rangle). \quad (59)$$

Next, we assign (3) with A_1 and A_{22} symmetry since we know that these states must have a doubly occupied site

$$\Psi_{A_1} = \frac{1}{\sqrt{6}} [(|dpe\rangle + |edp\rangle + |ped\rangle) + (|dep\rangle + |pde\rangle + |epd\rangle)] \quad (60)$$

$$\Psi_{A_{22}} = \frac{1}{\sqrt{6}} [(|dpe\rangle + |edp\rangle + |ped\rangle) - (|dep\rangle + |pde\rangle + |epd\rangle)]. \quad (61)$$

This explains why A_1 and A_{22} are degenerate for all U . Finally, we then can explain why the E_3 energy is lower than the A_1 and A_{22} energy for finite U . This is because the E_3 state can have a component of Bloch state (4) which is energetically lower for finite U than (3).

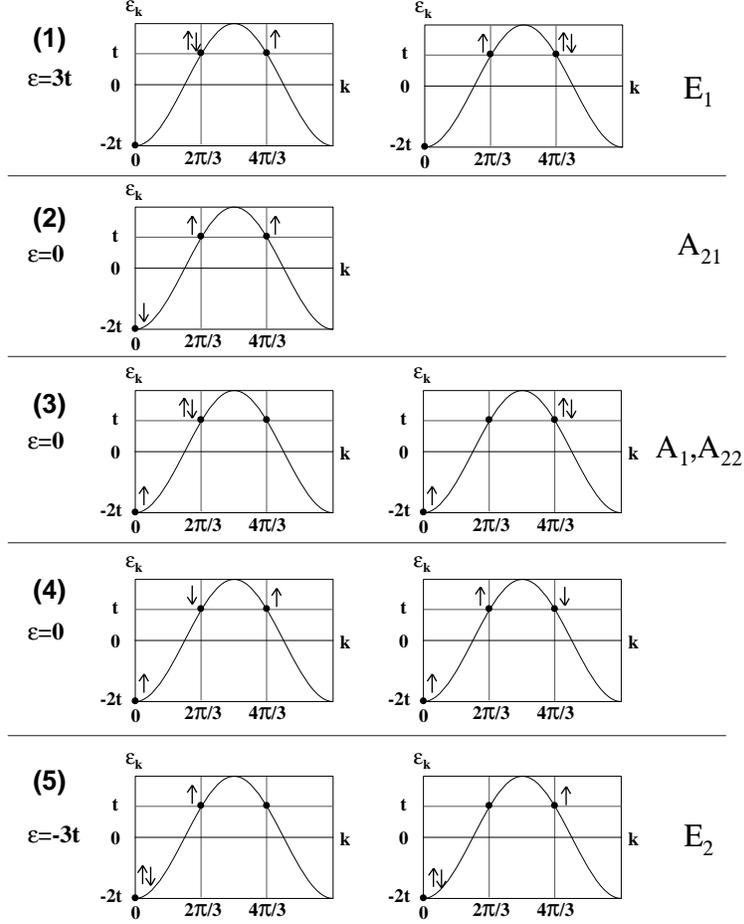


Figure 5: Bloch states with definite symmetry for the triangular cluster at half-filling.

The eigenvalues of the triangular cluster above half-filling, $N_e = 4$, and $S_z = 0$ are the following

$$\lambda_{A_{11}}^{N_e=4, S_z=0} = \frac{11U + 2t + \sqrt{(-11U - 2t)^2 - 4(30U^2 + 12Ut - 8t^2)}}{2} \quad (62)$$

$$\lambda_{A_{12}}^{N_e=4, S_z=0} = \frac{11U + 2t - \sqrt{(-11U - 2t)^2 - 4(30U^2 + 12Ut - 8t^2)}}{2} \quad (63)$$

$$\lambda_{A_2}^{N_e=4, S_z=0} = 5U - 2t \quad (64)$$

$$\lambda_{E_1}^{N_e=4, S_z=0} = 5U + t \quad (65)$$

$$\lambda_{E_2}^{N_e=4, S_z=0} = \frac{11U - t + \sqrt{(-11U + t)^2 - 4(30U^2 - 6Ut - 2t^2)}}{2} \quad (66)$$

$$\lambda_{E_3}^{N_e=4, S_z=0} = \frac{11U - t - \sqrt{(-11U + t)^2 - 4(30U^2 - 6Ut - 2t^2)}}{2} \quad (67)$$

and the eigenvalues below half-filling are

$$\lambda_{A_{11}}^{N_e=2, S_z=0} = \frac{5U - 2t + \sqrt{(-5U + 2t)^2 - 4(6U^2 - 6Ut - 8t^2)}}{2} \quad (68)$$

$$\lambda_{A_{12}}^{N_e=2, S_z=0} = \frac{5U - 2t - \sqrt{(-5U + 2t)^2 - 4(6U^2 - 6Ut - 8t^2)}}{2} \quad (69)$$

$$\lambda_{A_2}^{N_e=2, S_z=0} = 2U + 2t \quad (70)$$

$$\lambda_{E_1}^{N_e=2, S_z=0} = 2U - t \quad (71)$$

$$\lambda_{E_2}^{N_e=2, S_z=0} = \frac{5U + t + \sqrt{(-5U - t)^2 - 4(6U^2 + 3Ut - 2t^2)}}{2} \quad (72)$$

$$\lambda_{E_3}^{N_e=2, S_z=0} = \frac{5U + t - \sqrt{(-5U - t)^2 - 4(6U^2 + 3Ut - 2t^2)}}{2}. \quad (73)$$

Plots of the eigenvalues above half-filling for $N_e = 4$ and $S_z = 0$ are plotted in Fig.(8) with the constant term of the Hubbard Hamiltonian, $4U$, subtracted off. Fig.(8) shows the variation of the photoemission energies with U . The ground state energy of the half-filled system has been subtracted off of $\lambda^{N_e=4, S_z=0}$ and $\lambda^{N_e=4, S_z=0}$.

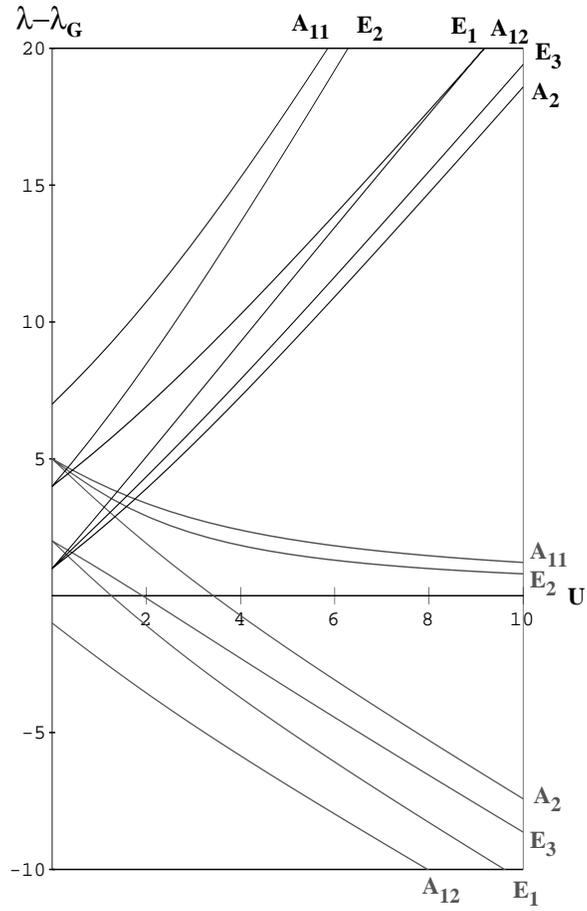


Figure 6: Photoemission energies verses U : $\lambda^{N_e=4, S_z=0} - \lambda_G$ in black and $\lambda^{N_e=4, S_z=0} - \lambda_G$ in gray.

A Triangular Cluster Data

In this section we present our findings for the triangular cluster for the following cases: half-filling, $N_e = 3$, for $S_z = \frac{1}{2}$; above half-filling, $N_e = 4$, for $S_z = 0, 1$; and, below half-filling, $N_e = 4$, for $S_z = 0, 1$.

A.1 Half-filling: $N_e = 3$ and $S_z = \frac{1}{2}$

For $S_z = \frac{1}{2}$ in the case of half-filling where $N_e = 3$ we have 9 elements in our bases. We choose our $\{\phi_n\}$ basis as follows

$$\begin{aligned}\phi_1 &= |mpp\rangle & \phi_2 &= |pmp\rangle & \phi_3 &= |ppm\rangle \\ \phi_4 &= |dpe\rangle & \phi_5 &= |edp\rangle & \phi_6 &= |ped\rangle \\ \phi_7 &= |dep\rangle & \phi_8 &= |pde\rangle & \phi_9 &= |epd\rangle\end{aligned}$$

In the case of half-filling the $\{\psi_n\}$ basis states generated by the C_{3v} projection operators happen all to be eigenvectors of SS , so here we do not get any reduction in block size using the total-spin. Therefore, the $\{\varphi_n\}$ basis is equivalent to $\{\psi_n\}$.

A.1.1 A_1 State with $S = \frac{1}{2}$

$$\psi_1 = (\phi_4 + \phi_5 + \phi_6 + \phi_7 + \phi_8 + \phi_9)/\sqrt{6} \quad \rightarrow \quad \langle H_{S=\frac{1}{2}}^{A_1} \rangle = (4U). \quad (74)$$

A.1.2 A_2 States with $S = \frac{1}{2}, \frac{3}{2}$

$$\psi_2 = (\phi_1 + \phi_2 + \phi_3)/\sqrt{3} \quad \rightarrow \quad \langle H_{S=\frac{3}{2}}^{A_2} \rangle = (3U) \quad (75)$$

$$\psi_3 = (\phi_4 + \phi_5 + \phi_6 - \phi_7 - \phi_8 - \phi_9)/\sqrt{6} \quad \rightarrow \quad \langle H_{S=\frac{1}{2}}^{A_2} \rangle = (4U) \quad (76)$$

A.1.3 E States with $S = \frac{1}{2}$

$$\left. \begin{aligned}\psi_4 &= (\phi_1 + \epsilon\phi_2 + \epsilon^*\phi_3)/\sqrt{6} \\ \psi_5 &= (\phi_4 + \epsilon\phi_5 + \epsilon^*\phi_6)/\sqrt{6} \\ \psi_6 &= (\phi_7 + \epsilon\phi_8 + \epsilon^*\phi_9)/\sqrt{6}\end{aligned} \right\} \quad \rightarrow \quad \langle H_{S=\frac{1}{2}}^E \rangle = \begin{pmatrix} 3U & (\epsilon^* - 1)t & (1 - \epsilon)t \\ (\epsilon - 1)t & 4U & (\epsilon^* - 1)t \\ (1 - \epsilon^*)t & (\epsilon - 1)t & 4U \end{pmatrix}. \quad (77)$$

A.2 Above Half-filling: $N_e = 4$ and $S_z = 0$

For $S_z = 0$, above half-filling where $N_e = 4$, we have 9 elements in our bases. We choose our $\{\phi_n\}$ basis as follows

$$\begin{aligned}\phi_1 &= |dmp\rangle & \phi_2 &= |pdm\rangle & \phi_3 &= |mpd\rangle \\ \phi_4 &= |dpm\rangle & \phi_5 &= |mdp\rangle & \phi_6 &= |pmd\rangle \\ \phi_7 &= |edd\rangle & \phi_8 &= |ded\rangle & \phi_9 &= |dde\rangle\end{aligned}$$

The $\{\varphi_n\}$ and $\{\psi_n\}$ basis are equivalent in the A_1 and A_2 representations, for $n = 1, 2, 3$.

A.2.1 A_1 States with $S = 0$

$$\left. \begin{aligned} \varphi_1 = \psi_1 &= (\phi_1 - \phi_2 + \phi_3 - \phi_4 + \phi_5 - \phi_6)/\sqrt{6} \\ \varphi_2 = \psi_2 &= (\phi_7 + \phi_8 + \phi_9)/\sqrt{3} \end{aligned} \right\} \rightarrow \langle H_{S=0}^{A_1} \rangle = \begin{pmatrix} 5U + 2t & \frac{4t}{\sqrt{2}} \\ \frac{4t}{\sqrt{2}} & 6U \end{pmatrix}. \quad (78)$$

A.2.2 A_2 State with $S = 1$

$$\varphi_3 = \psi_3 = (\phi_1 - \phi_2 + \phi_3 + \phi_4 - \phi_5 + \phi_6)/\sqrt{6} \rightarrow \langle H_{S=1}^{A_2} \rangle = (5U - 2t). \quad (79)$$

A.2.3 E States with $S = 0, 1$

$$\begin{aligned} \psi_4 &= (2\phi_1 + \phi_2 - \phi_3)/\sqrt{6} \\ \psi_5 &= (2\phi_4 + \phi_5 - \phi_6)/\sqrt{6} \\ \psi_6 &= (2\phi_7 - \phi_8 - \phi_9)/\sqrt{6} \end{aligned}$$

$$\varphi_4 = (\psi_4 + \psi_5)/\sqrt{2} \rightarrow \langle H_{S=1}^E \rangle = (5U + t) \quad (80)$$

$$\left. \begin{aligned} \varphi_5 &= (\psi_4 - \psi_5)/\sqrt{2} \\ \varphi_6 &= \psi_6 \end{aligned} \right\} \rightarrow \langle H_{S=0}^E \rangle = \begin{pmatrix} 5U - t & \frac{-2t}{\sqrt{2}} \\ \frac{-2t}{\sqrt{2}} & 6U \end{pmatrix}. \quad (81)$$

A.3 Above Half-filling: $N_e = 4$ and $S_z = 1$

For $S_z = 1$, above half-filling where $N_e = 4$, we have 3 elements in our bases. We choose our $\{\phi_n\}$ basis as follows

$$\phi_1 = |dpp\rangle \quad \phi_2 = |pdp\rangle \quad \phi_3 = |ppd\rangle. \quad (82)$$

The $\{\varphi_n\}$ and $\{\psi_n\}$ basis are equivalent. There are no states in the A_1 representation.

A.3.1 A_2 State with $S = 1$

$$\varphi_1 = \psi_1 = (\phi_1 - \phi_2 + \phi_3)/\sqrt{3} \rightarrow \langle H_{S=1}^{A_2} \rangle = (5U - 2t). \quad (83)$$

A.3.2 E State with $S = 1$

$$\varphi_2 = \psi_2 = (2\phi_1 + \phi_2 - \phi_3)/\sqrt{3} \rightarrow \langle H_{S=1}^E \rangle = (5U + t). \quad (84)$$

A.4 Below Half-filling: $N_e = 2$ and $S_z = 0$

For $S_z = 0$, below half-filling where $N_e = 2$, we have 9 elements in our bases. We choose our $\{\phi_n\}$ basis as follows

$$\begin{aligned}\phi_1 &= |emp\rangle & \phi_2 &= |pem\rangle & \phi_3 &= |mpe\rangle \\ \phi_4 &= |epm\rangle & \phi_5 &= |mep\rangle & \phi_6 &= |pme\rangle \\ \phi_7 &= |dee\rangle & \phi_8 &= |ede\rangle & \phi_9 &= |eed\rangle\end{aligned}$$

The $\{\varphi_n\}$ and $\{\psi_n\}$ basis are equivalent in the A_1 and A_2 representations, for $n = 1, 2, 3$.

A.4.1 A_1 States with $S = 0$

$$\left. \begin{aligned}\varphi_1 = \psi_1 &= (\phi_1 - \phi_2 + \phi_3 - \phi_4 + \phi_5 - \phi_6)/\sqrt{6} \\ \varphi_2 = \psi_2 &= (\phi_7 + \phi_8 + \phi_9)/\sqrt{3}\end{aligned} \right\} \rightarrow \langle H_{S=0}^{A_1} \rangle = \begin{pmatrix} 2U - 2t & \frac{4t}{\sqrt{2}} \\ \frac{4t}{\sqrt{2}} & 3U \end{pmatrix}. \quad (85)$$

A.4.2 A_2 State with $S = 1$

$$\varphi_3 = \psi_3 = (\phi_1 - \phi_2 + \phi_3 + \phi_4 - \phi_5 + \phi_6)/\sqrt{6} \rightarrow \langle H_{S=1}^{A_2} \rangle = (2U + 2t). \quad (86)$$

A.4.3 E States with $S = 0, 1$

$$\begin{aligned}\psi_4 &= (2\phi_1 + \phi_2 - \phi_3)/\sqrt{6} \\ \psi_5 &= (2\phi_4 + \phi_5 - \phi_6)/\sqrt{6} \\ \psi_6 &= (2\phi_7 - \phi_8 - \phi_9)/\sqrt{6}\end{aligned}$$

$$\varphi_4 = (\psi_4 + \psi_5)/\sqrt{2} \rightarrow \langle H_{S=1}^E \rangle = (2U - t) \quad (87)$$

$$\left. \begin{aligned}\varphi_5 &= (\psi_4 - \psi_5)/\sqrt{2} \\ \varphi_6 &= \psi_6\end{aligned} \right\} \rightarrow \langle H_{S=0}^E \rangle = \begin{pmatrix} 2U + t & \frac{-2t}{\sqrt{2}} \\ \frac{-2t}{\sqrt{2}} & 3U \end{pmatrix}. \quad (88)$$

A.5 Below Half-filling: $N_e = 2$ and $S_z = 1$

For $S_z = 1$, below half-filling where $N_e = 2$, we have 3 elements in our bases. We choose our $\{\phi_n\}$ basis as follows

$$\phi_1 = |epp\rangle \quad \phi_2 = |pep\rangle \quad \phi_3 = |ppe\rangle. \quad (89)$$

The $\{\varphi_n\}$ and $\{\psi_n\}$ basis are equivalent. There are no states in the A_1 representation.

A.5.1 A_2 State with $S = 1$

$$\varphi_1 = \psi_1 = (\phi_1 - \phi_2 + \phi_3)/\sqrt{3} \rightarrow \langle H_{S=1}^{A_2} \rangle = (2U + 2t). \quad (90)$$

A.5.2 *E* State with $S = 1$

$$\varphi_2 = \psi_2 = (2\phi_1 + \phi_2 - \phi_3)/\sqrt{3} \quad \rightarrow \quad \langle H_{S=1}^E \rangle = (2U - t) . \quad (91)$$

B Square Cluster Data

In this section we present our findings for the square cluster for the case of half-filling, $N_e = 4$, for $S_z = 0$.

B.1 Half-filling: $N_e = 4$ and $S_z = 0$

For $S_z = 0$ in the case of half-filling where $N_e = 4$ we have 36 elements in our bases. We choose our $\{\phi_n\}$ basis as follows

$$\begin{aligned}
& \phi_1 = |mpmp\rangle & \phi_2 = |pmmp\rangle \\
\phi_3 = |ppmm\rangle & \phi_4 = |mppm\rangle & \phi_5 = |mmpp\rangle & \phi_6 = |pmmp\rangle \\
\phi_7 = |demp\rangle & \phi_8 = |pdem\rangle & \phi_9 = |mpde\rangle & \phi_{10} = |empd\rangle \\
\phi_{11} = |dpme\rangle & \phi_{12} = |edpm\rangle & \phi_{13} = |medp\rangle & \phi_{14} = |pmed\rangle \\
\phi_{15} = |depm\rangle & \phi_{16} = |mdep\rangle & \phi_{17} = |pmde\rangle & \phi_{18} = |epmd\rangle \\
\phi_{19} = |dmpe\rangle & \phi_{20} = |edmp\rangle & \phi_{21} = |pedm\rangle & \phi_{22} = |mped\rangle \\
\phi_{23} = |dmep\rangle & \phi_{24} = |pdme\rangle & \phi_{25} = |epdm\rangle & \phi_{26} = |mepd\rangle \\
\phi_{27} = |dpem\rangle & \phi_{28} = |mdpe\rangle & \phi_{29} = |emdp\rangle & \phi_{30} = |pemd\rangle \\
& \phi_{31} = |dede\rangle & \phi_{32} = |eded\rangle \\
\phi_{33} = |ddee\rangle & \phi_{34} = |deed\rangle & \phi_{35} = |edde\rangle & \phi_{36} = |eedd\rangle
\end{aligned}$$

B.1.1 A_1 States with $S = 0, 1$

$$\begin{aligned}
\psi_1 &= (\phi_3 - \phi_4 + \phi_5 - \phi_6)/2 \\
\psi_2 &= (\phi_7 - \phi_8 + \phi_9 + \phi_{10} - \phi_{11} - \phi_{12} + \phi_{13} - \phi_{14})/\sqrt{8} \\
\psi_3 &= (\phi_{15} - \phi_{16} + \phi_{17} + \phi_{18} - \phi_{19} - \phi_{20} + \phi_{21} - \phi_{22})/\sqrt{8} \\
\psi_4 &= (\phi_{23} - \phi_{24} - \phi_{25} + \phi_{26} - \phi_{27} + \phi_{28} + \phi_{29} - \phi_{30})/\sqrt{8} \\
\psi_5 &= (\phi_{31} + \phi_{32})/\sqrt{2} \\
\psi_6 &= (\phi_{33} + \phi_{34} + \phi_{35} + \phi_{36})/2 \\
\varphi_1 &= (\psi_2 + \psi_3)/\sqrt{2} \quad \rightarrow \quad \langle H_{S=1}^{A_1} \rangle = (5U). \tag{92}
\end{aligned}$$

$$\left. \begin{aligned}
\varphi_2 &= \psi_4 \\
\varphi_3 &= \psi_1 \\
\varphi_4 &= (\psi_2 - \psi_3)/\sqrt{2} \\
\varphi_5 &= \psi_5 \\
\varphi_6 &= \psi_6
\end{aligned} \right\} \rightarrow \langle H_{S=0}^{A_1} \rangle = \begin{pmatrix} 5U & 0 & 0 & 0 & 0 \\ 0 & 4U & 2t & 0 & 0 \\ 0 & 2U & 5U & \frac{4t}{\sqrt{2}} & 2t \\ 0 & 0 & \frac{4t}{\sqrt{2}} & 6U & 0 \\ 0 & 0 & 2t & 0 & 6U \end{pmatrix}. \tag{93}$$

It is interesting that φ_6 does not mix with any of the other states in its sub-basis.

B.1.2 A_2 States with $S = 0, 1$

$$\begin{aligned}
\psi_7 &= (\phi_1 - \phi_2)/\sqrt{2} \\
\psi_8 &= (\phi_7 - \phi_8 + \phi_9 + \phi_{10} + \phi_{11} + \phi_{12} - \phi_{13} + \phi_{14})/\sqrt{8} \\
\psi_9 &= (\phi_{15} - \phi_{16} + \phi_{17} + \phi_{18} + \phi_{19} + \phi_{20} - \phi_{21} + \phi_{22})/\sqrt{8} \\
\psi_{10} &= (\phi_{23} - \phi_{24} - \phi_{25} + \phi_{26} + \phi_{27} - \phi_{28} - \phi_{29} + \phi_{30})/\sqrt{8}
\end{aligned}$$

$$\left. \begin{aligned}
\varphi_7 &= \psi_7 \\
\varphi_8 &= \psi_{10} \\
\varphi_9 &= (\psi_8 + \psi_9)/\sqrt{2}
\end{aligned} \right\} \rightarrow \langle H_{S=1}^{A_2} \rangle = \begin{pmatrix} 4U & 0 & \frac{4t}{\sqrt{2}} \\ 0 & 5U & \frac{-4t}{\sqrt{2}} \\ \frac{4t}{\sqrt{2}} & \frac{-4t}{\sqrt{2}} & 5U \end{pmatrix}. \quad (94)$$

$$\varphi_{10} = (\psi_8 - \psi_9)/\sqrt{2} \rightarrow \langle H_{S=0}^{A_2} \rangle = (5U). \quad (95)$$

B.1.3 B_1 States with $S = 0, 1$

$$\begin{aligned}
\psi_{11} &= (\phi_7 + \phi_8 + \phi_9 - \phi_{10} - \phi_{11} + \phi_{12} + \phi_{13} + \phi_{14})/\sqrt{8} \\
\psi_{12} &= (\phi_{15} + \phi_{16} + \phi_{17} - \phi_{18} - \phi_{19} + \phi_{20} + \phi_{21} + \phi_{22})/\sqrt{8} \\
\psi_{13} &= (\phi_{23} + \phi_{24} - \phi_{25} - \phi_{26} - \phi_{27} - \phi_{28} + \phi_{29} + \phi_{30})/\sqrt{8} \\
\psi_{14} &= (\phi_{31} - \phi_{32})/\sqrt{2}
\end{aligned}$$

$$\varphi_{11} = (\psi_{11} + \psi_{12})/\sqrt{2} \rightarrow \langle H_{S=1}^{B_1} \rangle = (5U). \quad (96)$$

$$\left. \begin{aligned}
\varphi_{12} &= (\psi_{11} - \psi_{12})/\sqrt{2} \\
\varphi_{13} &= \psi_{13} \\
\varphi_{14} &= \psi_{14}
\end{aligned} \right\} \rightarrow \langle H_{S=0}^{B_1} \rangle = \begin{pmatrix} 5U & \frac{-4t}{\sqrt{2}} & \frac{4t}{\sqrt{2}} \\ \frac{-4t}{\sqrt{2}} & 5U & 0 \\ \frac{4t}{\sqrt{2}} & 0 & 6U \end{pmatrix}. \quad (97)$$

B.1.4 B_2 States with $S = 0, 1, 2$

$$\begin{aligned}
\psi_{15} &= (\phi_1 + \phi_2)/\sqrt{2} \\
\psi_{16} &= (\phi_3 + \phi_4 + \phi_5 + \phi_6)/2 \\
\psi_{17} &= (\phi_7 + \phi_8 + \phi_9 - \phi_{10} + \phi_{11} - \phi_{12} - \phi_{13} - \phi_{14})/\sqrt{8} \\
\psi_{18} &= (\phi_{15} + \phi_{16} + \phi_{17} - \phi_{18} + \phi_{19} - \phi_{20} - \phi_{21} - \phi_{22})/\sqrt{8} \\
\psi_{19} &= (\phi_{23} + \phi_{24} - \phi_{25} - \phi_{26} + \phi_{27} + \phi_{28} - \phi_{29} - \phi_{30})/\sqrt{8} \\
\psi_{20} &= (\phi_{33} - \phi_{34} - \phi_{35} + \phi_{36})/\sqrt{4}
\end{aligned}$$

$$\varphi_{15} = (\psi_{15}/\sqrt{2} + \psi_{16})/\sqrt{3/2} \rightarrow \langle H_{S=2}^{B_2} \rangle = (4U). \quad (98)$$

$$\left. \begin{aligned}
\varphi_{16} &= (\psi_{17} + \psi_{18})/\sqrt{2} \\
\varphi_{17} &= \psi_{19}
\end{aligned} \right\} \rightarrow \langle H_{S=1}^{B_2} \rangle = \begin{pmatrix} 5U & 0 \\ 0 & 5U \end{pmatrix}. \quad (99)$$

$$\left. \begin{aligned} \varphi_{18} &= (-2\psi_{15}/\sqrt{2} + \psi_{16})/\sqrt{3} \\ \varphi_{19} &= (\psi_{17} - \psi_{18})/\sqrt{2} \\ \varphi_{20} &= \psi_{20} \end{aligned} \right\} \rightarrow \langle H_{S=0}^{B_2} \rangle = \begin{pmatrix} 4U & \frac{-6t}{\sqrt{3}} & 0 \\ \frac{-6t}{\sqrt{3}} & 5U & -2t \\ 0 & -2t & 6U \end{pmatrix}. \quad (100)$$

Although φ_{16} and φ_{17} have the same total-spin, not that they happen to be eigenvectors the Hamiltonian.

B.1.5 E States with $S = 0, 1$

$$\begin{aligned} \psi_{21} &= (\phi_3 - I\phi_4 - \phi_5 + I\phi_6)/2 \\ \psi_{22} &= (\phi_7 - I\phi_8 - \phi_9 - I\phi_{10})/2 \\ \psi_{23} &= (\phi_{11} + I\phi_{12} + \phi_{13} - I\phi_{14})/2 \\ \psi_{24} &= (\phi_{15} - I\phi_{16} - \phi_{17} - I\phi_{18})/2 \\ \psi_{25} &= (\phi_{19} + I\phi_{20} + \phi_{21} - I\phi_{22})/2 \\ \psi_{26} &= (\phi_{23} - I\phi_{24} + \phi_{25} - I\phi_{26})/2 \\ \psi_{27} &= (\phi_{27} - I\phi_{28} + \phi_{29} - I\phi_{30})/2 \\ \psi_{28} &= (\phi_{33} - I\phi_{34} + I\phi_{35} - \phi_{36})/2 \end{aligned}$$

$$\left. \begin{aligned} \varphi_{21} &= \psi_{21} \\ \varphi_{22} &= (\psi_{26} + \psi_{27})/\sqrt{2} \\ \varphi_{23} &= (\psi_{23} + \psi_{25})/\sqrt{2} \\ \varphi_{24} &= (\psi_{22} + \psi_{24})/\sqrt{2} \end{aligned} \right\} \rightarrow \langle H_{S=1}^E \rangle = \begin{pmatrix} 4U & 0 & \frac{-2t}{\sqrt{2}} & \frac{2it}{\sqrt{2}} \\ 0 & 5U & (-1+i)t & (-1-i)t \\ \frac{-2t}{\sqrt{2}} & (-1-i)t & 5U & 0 \\ \frac{-2t}{\sqrt{2}} & (-1+i)t & 0 & 5U \end{pmatrix}. \quad (101)$$

$$\left. \begin{aligned} \varphi_{25} &= (-\psi_{23} + \psi_{25})/\sqrt{2} \\ \varphi_{26} &= (-\psi_{22} + \psi_{24})/\sqrt{2} \\ \varphi_{27} &= (\psi_{26} - \psi_{27})/\sqrt{2} \\ \varphi_{28} &= \psi_{28} \end{aligned} \right\} \rightarrow \langle H_{S=0}^E \rangle = \begin{pmatrix} 5U & 0 & (-1+i)t & \frac{2t}{\sqrt{2}} \\ 0 & 5U & (1+i)t & \frac{2it}{\sqrt{2}} \\ (-1-i)t & (1-i)t & 5U & 0 \\ \frac{2t}{\sqrt{2}} & \frac{-2it}{\sqrt{2}} & 0 & 6U \end{pmatrix}. \quad (102)$$

C Hubbard Package: Mathematica Code

```
(*
 * Description:
 *
 * Hubbard model package to calculate for small lattice clusters the hamiltonian
 * matrix of elements given a list of basis states. The number of sites of the
 * cluster in principle is arbitrary, constrained only by computation time.
 * Further, the interactions, i.e. the bonds, between sites in the lattice is
 * also arbitrary a must be given is a list.
 *
 * Package also generates a linear combination of basis state by using the C3v
 * symmetry group to block diagonalize a Hamiltonian matrix of elements.
 * The particles comprising the system are assumed to be fermions, so phase
 * changes due to symmetry operations are taken into account.
 * This package depends on the Braket operator defined in the Hubbard package.
 *
 * Version: 1.10
 *)

BeginPackage["hubbard`"]

p::usage = "spin up electron"
m::usage = "spin down electron"
d::usage = "double electrons: pm"
e::usage = "empty site"
t::usage = "Hopping kinetic energy"
U::usage = "Intersite Coulomb potential energy"

Z::usage = "Z[state]\n
Symbolic state vector in the number representation"

c::usage = "c[spin, site, Z[state]]\n
Fermion destruction operator for a given spin and site"

c::usage = "c[spin, site, Z[state]]\n
Fermion creation operator for a given spin and site"

number::usage = "number[spin, site, Z[state]] is the number operator"

H::usage = "H[Z[state],bonds]\n
Hubbard hamiltonian applied onto Z[state]
where state is a list of n spins and bonds is a list of all the site interactions.
For example, for a three site lattice, we may let bonds={{1,2},{2,1},{2,3},{3,2},{3,1},{1,3}}.\n
The spin notations for the state is as follows:\n p=up\n m=down\n d=double\n e=empty\n
Then for our three site lattice, a state with total spin=1 may be written: state = {p,p,m}.
Off-site interactions have t as the kinetic energy hopping term and on-site
interactions have U as the Coulomb term.
The return value is the new state, Z'[state] = H[Z[state],bonds]."
```

```
Braket::usage = "Braket[Z[state1], Z[state2]]\n
Takes the dot product of two state vectors.
The second argument, Z[state2] may be any linear combination of basis states."
```

```
MatrixElements::usage = "MatrixElements[basis, basis, bonds]\n
Calculates the matrix elements of the Hubbard hamiltonian using a list of general states, basis, and a conjugate list, basis*, al
```

```
fermflip::usage = "fermflip[site_A, site_B, Z[state]]\n
General fermionic site interchange operator. Exchanges spins between sites A and B
given any linear combination of basis states."
```

```
C3v::usage = "C3v[op, a Z[state] + ... ] is the group operator acting on a general state\n
op = 1 -> E      - Identity\n
op = 2 -> C3     - Rotation by 120 degrees\n
```

```

op = 3 -> C3^2 - Rotation by 240 degrees\n
op = 4 -> Sigma1 - Reflection about site 1\n
op = 5 -> Sigma2 - Reflection about site 2\n
op = 6 -> Sigma3 - Reflection about site 3\n
\n
Fermionic particles is assumed.
"
C3vOpMatrix::usage = "C3vOpMatrix[op, basis, basis] generates a matrix for each operation"

C4v::usage = "C4v[op, a Z[state] + ... ] is the group operator acting on a general state\n
op = 1 -> E - Identity\n
op = 2 -> C4 - Rotation by 90 degrees\n
op = 3 -> C2 - Rotation by 180 degrees\n
op = 4 -> C4^3 - Rotation by 270 degrees\n
op = 5 -> Sigma - Reflection about site 1 and site 3\n
op = 6 -> Sigma - Reflection about site 2 and site 4\n
op = 7 -> Sigma - Reflection about vertical\n
op = 8 -> Sigma - Reflection about horizontal\n
\n
Fermionic particles is assumed.
"

C4vOpMatrix::usage = "C4vOpMatrix[op, basis, basis] generates a matrix for each operation"

SS::usage = "SS[Z[state]], where Z[state] may be a general state"

SSMatrix::usage = "SSMatrix[basis, basis] generates a total spin squared matrix given a general basis"

SSij::usage = "SSij[site1, site2, Z] total spin coorelation between two sites"

Begin["private"]

(*****
*****
** **
** Second Quantized Operators **
** and the **
** Hubbard Hamiltonian **
** **
*****
*****)

(*
*
* Define basic site-independent creation
* and annihilation operators
*
*)

cp[p] = 0
cp[m] = d
cp[d] = 0
cp[e] = p
cp[0] = 0

cm[p] = d
cm[m] = 0
cm[d] = 0
cm[e] = m
cm[0] = 0

cp[p] = e
cp[m] = 0
cp[d] = m
cp[e] = 0
cp[0] = 0

cm[p] = 0

```

```

cm[m] = e
cm[d] = p
cm[e] = 0
cm[0] = 0

(*
 *
 * Define the state operator property
 *
 *)

Z[Z[state_]] := state

(*
 *
 * Define nulstate to handle Pauli exclusion
 * and destruction on the vacuum
 *
 *)

nulstate = 0

(*
 *
 * Define basis site and spin specific creation
 * and annihilation operators with arbitrary phase
 *
 *)
c[spin_, site_, phase_:1 Z[state_]] := Block[
{1, lstate, lphase},

lstate = state = Z[Z[state]];
lphase = phase ;

(* Apply anti-commutation upto the indexed site *)
For[l=1, l<site, l++,
If[state[[l]] == p || state[[l]] == m,
  lphase ** -1
]
] ;

(* Apply creation/destruction operator of given spin
on the indexed site *)
Switch[spin,
p, lstate[[site]] = cp[state[[site]] ,
  m, If[lstate[[site]] == p, lphase ** -1] ;
  lstate[[site]] = cm[state[[site]]
] ;
Which[ lstate[[site]] == 0, nulstate,
lstate == lstate, lphase Z[lstate]
]
]
c[spin_, site_, phase_:1 Z[state_]] := Block[
{1, lstate, lphase},

lstate = state = Z[Z[state]];
lphase = phase ;

(* Apply anti-commutation upto the indexed site *)
For[l=1, l<site, l++,
If[state[[l]] == p || state[[l]] == m,
  lphase ** -1
]
] ;

(* Apply creation/destruction operator of given spin
on the indexed site *)

```

```

Switch[spin,
p, lstate[[site]] = cp[state[[site]]],
      m, If[lstate[[site]] == d, lphase *=- -1] ;
      lstate[[site]] = cm[state[[site]]]
      ] ;
Which[ lstate[[site]] == 0, nulstate,
lstate == lstate, lphase Z[lstate]
]
]

(*
*
* Handle the case when the state is null
*
*)

c[spin_, index_, nulstate] = nulstate
c[spin_, index_, nulstate] = nulstate

(*
*
* Handle by recursion the case when the given state
* is a linear combination of basis states
*
*)

c[spin_, site_, a_. Z[state_] + b_.] := a c[spin, site, Z[state]] + c[spin, site, b]
c[spin_, site_, a_. Z[state_] + b_.] := a c[spin, site, Z[state]] + c[spin, site, b]

(*
* Handle case when the state is written in factored form
*
*)

c[spin_, site_, Z_] := c[spin, site, Expand[Z]]
c[spin_, site_, Z_] := c[spin, site, Expand[Z]]

(*
* Number of operator with specified spin at a certain site
*)

number[spin_, site_, Z_] := c[spin,site, c[spin, site, Z]]
number[spin_, site_, nulstate] = nulstate

(*
* Hubbard hamiltonian for N-sites
*)

H[Z[state_], bonds_] := Block[
{i, j, Zo, lstate, nsites, nbonds},

lstate = Z[Z[state]] ;
nsites = Length[lstate] ;
nbonds = Length[bonds] ;

Zo = 0 ;

For[ i=1, i<=nbonds, i++,
Zo += -t c[m,bonds[[i]][[1]],c[m,bonds[[i]][[2]],Z[state]]] +
-t c[p,bonds[[i]][[1]],c[p,bonds[[i]][[2]],Z[state]]]
] ;

For[ i=1, i<=nsites, i++,
Zo += U number[p,i, number[m,i,Z[state]]]
+ U number[p,i, Z[state]] + U number[m,i,Z[state]]
] ;

```

```

    Zo
]

H[a_:1 Z[state_] + b_., bonds_] := a H[Z[state], bonds] + H[b, bonds]
H[nulstate, bonds_] = nulstate

(*
 * Recursive definition of state vector orthogonality
 * Note: If Braket cannot compute the value it will return Error
 *)

SumList[alist_] := Block[{i, sum, size},
sum = 0 ;
size = Length[alist] ;
Do[ sum += alist[[i]], {i,1,size} ] ;
If[size==0, Error, sum]
]

Braket [a_:1 Z[s_], b_:1 Z[s_] ] := a b
Braket [a_:1 Z[s1_], b_:1 Z[s2_] ] := 0
Braket [a_:1 Z[s_]/d1_:1 , c_:1 Z[s_]/d2_:1 ] := (a c)/(d1 d2)
Braket [a_:1 Z[s1_]/d1_:1, c_:1 Z[s2_]/d2_:1 ] := 0

Braket[a_:1 Z[s_], Z2_] := a SumList[Flatten[Outer[Braket,{Z[s]},Level[Collect[Expand[Z2],{Z}],1]]]]
Braket[Z1_, a_:1 Z[s_]] := a SumList[Flatten[Outer[Braket,Level[Collect[Expand[Z1],{Z}],1],{Z[s]}]]]]
Braket[Z1_, Z2_] := SumList[Flatten[Outer[Braket,Level[Z1],1],Level[Collect[Expand[Z2],{Z}],1]]]]

Braket[nulstate, __ ] = nulstate
Braket[_, nulstate] = nulstate
Braket[nulstate, nulstate] = nulstate

(*
 * Calculate the matrix of elements using the Hubbard
 * hamiltonian and the Braket operator
 *)

MatrixElements[basis_, basis_, bonds_] := Block[{i,j, num, ME, M},

num = Length[basis] ;
ME = {};

For[j=1, j<= num, j++,
(* Print["Z[" ,j," ] = ", basis[[j]] ] ; *)
Print["[" ,j," ]" ] ;
M = {};
Do[ AppendTo[M, Braket[ basis[[j]], H[ basis[[i]] , bonds] ]], {i,1,num}];
AppendTo[ME,M]
];
ME
]

(*****
*****
** **
** Site Interchange Operator for Fermions **
** based on Conditional Creation/Annihilation Operators **
** **
*****
*****
)

(*

```

```

* Occupation operator of a given spin and site.
* Returns 1 if present or 0 if not, and applies only to basis states.
*)

occupy[spin_, site_, Z[state_] ] := number[spin,site,Z[state]]/Z[state]

(*
* Conditional destruction and annihilation operators for given spin and site.
* That is, destruction and annihilation operators apply only if
* occupancy is 1. Equivalent to destruction/annihilation operators raised to
* the power of the occupancy. These operators apply only to basis states.
*)

w[spin_,site_, a_:1 Z[state_] ] := If[occupy[spin,site,Z[state]]==1, c[spin,site, a Z[state]], a Z[state]]
w[spin_,osite_, site_, Z[ostate_] , a_:1 Z[state_] ] := If[occupy[spin,osite,Z[ostate]]==1
&& occupy[spin,site,Z[state]]==0,
c[spin,site, a Z[state]], a Z[state]]

(* Spin-independent conditional destruction and annihilation operators.
* These operators apply only to basis states and are defined only
* for convenience to simplify the production rules for the fermionic
* site interchange operators.
*)

ww[site_, a_:1 Z[state_]] := w[p, site, w[m, site, a Z[state]] ]
ww[osite_, site_, Z[ostate_] , a_:1 Z[state_]] := w[m, osite, site, Z[ostate], w[p, osite, site, Z[ostate], a Z[state]] ]

(*
* Fermionic site interchange operator. Exchanges spins between osite and site.
* This operator applies only to basis states.
*)

fflip[osite_,site_, a_:1 Z[state_]] := ww[osite, site, Z[state], ww[site, osite, Z[state], ww[site, ww[osite, a Z[state]]] ] ]

(*
* General fermionic site interchange operator. Exchanges spins between osite and site
* given any linear combination of basis states.
*)

fermflip[osite_,site_, ss_] := Distribute[fflip[osite,site,ss]]
fermflip[osite_, site_, 0 ] := 0

(*****
*****
** **
** Site Interchange Operator for Fermions **
** based on Pendelton's Operators **
** **
*****
*****)

P[spin_, s1_, s2_, Z_] := Z + c[spin,s2, c[spin,s1,Z]] + c[spin,s1, c[spin,s2,Z]] -
c[spin,s1, c[spin,s1,Z]] - c[spin,s2, c[spin,s2,Z]]

fermx[s1_, s2_ , Z_] := P[m,s1,s2, P[p,s1,s2,Z] ]

(*****
*****
** **
** C3v Group Operators for Fermions **
** **
*****
*****)

C3v[op_, Z_] := Block[
{Y},

```

```

Switch[ op,
1>(* E - Identity Operator *)
Y = Z,

2>(* C3 = sigma1 sigma3 - Rotation by 120 degrees *)
Y = fermx[1,2, fermx[2,3,Z] ],

3>(* C3^2 = sigma3 sigma1 - Rotation by 240 degrees *)
Y = fermx[2,3, fermx[1,2,Z] ],

4>(* Sigma1 - Reflection about site 1 *)
Y = fermx[2,3,Z],

5>(* Sigma1 - Reflection about site 2 *)
Y = fermx[3,1,Z],

6>(* Sigma1 - Reflection about site 3 *)
Y = fermx[1,2,Z],
] ;

Y
]

(*
* Generate C3v matrices for each group operation
*)

C3vOpMatrix[op_, basis_, basis_] := Block[
{i,j, num, Row},

num = Length[basis] ;
OpMatrix = {};

For[j=1, j<= num, j++,
Row = {};
Do[ AppendTo[Row, Braket[ basis[[j]], C3v [op, basis[[i]] ] ]], {i,1,num}];
AppendTo[OpMatrix,Row]
] ;
OpMatrix
]

(*****
*****
** **
** C4v Group Operators for Fermions **
** **
*****
*****)

C4v[op_, Z_] := Block[
{Y},

Switch[ op,
1>(* E - Identity Operator *)
Y = Z,

2>(* C4 - Rotation by 90 degrees *)
Y = fermx[1,2, fermx[2,3, fermx[3,4,Z] ]],

3>(* C4^2 = C2 - Rotation by 180 degrees *)
Y = fermx[1,3, fermx[2,4,Z] ],

4>(* C4^2 - Rotation by 270 degrees *)
Y = fermx[3,4, fermx[2,3, fermx[1,2,Z] ]],

5>(* Sigma - Reflection about site 1 and site 3 *)

```

```

Y = fermx[2,4,Z],

6,(* Sigma - Reflection about site 2 and site 4 *)
Y = fermx[1,3,Z],

7,(* Sigma - Reflection about vertical *)
Y = fermx[1,2, fermx[3,4,Z] ],

8,(* Sigma - Reflection about horizontal *)
Y = fermx[1,4, fermx[2,3,Z] ],
] ;

      Y
]

(*
 * Generate C4v matrices for each group operation
 *)

C4vOpMatrix[op_, basis_, basis_] := Block[
{i,j, num, Row},

num = Length[basis] ;
OpMatrix = {};

      For[j=1, j<= num, j++,
        Row = {};
        Do[ AppendTo[Row, Braket[ basis[[j]], C4v [op, basis[[i]] ] ]], {i,1,num}];
AppendTo[OpMatrix,Row]
] ;
OpMatrix
]

(*****
*****
** **
**   General Spin Operators       **
** **
*****
*****)

(*
 * Site specific spin operators
 *)

sx[site_, Z_] := c[p, site, c[m, site, Z]]/2 + c[m, site, c[p, site, Z]]/2
sy[site_, Z_] := - I c[p, site, c[m, site, Z]]/2 + I c[m, site, c[p, site, Z]]/2
sz[site_, Z_] := c[p, site, c[p, site, Z]]/2 - c[m, site, c[m, site, Z]]/2

(*
 * Site-to-site product spin operators: sx * sx , sy * sy, sz * sz
 *)

sxsx[site1_, site2_, Z_] := c[p, site1, c[m, site1, c[p, site2, c[m, site2, Z ]]]/4 +
c[m, site1, c[p, site1, c[m, site2, c[p, site2, Z ]]]/4 +
c[p, site1, c[m, site1, c[m, site2, c[p, site2, Z ]]]/4 +
c[m, site1, c[p, site1, c[p, site2, c[m, site2, Z ]]]/4

sysy[site1_, site2_, Z_] := - c[p, site1, c[m, site1, c[p, site2, c[m, site2, Z ]]]/4 -
c[m, site1, c[p, site1, c[m, site2, c[p, site2, Z ]]]/4 +
c[p, site1, c[m, site1, c[m, site2, c[p, site2, Z ]]]/4 +
c[m, site1, c[p, site1, c[p, site2, c[m, site2, Z ]]]/4

szsz[site1_, site2_, Z_] := c[p, site1, c[p, site1, c[p, site2, c[p, site2, Z ]]]/4 -
c[m, site1, c[m, site1, - c[m, site2, c[m, site2, Z ]]]/4 +
c[p, site1, c[p, site1, - c[m, site2, c[m, site2, Z ]]]/4 -
c[m, site1, c[m, site1, c[p, site2, c[p, site2, Z ]]]/4

```

```

(*)
* Total spin squared operator
*)

SS[Z[state_]] := Block[
{i, j, nsites, lstate, Zo},

lstate = Z[Z[state]] ;
nsites = Length[lstate] ;
Zo = 0 ;

For[ i=1, i<=nsites, i++,
For[ j=1, j<=nsites, j++,

    Zo += sxsx[i,j,Z[state]] + sysy[i,j,Z[state]] + szsz[i,j,Z[state]]
]
] ;

Expand[Zo] ;
Zo

]
SS[a_:1 Z[state_] + b_.] := a SS[Z[state]] + SS[b]
SS[nulstate] = nulstate

(*)
* Matrix of total spin squared operator given a general basis
*)

SSMatrix[basis_, basisc_] := Block[{i,j, num, SSE, M, ZY},

num = Length[basis] ;
SSE = {};

For[j=1, j<= num, j++,
(* Print["Z[" ,j," ] = ", basis[[j]] ] ; *)
Print["[" ,j," ]" ;
M = {};
ZY = Expand[ SS[ basis[[j]] ] ] ;
Do[ AppendTo[M, Braket[ basisc[[i]], ZY]], {i,1,num}];
AppendTo[SSE,M]
];
SSE
]

(*)
* Total Spin Correlation
*)

SSij[s1_, s2_, Z_] := sxsx[s1,s2,Expand[Z]] + sysy[s1,s2,Expand[Z]] + szsz[s1,s2,Expand[Z]]

End[]

EndPackage[]

Null

```

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