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The Relevant Operators for the Hubbard Hamiltonian with a magnetic field term

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Abstract

The Hubbard Hamiltonian and its variants/generalizations continue to dominate the theoretical modelling of important problems such as high temperature superconductivity. In this note we identify the set of relevant operators for the Hubbard Hamiltonian with a magnetic field term.

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I. INTRODUCTION

The Hubbard Hamiltonian [HH] and its extensions dominate the study of strongly correlated electrons systems and the insulator metal transition [1]. One of the attractive feature of the Hubbard Model is its simplicity. It is well known that in the HH the band electrons interact via a two-body repulsive Coulomb interaction; there are no phonons in this model and neither in general are attractive interactions incorporated. With these points in mind it is not surprising that the HH was mainly used to study magnetism. In contrast superconductivity was understood mainly in light of the BCS theory, namely as an instability of the vacuum [ground-state] arising from effectively attractive interactions between electron and phonons. However Anderson [2] suggested that the superconductivity in high T_c material could arise from purely repulsive interaction. The rationale of this suggestion is grounded in the observation that superconductivity in such materials arises from the doping of an otherwise insulating state. Thus following this suggestion the electronic properties in such a high T_c superconductor material close to a insulator-metal transition must be considered. In particular the one-dimensional HH is considered to be the most simple model which can account for the main properties of strongly correlated electron systems including the metal-insulator transition. Long range anti-ferromagnetic order at half-filling has been reported in the numerical studies of this model [3,4]. Away from half-filling this model has been studied in [5,6].

The Maximal Entropy Principle [MEP] is a useful tool to get the dynamical and thermodynamical descriptions. The main advantage of this formalism is to provide a definite prescription to determine the complete set of operators [i.e. relevant operators] related to the problem under considerations. An attractive feature of the relevant operators is that they are group theory based and hence once a Hamiltonian for a system can be written down, the task of identifying the relevant operators can proceed in principle. Relevant operators for a given physical system along with the Hamiltonian in essence describe the essential bare bones of the physical system. In a series of papers [7–9], the generalized time-dependent Jaynes-Cummings Hamiltonian in the context of Maximum Entropy Principle [MEP] and group theory based methods [10] was studied. In particular, in [7] the MEP formalism

was used to solve time-dependent N-level systems. A set of generalized Bloch equations, in terms of relevant operators was obtained and as an example the $N = 2$ case was solved. It was thus demonstrated in [7] that the dynamics and thermodynamics of a two-level system coupled to a classical field can be fully described in the framework of MEP and group theory based methods. Further in [8] a time-dependent generalization of the JCM was studied and by showing that the initial conditions of the operators are determined by the MEP density matrix the authors were able to demonstrate that inclusion of temperature turns the problem into a thermodynamical one. An exact solution was also presented in the time independent case. Finally in [9] more detailed analysis of the three set of relevant operators was given. These set of operators are related to each other by isomorphisms which allowed the authors to consider the case of mixed initial conditions. The mean values of the field's population, correlation functions and nth-order coherence functions are of interest and useful in several applications. The MEP formalism allows us to describe a Hamiltonian system in terms of those, and only those, quantum operators *relevant* to the problem at hand. Thus, this formalism is suitable to study the Hamiltonian given in [8,9]. In [8,9] the *population of each level and not their difference* is considered therefore the resulting Hamiltonian is called a *generalized* time-dependent JCH. Recently the relevant operators for the generalized time-dependent m-photon Jaynes-Cummings Hamiltonian were determined in [11].

The HH for different band-fillings is studied in the context of MEP by Aliga and Proto [12]. The HH with a magnetic field was considered by Alam and Proto [13] using MEP techniques. In the present note we incorporate a magnetic field term in HH and identify the relevant operators. The set of relevant operators and their evolution equations without the magnetic field term considered by Aliga and Proto has also been independently checked by us. Moreover by neglecting the magnetic field term we easily recover the case considered by Aliga and Proto which provides a check on our calculations. It is interesting to note that Essler et al. [14,15] have suggested an extended Hubbard model which contains the t-J model as a special case. In fact this model is a mixture of the Hubbard and the t-J model. The model of Essler et al. [14] contains a magnetic field term. On a one-dimensional lattice Essler et al. [14] present an exact solution to their model via Bethe ansatz. It is further claimed that by using η-pairing mechanism one can construct eigenstates of the

Hamiltonian with off-diagonal long-range order and that in the attractive case the exact ground state is superconducting in any numbers of dimensions. The model of Essler et al. [14,15] is motivated by high-T_c superconductivity and is expected to describe a system of strongly correlated electrons. The model of Essler et al. [14] possesses a huge symmetry group [for example it has eight supersymmetries] and it would be interesting to obtain the set of relevant operators corresponding to it.

The main purpose of this paper is to answer the question: Can we identify a set of relevant operators for the Hubbard Hamiltonian including a magnetic field term? The aims of this short note is to give such a set and the evolution equations for it. The layout of this paper is as follows. Section two contains discussion and definitions relevant to Hubbard Hamiltonian in the context of mean field method. In section three we recall some well-known results of the group theory based MEP formalism. In section four we give the relevant operators and the evolution equations for their expectation values in the context of the Hubbard Hamiltonian without and with an a magnetic field term present. Conclusions are given in the last section.

II. HUBBARD HAMILTONIAN AND THE MEAN FIELD METHOD

The Hubbard Hamiltonian can be written as

$$\hat{H} = -\tau' \sum_{<i,j>,\ \sigma} \hat{c}^{\dagger}_{i\sigma}\hat{c}_{j\sigma} + U\sum_{i} \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}. \tag{1}$$

τ' is the hopping parameter between the nearest neighbours, $\hat{c}^{\dagger}_{i\sigma}$ creates an electron with spin σ at site i, $\hat{c}_{i\sigma}$ destroys an electron with spin σ at site i, U is the on-site Coulomb interaction and $\hat{n}_{i\sigma} = \hat{c}^{\dagger}_{i\sigma}\hat{c}_{i\sigma}$ is the number operator for spin σ at site i.

A modified Hubbard Hamiltonian,

$$\hat{H}_1 = -\tau' \sum_{<i,j>,\ \sigma} \hat{c}^{\dagger}_{i\sigma}\hat{c}_{j\sigma} + U\sum_{i}[\hat{n}_{i\uparrow} - \frac{1}{2}][\hat{n}_{i\downarrow} - \frac{1}{2}]], \tag{2}$$

is also used by some authors [5,6]. One may rewrite $\hat{H}_1$ in terms of $\hat{H}$

$$\hat{H}_1 = -\tau' \sum_{<i,j>,\,\sigma} \hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma} + U\sum_i [\hat{n}_{i\uparrow}\hat{n}_{i\downarrow} - \frac{1}{2}(\hat{n}_{i\uparrow} + \hat{n}_{i\downarrow}) + \frac{1}{4}]$$
$$= H - \frac{U}{2}\sum_i [\hat{n}_{i\uparrow} + \hat{n}_{i\downarrow}] + \frac{1}{4}NU\hat{I}. \tag{3}$$

N in Eq. 3 is the number of sites. It is important to note that the Hamiltonians given in Eq. 1 and Eq. 3 cannot be considered as equivalent even when they lead to the same set of the relevant operators, since the g matrix [see Eq. 22 below] associated with the Hamiltonian in Eq. 1 is different from that which corresponds to the Hamiltonian in Eq. 3.

In order to get solvable model, in this note, we resort to the mean-field method. Our main approximation is to replace the product of operators in the hopping term by averages according the rule

$$\hat{A}\hat{B} =< \hat{A} > \hat{B} + \hat{A} < \hat{B} > - < \hat{A} >< \hat{B} > . \tag{4}$$

It is important to note that in contrast to [16] the mean-field approximation in our case,like [17], has been applied to the hopping term. In [16] the mean-field approximation is applied to the Coulomb term. In our approximation the Hamiltonian can be written in site-diagonal form, the sites being coupled only by the mean-field parameter Δ_σ, for the definition of Δ_σ, see Eq. 7 below.

In order to apply the above rule, viz Eq. 4 to the hopping term we rewrite the latter as

$$\sum_{<i,j>,\,\sigma} \hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma} = \hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma} + \hat{c}^\dagger_{j\sigma}\hat{c}_{i\sigma},$$
$$= [\hat{c}^\dagger_{i\sigma} + \hat{c}^\dagger_{j\sigma}][\hat{c}_{i\sigma} + \hat{c}_{j\sigma}] - \hat{n}_{i\sigma} - \hat{n}_{j\sigma}, \tag{5}$$

Applying the definition of the averaging procedure, viz Eq. 4 to the hopping term written as in Eq. 5 we obtain

$$\sum_{<i,j>,\,\sigma} \hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma} = \sum_\sigma \hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma} + \hat{c}^\dagger_{j\sigma}\hat{c}_{i\sigma},$$
$$\approx \sum_\sigma \Delta^*_\sigma < \hat{c}^\dagger_{i\sigma} + \hat{c}^\dagger_{j\sigma} > + \Delta_\sigma < \hat{c}_{i\sigma} + \hat{c}_{j\sigma} >$$
$$-| < \Delta_\sigma > |^2 I - \hat{n}_{i\sigma} - \hat{n}_{j\sigma}, \tag{6}$$

where we have used the definitions

$$\Delta_\sigma = < \hat{c}^\dagger_{i\sigma} + \hat{c}^\dagger_{j\sigma} >,$$
$$\Delta^*_\sigma = < \hat{c}_{i\sigma} + \hat{c}_{j\sigma} > . \tag{7}$$

Using the reduction given in Eq. 6 we may write the Hubbard Hamiltonian in Eq. 1 as

$$\hat{H} = \tau' \sum_\sigma \hat{n}_{i\sigma} + \hat{n}_{j\sigma} - \tau' \sum_\sigma \Delta_\sigma [\hat{c}_{i\sigma} + \hat{c}_{j\sigma}] - \tau' \sum_\sigma \Delta^*_\sigma [\hat{c}^\dagger_{i\sigma} + \hat{c}^\dagger_{j\sigma}]$$
$$+\tau' \sum_\sigma | < \Delta_\sigma > |^2 I + U \sum_i \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}. \tag{8}$$

Next we want to write the HH in terms of one site only to this end we observe that in one dimension [1-d] each site has two nearest neighbours, in 2-d each site as 4 nearest neighbours and so on. Denoting the number of nearest neighbours by m we define

$$\tau \stackrel{\text{def}}{=} m\tau',$$
$$|\Delta|^2 \stackrel{\text{def}}{=} \frac{|\Delta_\uparrow|^2 + |\Delta_\downarrow|^2}{2} \tag{9}$$

Using these definitions we may write the one-site equivalent of Eq. 8

$$\hat{H}_i = \tau \sum_\sigma \hat{n}_{i\sigma} - \tau \sum_\sigma \Delta_\sigma \hat{c}_{i\sigma} - \tau \sum_\sigma \Delta^*_\sigma \hat{c}^\dagger_{i\sigma}$$
$$+\tau |\Delta|^2 \hat{I} + U \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}. \tag{10}$$

Eq. 10 allows us to rewrite the Hamiltonian in Eq. 3 in the form

$$\hat{H}_{1i} = (\tau - \frac{U}{2}) \sum_\sigma \hat{n}_{i\sigma} - \tau \sum_\sigma \Delta_\sigma \hat{c}_{i\sigma} - \tau \sum_\sigma \Delta^*_\sigma \hat{c}^\dagger_{i\sigma}$$
$$+(\tau |\Delta|^2 + \frac{U}{4})\hat{I} + U \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}. \tag{11}$$

It is convenient to introduce a compact notation

$$\hat{H}_i = \alpha \hat{n}_i - \tau \hat{x}_i + \gamma \hat{I} + U \hat{r}_i, \tag{12}$$

where we have defined

$$\hat{n}_i \stackrel{\text{def}}{=} \hat{n}_{i\uparrow} + \hat{n}_{i\downarrow},$$
$$\hat{x}_i \stackrel{\text{def}}{=} \Delta^*_\uparrow \hat{c}^\dagger_{i\uparrow} + \Delta^*_\downarrow \hat{c}^\dagger_{i\downarrow} + \Delta_\uparrow \hat{c}_{i\uparrow} + \Delta_\downarrow \hat{c}_{i\downarrow},$$
$$\hat{r}_i \stackrel{\text{def}}{=} \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}. \tag{13}$$

$\hat{n}_i$ is the number of electrons at site i, $\hat{x}_i$ is the mean field hopping interaction between neighbouring sites and $\hat{r}_i$ measures the double occupancy probability or simply the number of pairs at the site i.

The Hamiltonian in Eq. 10 is a special case of the Hamiltonian form in Eq. 12 with the identifications $\alpha = \tau$ and $\gamma = \tau|\Delta|^2$. If we set $\alpha = \tau - \frac{U}{2}$ and $\gamma = \tau|\Delta|^2 + \frac{U}{4}$ in Eq. 12 we recover the Hamiltonian form given in Eq. 11.

The magnetic field can be readily accommodated by adding the term $h(\hat{n}_{i\uparrow} - \hat{n}_{i\downarrow})$ to the Hamiltonian form in Eq. 12, viz,

$$\hat{H}_i = \alpha\hat{n}_i - \tau\hat{x}_i + \gamma\hat{I} + U\hat{r}_i + h\hat{N}_i, \tag{14}$$

where we have defined

$$\hat{N}_i \stackrel{\text{def}}{=} \hat{n}_{i\uparrow} - \hat{n}_{i\downarrow}. \tag{15}$$

$\hat{n}_i$ and $\hat{N}_i$ respectively represent the symmetric and antisymmetric sums of the number operators for both types of spin. We define $|\tilde{\Delta}|^2$ in analogy with $|\Delta|^2$ as

$$\begin{aligned} |\tilde{\Delta}|^2 &\stackrel{\text{def}}{=} \frac{|\Delta_\uparrow|^2 - |\Delta_\downarrow|^2}{2}, \\ |\Delta_\uparrow|^2 &= |\Delta|^2 + \tilde{\Delta}|^2, \\ |\Delta_\downarrow|^2 &= |\Delta|^2 - \tilde{\Delta}|^2, \end{aligned} \tag{16}$$

where we have written $|\Delta_\uparrow|^2$ and $|\Delta_\downarrow|^2$ in terms of $|\Delta|^2$ and $|\tilde{\Delta}|^2$.

III. OUTLINE OF THE MEP FORMALISM

It is instructive to summarize the principal concepts of the MEP [7–9,18,19]. A summary of MEP formalism has been given in [11]. Here we again outline it for the benefit of the readers not familiar with [11].

Given the expectation values $<\hat{O}_j>$ of the operators $\hat{O}_j$, the statistical operator $\hat{\rho}(t)$ is defined by

$$\hat{\rho}(t) = \exp\left(-\lambda_0\hat{I} - \sum_{j=1}^{L}\lambda_j\hat{O}_j\right), \tag{17}$$

where L is a natural number or infinity, and the $L+1$ Lagrange multipliers λ_j, are determined to fulfill the set of constraints

$$<\hat{O}_j>= \mathrm{Tr}\,[\,\hat{\rho}(t)\,\hat{O}_j\,]\,, \qquad \mathrm{j} = 0,\,1,\,\ldots,\,\mathrm{L}\,, \tag{18}$$

($\hat{O}_0 = \hat{I}$ is the identity operator) and the normalization in order to maximize the entropy, defined (in units of the Boltzmann constant) by

$$S(\hat{\rho}) = -\mathrm{Tr}\,[\,\hat{\rho}\,\ln\hat{\rho}\,]\,. \tag{19}$$

Eq. 17 is a generalization of the more familiar density operator. For e.g. in open system, where we have Grand Canonical Ensemble there are two Lagrange multipliers, $\beta = \frac{1}{k_B T}$ and μ are present, and we write the density operator as [20]

$$\hat{\rho}(t) = \exp\left(\beta\Omega(T,V,\mu) - \beta\hat{H} + \beta\mu\hat{N}\right), \tag{20}$$

As is well-known the dynamics are governed by the time evolution of the statistical operator. The time evolution of the statistical operator is given by

$$i\hbar\frac{d\hat{\rho}}{dt} = [\,\hat{H}(t),\hat{\rho}(t)\,]\,. \tag{21}$$

The essence of the MEP formalism in conjunction with the group theory method is to find the relevant operators entering Eq. 17) so as to guarantee not only that S is maximum, but also is a constant of motion. Introducing the natural logarithm of Eq. 17 into Eq. 21) it can be easily verified that the **relevant operators** are those that close a semi-Lie algebra under commutation with the Hamiltonian $\hat{H}$, i.e.

$$[\,\hat{H}(t),\hat{O}_j\,] = i\hbar\sum_{i=0}^{L} g_{ij}(t)\hat{O}_i\,. \tag{22}$$

Thus the relevant operators may be defined as those satisfying the above equation. Equation 22) defines an $L \times L$ matrix G and constitutes the central requirement to be fulfilled by the operators entering in the density matrix. The Liouville Eq. 21 can be replaced by a set of coupled equations for the mean values of the relevant operators or the Lagrange multipliers as follows [21]:

$$\frac{d<\hat{O}_j>_t}{dt} = -\sum_{i=0}^{L} g_{ij} <\hat{O}_i> , \qquad \text{j} = 0, 1, \ldots, \text{L} , \tag{23}$$

$$\frac{d\lambda_j}{dt} = \sum_{i=0}^{L} \lambda_i g_{ji}, \qquad \text{j} = 0, 1, \ldots, \text{L}. \tag{24}$$

In the MEP formalism, the mean value of the operators and the Lagrange multipliers belongs to dual spaces which are related by [19]

$$<\hat{O}_j> = -\frac{\partial \lambda_0}{\partial \lambda_j}. \tag{25}$$

IV. THE RELEVANT OPERATORS AND EVOLUTION EQUATIONS FOR THE HUBBARD HAMILTONIAN WITH A MAGNETIC FIELD TERM

For notational convenience we now drop the subscript i, in all formulae from now on. The set of relevant operators for the HH with a magnetic field term is more than twice the number of relevant operators without it. It is thus informative and useful to give the set of the relevant operators for the HH without the magnetic field. To this end we first consider the Hamiltonian form given in Eq. 12. A little work shows that number operator n does not commute with the Hamiltonian, after some calculation we obtain

$$\left[\hat{H}, \hat{n}\right] = -i\tau\hat{p}, \tag{26}$$

where $\hat{p}$ is given by

$$\hat{p} \stackrel{\text{def}}{=} i(\Delta_\uparrow^* \hat{c}_\uparrow^\dagger + \Delta_\downarrow^* \hat{c}_\downarrow^\dagger - \Delta_\uparrow \hat{c}_\uparrow - \Delta_\downarrow \hat{c}_\downarrow). \tag{27}$$

$\hat{p}$ is the mean field electron's current. Thus so far we have introduced three operators besides the Hamiltonian, namely $\hat{n}$, $\hat{x}$ and $\hat{p}$ belonging to the relevant operator set. To determine the whole set we must proceed by finding the commutation relations of all the operators with the Hamiltonian until we get the complete set. The commutation relation of $\hat{x}$ with the Hamiltonian yields

$$\left[\hat{H}, \hat{x}\right] = -i\alpha\hat{p} - iU\hat{l}_-, \tag{28}$$

where $\hat{l}_-$ is the mean field pair's current and can be written as

$$\hat{l}_- \stackrel{\text{def}}{=} i([\Delta_\uparrow^* \hat{c}_\uparrow^\dagger - \Delta_\uparrow \hat{c}_\uparrow]\hat{n}_\downarrow + \hat{n}_\uparrow[\Delta_\downarrow^* \hat{c}_\downarrow^\dagger - \Delta_\downarrow \hat{c}_\downarrow]). \tag{29}$$

We note that since the c's are fermion operators they anticommute, hence as a consequence of this $\hat{c}_\downarrow$ commutes with $\hat{n}_\uparrow$, viz, explicitly, $\hat{c}_\downarrow \hat{n}_\uparrow = \hat{c}_\downarrow \hat{c}_\uparrow^\dagger \hat{c}_\uparrow = -\hat{c}_\uparrow^\dagger \hat{c}_\downarrow \hat{c}_\uparrow = \hat{c}_\uparrow^\dagger \hat{c}_\uparrow \hat{c}_\downarrow = \hat{n}_\uparrow \hat{c}_\downarrow$.

The commutation relation of $\hat{p}$ with the Hamiltonian introduces yet another two operators $\hat{l}_+$ and $\hat{\omega}_1$. $\hat{l}_+$ represents the mean field pair's interaction.

$$\left[\hat{H}, \hat{p}\right] = i\alpha\hat{x} + iU\hat{l}_+ - i4\tau\hat{\omega}_1, \tag{30}$$

where $\hat{l}_+$ and $\hat{\omega}_1$ are defined as

$$\begin{aligned} \hat{l}_+ &\stackrel{\text{def}}{=} ([\Delta_\uparrow^* \hat{c}_\uparrow^\dagger + \Delta_\uparrow \hat{c}_\uparrow]\hat{n}_\downarrow + \hat{n}_\uparrow[\Delta_\downarrow^* \hat{c}_\downarrow^\dagger + \Delta_\downarrow \hat{c}_\downarrow]), \\ \hat{\omega}_1 &\stackrel{\text{def}}{=} \frac{|\Delta_\uparrow|^2}{2}\left[\hat{c}_\uparrow, \hat{c}_\uparrow^\dagger\right] + \frac{|\Delta_\downarrow|^2}{2}\left[\hat{c}_\downarrow, \hat{c}_\downarrow^\dagger\right] + \Delta_\downarrow \Delta_\uparrow^* \hat{c}_\downarrow \hat{c}_\uparrow^\dagger + \Delta_\uparrow \Delta_\downarrow^* \hat{c}_\uparrow \hat{c}_\downarrow^\dagger \end{aligned} \tag{31}$$

The commutator of $\hat{l}_-$ with the Hamiltonian yields the final relevant operator of the present set, namely $\hat{\omega}_2$,

$$\left[\hat{H}, \hat{l}_-\right] = i(\alpha + U)\hat{l}_+ - i\tau\hat{\omega}_2, \tag{32}$$

$\hat{\omega}_2$ is given by the following expression

$$\hat{\omega}_2 \stackrel{\text{def}}{=} 2(\frac{|\Delta_\uparrow|^2}{2}\left[\hat{c}_\uparrow, \hat{c}_\uparrow^\dagger\right]\hat{n}_\downarrow + \frac{|\Delta_\downarrow|^2}{2}\hat{n}_\uparrow\left[\hat{c}_\downarrow, \hat{c}_\downarrow^\dagger\right] + \Delta_\downarrow\Delta_\uparrow^*\hat{c}_\downarrow\hat{c}_\uparrow^\dagger + \Delta_\uparrow\Delta_\downarrow^*\hat{c}_\uparrow\hat{c}_\downarrow^\dagger). \tag{33}$$

The three remaining commutation relations required to close the algebra can be expressed entirely in terms of operators already defined. These read

$$\begin{aligned}\left[\hat{H}, \hat{l}_+\right] &= -i(\alpha + U)\hat{l}_-,\\ \left[\hat{H}, \hat{\omega}_1\right] &= i2|\Delta|^2\tau\hat{p},\\ \left[\hat{H}, \hat{\omega}_2\right] &= i8|\Delta|^2\tau\hat{l}_-.\end{aligned} \tag{34}$$

Thus we have a set of seven relevant operators, namely $\hat{n}$, $\hat{x}$, $\hat{p}$, $\hat{l}_-$, $\hat{l}_+$, $\hat{\omega}_1$ and $\hat{\omega}_2$ which close the algebra as is clear from Eqs. 26, 28, 30, 32 and 34. Using Eqs. 22 and 23, the evolution equations for the present set of relevant operators immediately follow and are

$$\frac{d<\hat{n}>_t}{dt} = \frac{\tau}{\hbar}<\hat{p}>_t, \tag{35}$$

$$\frac{d<\hat{x}>_t}{dt} = \frac{\alpha}{\hbar}<\hat{p}>_t + \frac{U}{\hbar}<\hat{l}_->_t, \tag{36}$$

$$\frac{d<\hat{p}>_t}{dt} = -\frac{\alpha}{\hbar}<\hat{x}>_t - \frac{U}{\hbar}<\hat{l}_+>_t + \frac{4\tau}{\hbar}<\hat{\omega}_1>_t, \tag{37}$$

$$\frac{d<\hat{l}_+>_t}{dt} = \frac{(\alpha+U)}{\hbar}<\hat{l}_->_t, \tag{38}$$

$$\frac{d<\hat{l}_->_t}{dt} = -\frac{(\alpha+U)}{\hbar}<\hat{l}_->_t + \frac{\tau}{\hbar}<\hat{\omega}_2>_t, \tag{39}$$

$$\frac{d<\hat{\omega}_1>_t}{dt} = -\frac{2|\Delta|^2\tau}{\hbar}<\hat{p}>_t, \tag{40}$$

$$\frac{d<\hat{\omega}_2>_t}{dt} = -\frac{8|\Delta|^2\tau}{\hbar}<\hat{l}_->_t, \tag{41}$$

$$\tag{42}$$

The magnetic field term modifies the HH by a simple looking term, viz $\hat{N}$, as is immediately apparent from the Hamiltonian form in Eq. 14. We observe that $\hat{N}$ differs by a negative sign between the number operators of spin-up and spin-down states from $\hat{n}$. This observation leads us to expect that like $\hat{n}$, $\hat{N}$ when commuted with the Hamiltonian will lead to a set of relevant operators parallel to the ones obtained in case of $\hat{n}$.

$$\left[\hat{H}, \hat{N}\right] = -i\tau\hat{P}, \tag{43}$$

where $\hat{P}$ is given by

$$\hat{P} \stackrel{\text{def}}{=} i(\Delta_\uparrow^* \hat{c}_\uparrow^\dagger - \Delta_\downarrow^* \hat{c}_\downarrow^\dagger - \Delta_\uparrow \hat{c}_\uparrow + \Delta_\downarrow \hat{c}_\downarrow). \tag{44}$$

$$\left[\hat{H}, \hat{X}\right] = -i\alpha\hat{P} - iU\hat{L}_- - ih\hat{p} + i4\tau\hat{\Omega}_1 \tag{45}$$

where $\hat{X}$, $\hat{L}_-$, $\hat{\Omega}_1$ are given by

$$\begin{aligned}
\hat{X} &\stackrel{\text{def}}{=} \Delta_\uparrow^* \hat{c}_\uparrow^\dagger - \Delta_\downarrow^* \hat{c}_\downarrow^\dagger + \Delta_\uparrow \hat{c}_\uparrow - \Delta_\downarrow \hat{c}_\downarrow, \\
\hat{L}_- &\stackrel{\text{def}}{=} i([\Delta_\uparrow^* \hat{c}_\uparrow^\dagger - \Delta_\uparrow \hat{c}_\uparrow]\hat{n}_\downarrow - \hat{n}_\uparrow[\Delta_\downarrow^* \hat{c}_\downarrow^\dagger - \Delta_\downarrow \hat{c}_\downarrow]), \\
\hat{\Omega}_1 &\stackrel{\text{def}}{=} i(\Delta_\uparrow^* \Delta_\downarrow^* \hat{c}_\uparrow^\dagger \hat{c}_\downarrow^\dagger + \Delta_\uparrow \Delta_\downarrow \hat{c}_\uparrow \hat{c}_\downarrow + \Delta_\uparrow \Delta_\downarrow^* \hat{c}_\uparrow \hat{c}_\downarrow^\dagger + \Delta_\uparrow^* \Delta_\downarrow \hat{c}_\uparrow^\dagger \hat{c}_\downarrow).
\end{aligned} \tag{46}$$

$$\left[\hat{H}, \hat{P}\right] = i\alpha\hat{X} + iU\hat{L}_+ + ih\hat{x} - i4\tau\hat{\Omega}_2, \tag{47}$$

where $\hat{L}_+$, $\hat{\Omega}_2$ read

$$\begin{aligned}
\hat{L}_+ &\stackrel{\text{def}}{=} ([\Delta_\uparrow^* \hat{c}_\uparrow^\dagger + \Delta_\uparrow \hat{c}_\uparrow]\hat{n}_\downarrow - \hat{n}_\uparrow[\Delta_\downarrow^* \hat{c}_\downarrow^\dagger + \Delta_\downarrow \hat{c}_\downarrow]), \\
\hat{\Omega}_2 &\stackrel{\text{def}}{=} (-\frac{|\Delta_\uparrow|^2}{2}\left[\hat{c}_\uparrow, \hat{c}_\uparrow^\dagger\right] + \frac{|\Delta_\downarrow|^2}{2}\left[\hat{c}_\downarrow, \hat{c}_\downarrow^\dagger\right] + \Delta_\uparrow^* \Delta_\downarrow^* \hat{c}_\uparrow^\dagger \hat{c}_\downarrow^\dagger + \Delta_\downarrow \Delta_\uparrow \hat{c}_\downarrow \hat{c}_\uparrow).
\end{aligned} \tag{48}$$

The commutators of $\hat{L}_+$ and $\hat{L}_-$ with the Hamiltonian are

$$\left[\hat{H}, \hat{L}_+\right] = -i(\alpha + U)\hat{L}_- - ih\hat{l}_- - i2\tau\hat{\Omega}_1, \tag{49}$$

and

$$\left[\hat{H}, \hat{L}_-\right] = i(\alpha + U)\hat{L}_+ + ih\hat{l}_+ + i2\tau\hat{\Omega}_2. \tag{50}$$

The commutators of $\hat{n}$, $\hat{x}$, $\hat{p}$, with the Hamiltonian in presence of magnetic field are

$$\begin{aligned}
\left[\hat{H}, \hat{n}\right] &= -i\tau\hat{p}, \\
\left[\hat{H}, \hat{x}\right] &= -i\alpha\hat{p} - iU\hat{l}_- - ih\hat{P}, \\
\left[\hat{H}, \hat{p}\right] &= i\alpha\hat{x} + iU\hat{l}_+ - i4\tau\hat{\omega}_1 + ih\hat{X}, \\
\left[\hat{H}, \hat{l}_+\right] &= -i(\alpha + U)\hat{l}_- - ih\hat{L}_-, \\
\left[\hat{H}, \hat{l}_-\right] &= i(\alpha + U)\hat{l}_+ - i\tau\hat{\omega}_2 + ih\hat{L}_+, \\
\left[\hat{H}, \hat{\omega}_1\right] &= i2|\Delta|^2\tau\hat{p} - i2h\hat{\Omega}_3, \\
\left[\hat{H}, \hat{\omega}_2\right] &= i8|\Delta|^2\tau\hat{l}_- - i4h\hat{\Omega}_3.
\end{aligned} \tag{51}$$

If we set h to zero we recover the equations obtained before, which provides a check on our calculations. Ω_3 and Ω_4 are defined as

$$\begin{aligned}
\hat{\Omega}_3 &\stackrel{\text{def}}{=} i(\Delta_\downarrow^*\Delta_\uparrow\hat{c}_\downarrow^\dagger\hat{c}_\uparrow + \Delta_\downarrow\Delta_\uparrow^*\hat{c}_\downarrow\hat{c}_\uparrow^\dagger), \\
\hat{\Omega}_4 &\stackrel{\text{def}}{=} \Delta_\downarrow^*\Delta_\uparrow\hat{c}_\downarrow^\dagger\hat{c}_\uparrow - \Delta_\downarrow\Delta_\uparrow^*\hat{c}_\downarrow\hat{c}_\uparrow^\dagger.
\end{aligned} \tag{52}$$

In addition we define two more operators Ω_5 and Ω_6

$$\begin{aligned}
\hat{\Omega}_5 &\stackrel{\text{def}}{=} \Delta_\uparrow^*\Delta_\downarrow^*\hat{c}_\uparrow^\dagger\hat{c}_\downarrow^\dagger + \Delta_\downarrow\Delta_\uparrow\hat{c}_\downarrow\hat{c}_\uparrow, \\
\hat{\Omega}_6 &\stackrel{\text{def}}{=} i(\Delta_\uparrow^*\Delta_\downarrow^*\hat{c}_\uparrow^\dagger\hat{c}_\downarrow^\dagger - \Delta_\downarrow\Delta_\uparrow\hat{c}_\downarrow\hat{c}_\uparrow).
\end{aligned} \tag{53}$$

It is clear from the definitions of $\hat{\Omega}_1$, $\hat{\Omega}_3$ and $\hat{\Omega}_6$ given respectively in 46, 52 and 53 that

$$\hat{\Omega}_6 = \hat{\Omega}_1 + \hat{\Omega}_3. \tag{54}$$

Eq. 54 provides a check on our calculation since it implies that once we have independently calculated the time-evolution equations for $\hat{\Omega}_6$, $\hat{\Omega}_1$, and $\hat{\Omega}_3$ they must obey the relation

$$\frac{d<\hat{\Omega}_6>_t}{dt} = \frac{d<\hat{\Omega}_1>_t}{dt} + \frac{d<\hat{\Omega}_3>_t}{dt}. \tag{55}$$

Similarly it follows from definitions of $\hat{\Omega}_2$ [see 48], $\hat{\Omega}_5$ [see 53] and the definitions of $\hat{n}$ and $\hat{N}$ that

$$\hat{\Omega}_5 = \hat{\Omega}_2 + |\tilde{\Delta}|^2 \hat{I} - |\tilde{\Delta}|^2 \hat{n} - |\Delta|^2 \hat{N} \tag{56}$$

which implies that

$$\frac{d<\hat{\Omega}_5>_t}{dt} = \frac{d<\hat{\Omega}_2>_t}{dt} - |\tilde{\Delta}|^2 \frac{d<\hat{n}>_t}{dt} - |\tilde{\Delta}|^2 \frac{d<\hat{N}>_t}{dt}. \tag{57}$$

The commutators of $\hat{\Omega}_1$ through $\hat{\Omega}_6$ with the Hamiltonian are obtained after some calculation and may be displayed as

$$\begin{aligned}
\left[\hat{H}, \hat{\Omega}_1\right] &= i(2\alpha + U)\Omega_5 - i\ 2\ \tau[|\tilde{\Delta}|^2 \hat{x} - |\Delta|^2 \hat{X}] + i\ 2\ h\ \Omega_4, \\
\left[\hat{H}, \hat{\Omega}_2\right] &= -i(2\alpha + U)\Omega_6 - 2i\tau|\Delta|^2 \hat{P}, \\
\left[\hat{H}, \hat{\Omega}_3\right] &= i\tau|\tilde{\Delta}|^2 \hat{x} - i\tau|\Delta|^2 \hat{X} - i2h\Omega_4, \\
\left[\hat{H}, \hat{\Omega}_4\right] &= i\tau|\Delta|^2 \hat{p} - i\tau|\tilde{\Delta}|^2 \hat{P} - i2h\Omega_3, \\
\left[\hat{H}, \hat{\Omega}_5\right] &= -i(2\alpha + U)\Omega_6 - i\tau|\Delta|^2 \hat{P} - i\tau|\tilde{\Delta}|^2 \hat{p}, \\
\left[\hat{H}, \hat{\Omega}_6\right] &= i(2\alpha + U)\Omega_5 - i\tau|\tilde{\Delta}|^2 \hat{x} + i\tau|\Delta|^2 \hat{X}.
\end{aligned} \tag{58}$$

It follows from the above discussion that we have a set of eighteen relevant operators in the presence of the external magnetic field, namely $\hat{n}$, $\hat{x}$, $\hat{p}$, $\hat{l}_-$, $\hat{l}_+$, $\hat{\omega}_1$, $\hat{\omega}_2$, $\hat{N}$, $\hat{X}$, $\hat{P}$, $\hat{L}_-$, $\hat{L}_+$, $\hat{\Omega}_1$, $\hat{\Omega}_2$, $\hat{\Omega}_3$, $\hat{\Omega}_4$, $\hat{\Omega}_5$, and $\hat{\Omega}_6$ which close the algebra as is clear from Eqs. 26, 28, 30, 32, 34, 43, 45, 47, 50, 49 and 58. However not all of the operators are independent as is clear from the relations given in Eqs. 54 and 56. Using Eqs. 22 and 23, the evolution equations for the present set of relevant operators can be written as

$$\frac{d<\hat{n}>_t}{dt} = \frac{\tau}{\hbar} <\hat{p}>_t, \tag{59}$$

$$\frac{d<\hat{x}>_t}{dt} = \frac{\alpha}{\hbar} <\hat{p}>_t + \frac{U}{\hbar} <\hat{l}_->_t + \frac{h}{\hbar} <\hat{P}>_t, \tag{60}$$

$$\frac{d<\hat{p}>_t}{dt} = -\frac{\alpha}{\hbar} <\hat{x}>_t - \frac{U}{\hbar} <\hat{l}_+>_t + \frac{4\tau}{\hbar} <\hat{\omega}_1>_t - \frac{h}{\hbar} <\hat{X}>_t, \tag{61}$$

$$\frac{d<\hat{l}_+>_t}{dt} = \frac{(\alpha+U)}{\hbar}<\hat{l}_->_t + \frac{h}{\hbar}<\hat{L}_->_t, \tag{62}$$

$$\frac{d<\hat{l}_->_t}{dt} = -\frac{(\alpha+U)}{\hbar}<\hat{l}_->_t + \frac{\tau}{\hbar}<\hat{\omega}_2>_t - \frac{h}{\hbar}<\hat{L}_+>_t, \tag{63}$$

$$\frac{d<\hat{\omega}_1>_t}{dt} = -\frac{2|\Delta|^2\tau}{\hbar}<\hat{p}>_t + 2\frac{h}{\hbar}<\hat{\Omega}_3>_t, \tag{64}$$

$$\frac{d<\hat{\omega}_2>_t}{dt} = -\frac{8|\Delta|^2\tau}{\hbar}<\hat{l}_->_t + 4\frac{h}{\hbar}<\hat{\Omega}_3>_t, \tag{65}$$

$$\frac{d<\hat{N}>_t}{dt} = \frac{\tau}{\hbar}<\hat{P}>_t, \tag{66}$$

$$\frac{d<\hat{X}>_t}{dt} = \frac{\alpha}{\hbar}<\hat{P}>_t + \frac{U}{\hbar}<\hat{L}_->_t + \frac{h}{\hbar}<\hat{p}>_t - 4\frac{\tau}{\hbar}<\hat{\Omega}_1>_t, \tag{67}$$

$$\frac{d<\hat{P}>_t}{dt} = -\frac{\alpha}{\hbar}<\hat{X}>_t - \frac{U}{\hbar}<\hat{L}_+>_t - \frac{h}{\hbar}<\hat{x}>_t + 4\frac{\tau}{\hbar}<\hat{\Omega}_2>_t, \tag{68}$$

$$\frac{d<\hat{L}_+>_t}{dt} = \frac{(\alpha+U)}{\hbar}<\hat{L}_->_t + \frac{h}{\hbar}<\hat{l}_->_t + 2\frac{\tau}{\hbar}<\hat{\Omega}_1>_t, \tag{69}$$

$$\frac{d<\hat{L}_->_t}{dt} = -\frac{(\alpha+U)}{\hbar}<\hat{L}_+>_t - \frac{h}{\hbar}<\hat{l}_+>_t - 2\frac{\tau}{\hbar}<\hat{\Omega}_2>_t, \tag{70}$$

$$\frac{d<\hat{\Omega}_1>_t}{dt} = -\frac{(2\alpha+U)}{\hbar}<\hat{\Omega}_5>_t - 2\frac{h}{\hbar}<\hat{\Omega}_4>_t + 2\frac{\tau}{\hbar}[|\tilde{\Delta}|^2<\hat{x}>_t - |\Delta|^2<\hat{X}>_t], \tag{71}$$

$$\frac{d<\hat{\Omega}_2>_t}{dt} = +\frac{(2\alpha+U)}{\hbar}<\hat{\Omega}_6>_t + 2\frac{\tau}{\hbar}|\Delta|^2<\hat{P}>_t, \tag{72}$$

$$\frac{d<\hat{\Omega}_3>_t}{dt} = -\frac{\tau}{\hbar}|\tilde{\Delta}|^2<\hat{x}>_t + \frac{\tau}{\hbar}|\Delta|^2<\hat{X}>_t + 2\frac{h}{\hbar}<\Omega_4>_t, \tag{73}$$

$$\frac{d<\hat{\Omega}_4>_t}{dt} = -\frac{\tau}{\hbar}|\Delta|^2<\hat{p}>_t + \frac{\tau}{\hbar}|\tilde{\Delta}|^2<\hat{P}>_t + 2\frac{h}{\hbar}<\Omega_3>_t, \tag{74}$$

$$\frac{d<\hat{\Omega}_5>_t}{dt} = +\frac{(2\alpha+U)}{\hbar}<\Omega_6>_t - \frac{\tau}{\hbar}|\tilde{\Delta}|^2<\hat{p}>_t + \frac{\tau}{\hbar}|\Delta|^2<\hat{P}>_t, \tag{75}$$

$$\frac{d<\hat{\Omega}_6>_t}{dt} = -\frac{(2\alpha+U)}{\hbar}<\Omega_5>_t + \frac{\tau}{\hbar}|\tilde{\Delta}|^2<\hat{x}>_t - \frac{\tau}{\hbar}|\Delta|^2<\hat{X}>_t, \tag{76}$$

$$\tag{77}$$

To check the identity given in 55 we add Eqs. 71 and 73 and see if the sum of these two equations agrees with Eq. 76. We can immediately see that indeed this is the case. Likewise using Eqs. 59, 66, 72 and 75 we can see that the relation given in Eq. 57 holds. Thus we have an independent check of our stated relations.

The following remark is in order in context of future outlook. The MEP formalism is limited to the mean-field approach. However the group theory based approach of identifying the set of operators which close the partial Lie algebra under commutation with the Hamiltonian, is quite general. It is thus tempting to go beyond the mean-field formalism and use the set of relevant operators and their evolution equations to develop a technique which can take into account the quantum fluctuations.

V. CONCLUSIONS

We have given the set of relevant operators and the corresponding temporal evolution equations for the Hubbard Hamiltonian in the mean field approximation in the context of the maximal entropy formalism. The mean field approximation has been applied to the hopping term in the Hubbard term. As intuitively expected the inclusion of the external magnetic field leads to much larger set of the relevant operators than present in the case where the magnetic field is absent.

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