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# Group theoretical classification of the Hartree–Fock solutions of the Hubbard model on a triangular lattice

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**Abstract.** Group theoretically possible spin density waves (SDWs) of the Hubbard model on a triangular lattice are found and classified for ordering vectors $q$ of K and M in the Brillouin zone by finding the maximal subgroups of the symmetry group of the Hamiltonian. It is found that classifications of SDWs with these ordering vectors are reduced to classifications of SDWs on molecules with $D_3$ and $T_d$ symmetries, respectively. From this reduction we found two axial-type SDWs (ASDW) and one plane-type SDW (PSDW) for point K and three ASDWs, two PSDWs and one cubic- (three-dimensional-) type SDW (CSDW) for point M. The standard mean-field Hamiltonians and their invariance groups are listed for each class.

## 1. Introduction

Recently, the Hubbard model on a triangular lattice has been studied in order to understand the behaviour of adsorbed $^3$He on a substrate [1]. In order to discuss the possible types of long- or short-range orders realized in different fillings in this system, in this paper we find and classify various spin density wave (SDW) solutions of the model.

To perform such a work the group theoretical approach developed by Fukutome and Ozaki [2–4] provides a useful tool. They classified the Hartree–Fock (HF) solutions of the Hamiltonian with the symmetry

$$G_0 = \Gamma \times S \times T \tag{1}$$

where $\Gamma$ is the space group of the lattice structure, S is the group of the spin rotation and T is the group of the time reversal. When the electron–electron interaction is weak, its HF solution has the invariance group $G_0$. This solution is called the restricted HF (RHF) solution. As the interaction increases, the RHF solution becomes unstable and solutions with the lower symmetries or the symmetries of the subgroups of $G_0$ bifurcate. These solutions are called unrestricted HF (UHF) solutions. We can characterize a HF solution $|\Phi)$ of a Slater determinant by the invariance group which is defined by

$$G = \{g \in G_0 \mid g|\Phi) = \exp(i\alpha_g)|\Phi)\} \tag{2a}$$

or equivalently

$$G = \{g \in G_0 \mid gH_{MF} = H_{MF}\} \tag{2b}$$

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where $\exp(i\alpha_g)$ is a phase factor and $H_{MF}$ is the mean-field Hamiltonian corresponding to $|\Phi\rangle$. So, we can find and classify UHF solutions by finding and classifying the subgroups of $G_0$.

## 2. Formulation

The Hubbard Hamiltonian is given by

$$H = -\sum_{\sigma}\sum_{t,\tau} t_0(\tau) a^{\dagger}_{t+\tau\sigma} a_{t\sigma} + U\sum_{t} a^{\dagger}_{t\uparrow} a^{\dagger}_{t\downarrow} a_{t\downarrow} a_{t\uparrow} \tag{3}$$

where $a^{\dagger}_{t\sigma}(a_{t\sigma})$ is the operator which creates (annihilates) an electron of spin $\sigma$ at site $t$. $t_0(\tau)$ is the hopping parameter between atoms $t+\tau$ and $t$. With the use of the momentum and spinor representation

$$\tilde{a}^{\dagger}_{t\sigma} = \frac{1}{\sqrt{N}}\sum_{k} e^{-ik\cdot t}\tilde{a}^{\dagger}_{k\sigma} \qquad \tilde{a}^{\dagger} = (a^{\dagger}_{k\uparrow}, a^{\dagger}_{k\downarrow}) \tag{4}$$

the mean-field Hamiltonian can be written as

$$H_{MF} = \sum_{k} t(k)\tilde{a}^{\dagger}_{k}\tilde{a}_{k} + \sum_{i=0,x,y,z}\sum_{q} X^{i}_{q}\left(\sum_{k}\tilde{a}^{\dagger}_{k+q/2}\sigma_i\tilde{a}_{k-q/2}\right). \tag{5}$$

The $X^i_q$ are determined by the self-consistent field (SCF) conditions

$$X^0_q = \frac{U}{2}\rho_0(q) \qquad X^j_q = -\frac{U}{2}\rho_j(q) \qquad j = x,y,z \tag{6}$$

where $\sigma_0 = 1$ and $\sigma_i$ $(i = x,y,z)$ are $2\times 2$ Pauli matrixes, and

$$\rho_i(q) = \frac{1}{N}\sum_{k}\langle\tilde{a}^{\dagger}_{k-q/2}\sigma_i\tilde{a}_{k+q/2}\rangle \qquad i = 0,x,y,z. \tag{7}$$

$\rho_i(q)$ are order parameters characterizing the HF solutions. If there is no symmetry breaking, all the $\rho_i(q)$ except $\rho_0(\mathbf{0})$ are equal to zero.

Charge $(i=0)$ and spin $(i=x,y,z)$ densities are given by

$$\langle\tilde{a}^{\dagger}_{t}\sigma_i\tilde{a}_{t}\rangle = \sum_{q} e^{iq\cdot t}\rho_i(q) \qquad i = 0,x,y,z. \tag{8}$$

If $\rho_0(q)$ is not zero, the HF solution has a charge density wave (CDW) with wavevector $q$. If $\rho_i(q)$ $(i=x,y,z)$ is not zero, the HF solution has a SDW with wavevector $q$. Moreover, SDW solutions can be classified into three types according to the dimension of the component of the spin, that is axial (one), plane (two) and cubic (three) types. We call them ASDW, PSDW and CSDW, respectively.

The HF energy can be written as

$$E_{HF} = \sum_{k} t(k)\langle\tilde{a}^{\dagger}_{k}\tilde{a}_{k}\rangle + \frac{N}{4}U\sum_{q}|\rho_0(q)|^2 - \frac{N}{4}U\sum_{q}\sum_{i=x,y,z}|\rho_i(q)|^2. \tag{9}$$

From this expression we can see that the spin modulation $\rho_i(q)$ $(i = x, y, z)$ is stabilized while the charge modulation $\rho_0(q)$ is not favourable by positive $U$. Then we only consider the classification of SDW solutions.

From equation (5) the bases of the order parameters spaces are

$$\sum_k \tilde{a}^\dagger_{k+q/2}\sigma_i\tilde{a}_{k-q/2} = l_{i,q}. \tag{10}$$

Noting that

$$(l_{i,q})^\dagger = l_{i,-q} \tag{11}$$

we can define new Hermitian bases

$$l^+_{i,q} = \frac{1}{2}(l_{i,q} + l_{i,-q}) \qquad l^-_{i,q} = \frac{\mathrm{i}}{2}(l_{i,q} - l_{i,-q}). \tag{12}$$

If $-q$ is equivalent to $q$ then $l_{i,q} = l^+_{i,q}$.

Thus, $H_{\mathrm{MF}}$ can be determined by a vector in the vector space $V_0 = [l^\pm_{i,q}, i = 0, x, y, z]$, that is the space spanned by $l^\pm_{i,q}$ over the real number field. Moreover, $V_0$ is the representation space of the symmetry group $\mathrm{G}_0 = \Gamma \times \mathrm{S} \times \mathrm{T}$ of the Hamiltonian (3). $g \in \mathrm{G}_0$ transforms $l^\pm_{i,q}$ as follows.

(i) Translation:

$$\{1 \mid t\}(l^+_{i,q}, l^-_{i,q}) = (l^+_{i,q}, l^-_{i,q}) \begin{pmatrix} \cos q \cdot t & \sin q \cdot t \\ -\sin q \cdot t & \cos q \cdot t \end{pmatrix}. \tag{13}$$

(ii) Space rotation and inversion:

$$\{\alpha \mid \mathbf{0}\}(\mathbf{l}^+_{\mathbf{i},\mathbf{q}}, \mathbf{l}^-_{\mathbf{i},\mathbf{q}}) = (\mathbf{l}^+_{\mathbf{i},\mathbf{q}'}, \mathbf{l}^-_{\mathbf{i},\mathbf{q}'}) \qquad q' = \mathrm{R}(\alpha)q \tag{14}$$

where $R(\alpha)$ is the three-dimensional representation of the rotation $\alpha$.

(iii) Spin rotation:

$$u(e,\theta)l^\pm_{j,q} = \sum_{j'} R_{j'j}(e,\theta)l^\pm_{j',q} \qquad u(e,\theta)l^\pm_{0,q} = l^\pm_{0,q} \tag{15}$$

where $u(e,\theta)$ is the spin rotation around $e$ by angle $\theta$ and $R(u(e,\theta))$ is its three-dimensional rotation matrix.

(iv) Time reversal:

$$tl^\pm_{j,q} = -l^\pm_{j,q} \qquad (j = x, y, z) \qquad tl^\pm_{0,q} = l^\pm_{0,q}. \tag{16}$$

From equations (12) and (14), $l^+_{i,q}$ and $l^-_{i,q}$ have even and odd parities, respectively.

Since all broken-symmetry phases with a single order parameter can be derived from irreducible representations in the representation space $V_0$ [3, 4], we consider the SDW solutions belonging to an irreducible representation space $V_\lambda$ in $V_0$. Using Michel's theorem [5, 6], possible SDW solutions can be found by looking for the point $v \in V_\lambda$ such that the invariance group $\mathrm{G}_v$ of $v$:

$$\mathrm{G}_v = \{g \in \mathrm{G}_0 \mid gv = v, v \in V_\lambda\} \tag{17}$$

is maximal.

### 3. Classification of SDWs in a triangular lattice

Now we apply this method to a triangular lattice. The space symmetry of the triangular lattice is

$$\Gamma = L(t_a, t_b) \wedge D_{6h}. \tag{18}$$

Its fundamental translation vectors $t_a$ and $t_b$ are defined in figure 1(*a*). As we treat the single band model on the primitive two-dimensional lattice, it is sufficient to treat the space group with the proper rotational group, i.e. $\Gamma = L(t_a, t_b) \wedge D_6$. This is because the inversion of the space is equivalent to the $C_2$ rotation around the axis perpendicular to the plane. In figure 1(*a*) we also define two folded rotational axes in the plane and $x$ and $y$ axes. In figure 1(*b*) we show the reciprocal lattice vectors $G_a$ and $G_b$ and the first Brillouin zone. We find the possible SDW solutions which belong to the irreducible representations characterized by points K and M.

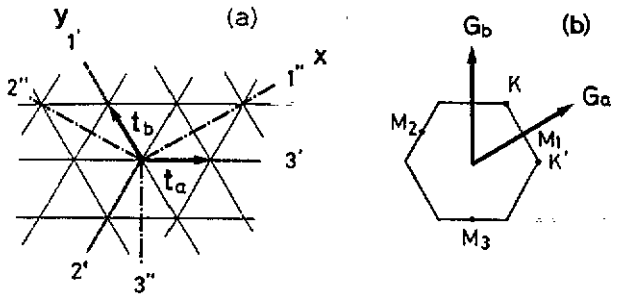


**Figure 1.** Fundamental translational vectors ($t_a$ and $t_b$) and two folded rotational axes (1', 2', 3', 1'', 2'' and 3'') (*a*); and fundamental reciprocal lattice vectors ($G_a$, and $G_b$) and the first Brillouin zone of the two-dimensional triangular lattice (*b*).

#### *3.1. SDWs characterized by point K*

The order parameter space characterized by point K (rigorously K and K') is

$$V_K = [l^{\pm}_{iQ},\ i = 0, x, y, z] \tag{19a}$$

where

$$Q = \tfrac{1}{3}(G_a + G_b). \tag{19b}$$

Any SDW in $V_K$ has the spatial symmetry

$$G_{V(K)} = L_3 \wedge D'_3 \tag{20a}$$

where

$$L_3 = L(2t_a + t_b, t_a + 2t_b) \qquad D'_3 = \{1, C^{+}_{3z}, C^{-}_{3z}, C_{21'}, C_{22'}, C_{23'}\}. \tag{20b}$$

$G_{V(K)}$ is a normal subgroup of $\Gamma$. Since $\Gamma/G_{V(K)} \simeq D_3$, the classification of SDWs characterized by point K is reduced to the classification of SDWs in a molecule

with $D_3$ symmetry. This has been solved in [3] and [4] so here we only give the results. We list in tables 1 and 2 the SDWs and their invariance groups and show in figure 2 their schematic spin and charge patterns on the triangular lattice with the corresponding patterns on the molecule with $D_3$ symmetry. $ASDW_1$ (figure 2(*a*)) and $ASDW_2$ (figure 2(*b*)) states are ferrimagnetic and antiferromagnetic, respectively. The former is similar to the cos structure and the latter is similar to the sin (partial disorder) structure proposed in the antiferromagnetic Ising model on the triangular lattice [7]. Since the base $l^+_{0,Q}$ is invariant under the invariance groups of $l^+_{z,Q}$ and $l^-_{z,Q}$, $ASDW_1$ and $ASDW_2$ are accompanied by a CDW. The vector space $V'$ in table 2 shows that CDWs inevitably accompany a SDW solution. The spin structure of the PSDW (figure 2(*c*)) is usually called $V_2$ or 120° structure. The ground states of the classical antiferromagnetic Heisenberg or $XY$ spin models on the triangular lattice have this spin structure. The invariance group of PSDW(K) includes the elements which consist of space translations coupled with spin rotations.

**Table 1.** The maximal invariance groups of the SDW solution on the triangular lattice. $u_{2m}(C_{2m})$ and $u^{\pm}_{im}$ ($C^{\pm}_{im}$) are two-folded and $i$-folded spin (space) rotations around the axis $m$, respectively. The axes $m$ are shown in figure 1 and [9].

| SDW | Invariance group | $N$ |
|---|---|---|
| K ASDW$_1$ | $NA(e_x)M(e_y)$ | $L_3 \wedge D_6$ |
| ASDW$_2$ | $N(1+\{C_{21''} \mid 0\}u_{21''})A(e_x)M(e_y)$ | $L_3 \wedge D'_3$ |
| PSDW | $N(1+\{1 \mid t_a\}u^+_{3z}+\{1 \mid -t_a\}u^-_{3z}+\{C_2 \mid 0\}u_{21''}$ $+\{C_{2z} \mid -t_a\}u_{22''}+\{C_{2z} \mid t_a\}u_{23''})M(e_z)$ | $L_3 \wedge D'_3$ |
| M ASDW$_1$ | $N(1+\{1 \mid t_a\}u_{21''})A(e_x)M(e_y)$ | $L_2 \wedge D_2$ |
| ASDW$_2$ | $N(1+\{1 \mid t_b\}u_{21''})A(e_x)M(e_y)$ | $L_4 \wedge D_2$ |
| ASDW$_3$ | $NA(e_x)M(e_y)$ | $L_4 \wedge D_6$ |
| PSDW$_1$ | $N(1+\{C^+_{3z} \mid 0\}u^+_{3z}+\{C^-_{3z} \mid 0\}u^-_{3z}+\{C_{21'} \mid 0\}u_{21'}$ $+\{C_{22'} \mid 0\}u_{22'}+\{C_{23'} \mid 0\}u_{23'})M(e_z)$ | $L_4 \wedge C_2$ |
| PSDW$_2$ | $N(1+\{1 \mid t_a\}u_{2x}+\{1 \mid t_b\}u_{2x}+\{1 \mid t_a+t_b\}u_{2y}+\{C_{23'} \mid 0\}u_{2b}$ $+\{C_{23'} \mid t_a\}u_{2a}+\{C_{23'} \mid t_b\}u^+_{4z}+\{C_{23'} \mid t_a+t_b\}u^-_{4z})M(e_z)$ | $L_4 \wedge C_2$ |
| CSDW | $N(1+\{1 \mid t_a\}u_{2z}+\{1 \mid t_b\}u_{2x}+\{1 \mid t_a+t_b\}u_{2y}$ $+\{C^+_{3z} \mid 0\}u^+_{31}+\{C^+_{3z} \mid t_a\}u^+_{33}+\{C^+_{3z} \mid t_b\}u^+_{34}+\{C^+_{3z} \mid t_a+t_b\}u^+_{32}$ $+\{C^-_{3z} \mid 0\}u^-_{31}+\{C^-_{3z} \mid t_a\}u^-_{34}+\{C^-_{3z} \mid t_b\}u^-_{32}+\{C^-_{3z} \mid t_a+t_b\}u^-_{33}$ $+\{C_{21'} \mid 0\}u_{2f}t+\{C_{21'} \mid t_a\}u^-_{4x}t+\{C_{21'} \mid t_b\}u_{2d}t+\{C_{23'} \mid t_a+t_b\}u^+_{4x}t$ $+\{C_{22'} \mid 0\}u_{2e}t+\{C_{22'} \mid t_a\}u^+_{4y}t+\{C_{22'} \mid t_b\}u^-_{4y}t+\{C_{22'} \mid t_a+t_b\}u_{2c}t$ $+\{C_{23'} \mid 0\}u_{2b}t+\{C_{23'} \mid t_a\}u_{2a}t+\{C_{23'} \mid t_b\}u^+_{4z}t+\{C_{23'} \mid t_a+t_b\}u^-_{4z}t)$ | $L_4 \wedge C_2$ |

$L_3 = L(2t_a + t_b, t_a + 2t_b)$; $L_2 = L(2t_a, t_b)$; $L_4 = L(t_a, t_b)$; $D'_3 = \{1, C^+_3, C^-_3, C_{21'}, C_{22'}, C_{23'}\}$; $D_2 = \{1, C_2, C_{21''}, C_{21'}\}$; $M(e_j) = \{1, u(e_j\pi)t\}$; $A(e_j) = \{u(e_j, \theta), 0 \leqslant \theta \leqslant 2\pi\}$.

### 3.2. *SDWs characterized by points M*

The order parameter space characterized by point M ($M_1$, $M_2$ and $M_3$) is

$$V(\mathrm{M}) = [l^+_{iQ(m)},\ i = 0, x, y, z;\ m = 1, 2, 3] \tag{21a}$$

where

$$Q(1) = \tfrac{1}{2}G_a \qquad Q(2) = -\tfrac{1}{2}G_a + \tfrac{1}{2}G_b \qquad Q(3) = -\tfrac{1}{2}G_b. \tag{21b}$$

**Table 2.** The order parameter spaces for the SDWs characterized by points M and K. The name of each SDW corresponds to that in table 1 and figures 2 and 3. $V$ is the space characterizing the SDW and $V'$ is the one inevitably accompanying the $V$. $Q$ and $Q(m)$ are defined in the text. $e_{i'}$ and $e_{i''}$ are unit vectors directed to the $i'$ and $i''$ axes, respectively.

| | SDW | $V$ | $V'$ |
|---|---|---|---|
| K | $ASDW_1$ | $l^+_{xQ}$ | $l_{x\mathbf{0}}l^+_{0Q}$ |
| | $ASDW_2$ | $l^-_{xQ}$ | $l^+_{0Q}$ |
| | PSDW | $l^+_Q \cdot e_x - l^-_Q \cdot e_y = l^+_{xQ} - l^-_{yQ}$ [a] | — |
| M | $ASDW_1$ | $l_{xQ(1)}$ | — |
| | $ASDW_3$ | $l_{xQ(2)} + l_{xQ(3)}$ | $l_{0Q(1)}$ |
| | $ASDW_2$ | $\sum_{j=1}^{3} l_{xQ(j)}$ | $\sum_{j=1}^{3} l_{0Q(j)}$ |
| | $PSDW_1$ | $\sum_{j=1}^{3} l_{Q(j)} \cdot e_{j'}$ | $\sum_{j=1}^{3} l_{0Q(j)}$ |
| | | $= l_{yQ(1)} + (-\frac{\sqrt{3}}{2} l_{xQ(2)} - \frac{1}{2} l_{yQ(2)}) + (\frac{\sqrt{3}}{2} l_{xQ(3)} - \frac{1}{2} l_{yQ(3)})$ | |
| | $PSDW_2$ | $l_{xQ(1)} + l_{yQ(2)}$ | — |
| | CSDW | $l_{xQ(1)} + l_{yQ(2)} + l_{xQ(3)}$ | — |

[a] $l^{\pm}_q = (l^{\pm}_{xq}, l^{\pm}_{yq}, l^{\pm}_{zq})$.

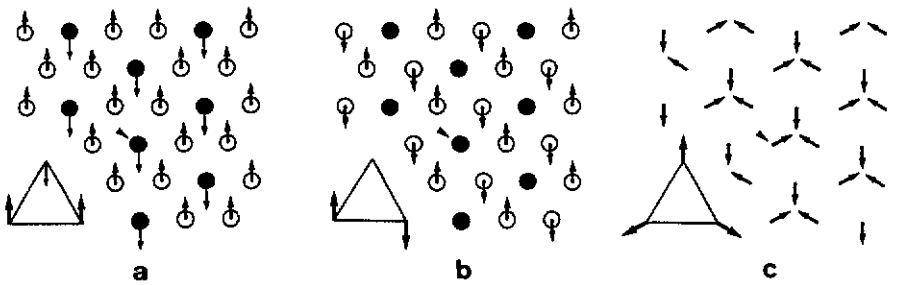


**Figure 2.** Schematic SDW patterns on the triangular lattice characterized by points K and K′ and their corresponding patterns on the molecule with $D_3$ symmetry: (*a*) $ASDW_1$, (*b*) $ASDW_2$, (*c*) PSDW. Full triangles indicate the centres of the invariance groups given in table 2. Open and full circles show different charge densities. The $xyz$ axes for the spins are the same as those shown in figure 1. The directions of the spins in the ASDW and PSDW states are perpendicular and parallel to the plane, respectively.

Any SDW characterized by M always has the spatial symmetry

$$G_{V(M)} = L_4 \wedge C_2 \tag{22a}$$

where

$$L_4 = L(2t_a, 2t_b) \qquad C_2 = \{1, C_{2z}\}. \tag{22b}$$

$G_{V(M)}$ is one of the normal subgroups of $\Gamma$. Since $\Gamma/G_{V(M)} \simeq T_d$, the classification of SDWs characterized by M is reduced to the classification in a molecule with $T_d$ symmetry [3, 4]. We list in tables 1 and 2 the order parameter spaces and their invariance groups which are found. In figure 3 we show their spin and charge density patterns on the triangular lattice with the corresponding patterns on the molecule with $T_d$ symmetry.

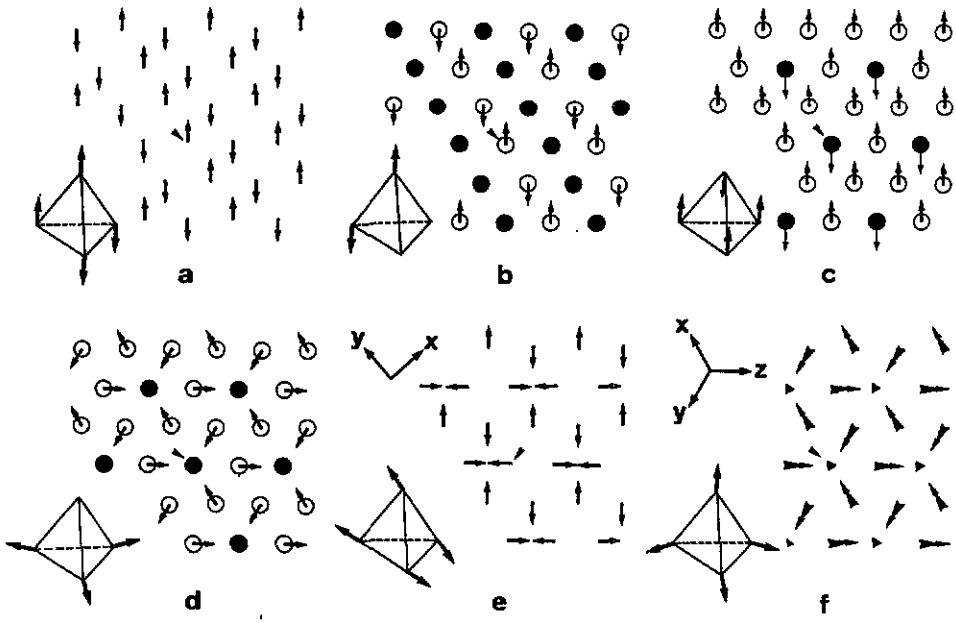


**Figure 3.** Schematic SDW patterns on the triangular lattice characterized by points $M_1$, $M_2$ and $M_3$ and their corresponding patterns on the molecule with the symmetry $T_d$: (*a*) $ASDW_1$, (*b*) $ASDW_2$, (*c*) $ASDW_3$, (*d*) $PSDW_1$, (*e*) $PSDW_2$ and (*f*) CSDW. The $xyz$ axes for spins are, except in (*e*) and (*f*), the same as those shown in figure 1. The $xyz$ axes in (*e*) and (*f*) are shown in the insets.

$ASDW_1$, $PSDW_2$ and CSDW are antiferromagnetic and all sites on them are equivalent. They are also characterized by one, two and three $q$ and can be called single-, double- and triple-$q$ states, respectively [8]. The other solutions are accompanied by CDWs. $ASDW_2$ and $PSDW_1$ are antiferromagnetic and $ASDW_3$ is ferrimagnetic.

From table 2 and equation (5), we can immediately get the $H_{MF}$. For example, $H_{MF}$ for $ASDW_1$(K) is

$$\sum_k t(k)\tilde{a}_k^\dagger \tilde{a}_k + X_0^z \sum_k \tilde{a}_k^\dagger \sigma_z \tilde{a}_k + X_Q^z \sum_k \tilde{a}_{k+Q/2}^\dagger \sigma_z \tilde{a}_{k-Q/2} + X_Q^0 \sum_k \tilde{a}_{k+Q/2}^\dagger \tilde{a}_{k-Q/2}. \tag{23}$$

The three order parameters $X_0^z$, $X_Q^z$ and $X_Q$ are determined by the SCF conditions given by equations (6) and (7).

In summary we have found out the possible SDWs on the triangular lattice which are characterized by points K and M. The results are listed in tables 1 and 2 and in figures 2 and 3. Our method naturally gives the mean-field Hamiltonian for each solution which includes a few order parameters determined by the SCF condition.

**Acknowledgments**

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