Semi-fermionic representation of SU($N$) Hamiltonians

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Abstract. We represent the generators of the SU($N$) algebra as bilinear combinations of Fermi operators with imaginary chemical potential. The distribution function, consisting of a minimal set of discrete imaginary chemical potentials, is introduced to satisfy the local constraints. This representation leads to the conventional temperature diagram technique with standard Feynman codex, except that the Matsubara frequencies are determined by neither integer nor half-integer numbers. The real-time Schwinger-Keldysh formalism is formulated in the framework of complex equilibrium distribution functions for auxiliary semi-fermionic fields. We discuss the continuous large $N$ and SU(2) large spin limits. We illustrate the application of this technique for magnetic and spin-liquid states of the Heisenberg model.

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Several approaches have been proposed for the description of spin systems in statistical physics. Methods of functional integration based on various representation of spin operators such as Fermi, Bose, Majorana, supersymmetric or Hubbard operators [1,2,3,4,5,6,7,8,9,10,11] have been applied to many problems involving quantum spins and pseudospins [2,12,13,14,15,16,17,18,19,20,21,22,23]. The difficulty with the representation of spin operators is connected with the fact that spins possess neither Fermi nor Bose statistics. The commutation relations for spins are determined by the SU(2) algebra, leading to the absence of a Wick theorem for SU(2) generators. The Gaudin [24] theorem existing instead makes it impossible to construct a simple diagram technique directly for spin operators. To resolve this problem, various representations [2,12,13,14,15,16,17,18,19,20,21,22,23] have been introduced. Nevertheless, the representation of spins as a bilinear combination of Fermi/Bose operators enlarges the dimensionality of Hilbert space where these operators act. Thus, the spurious (unphysical) states should be excluded from the consideration resulting in a constraint requirement. Basically, different representations cure the constraint problem in a different way. Nevertheless, the usual price for simplicity is the replacement of the local constraint on each point containing the spins by a so-called global constraint, so that the restriction is fulfilled only in the average over all sites. It is known that such a replacement results in uncontrollable approximations for quantum spins (especially in low dimensions). Although the use of a global constraint is questionable for SU(2) systems, it becomes more reasonable for higher SU($N$) groups, especially in the "large $N$ limit". The corresponding approach is known as "$1/N$ expansion" [14,15,18,19,20,21] successfully describing the strong coupling limits of the Kondo impurity [2], Anderson lattice [14,15,16,17,18,19,20,21] and Hubbard [16] models and also SU($N$) Heisenberg antiferromagnets on a square lattice [14,15,18,19,20,21] shedding light on the mechanism of high $T_c$ superconductivity in cuprate compounds. Although SU($N = 2$) models are of primary physical interest, the SU($N 
eq 2$) models can be considered as "approximate models" where an "exact solution" can be gained in contrast to "exact models" where the "approximate solution" is hard to obtain [20,21]. The simplification arises due to expansion in the inverse number of "flavors" $1/N$, making it possible to start with mean-field solution and systematically find corrections to it.

The goal of this paper is to consider a semi-fermionic representation for SU($N$) generators for arbitrary (not necessary large) $N$, applying a different idea of constraint realization. This idea is known as Popov-Fedotov [25] representation being initially proposed for $S = 1/2$ and $S = 1$ spins. Based on an exact representation of spin operators as fermions with imaginary chemical potential, this representation resulted in the conventional Feynman temperature diagram technique, nevertheless providing a rigorous treatment of the local constraint. [21,25,32,33] In this paper we give a generalization of this method to SU($N$) and we also construct the real-time formalism for the semi-fermionic spin representation.

SU($N$) algebra is determined by the generators obeying the following commutational relations:

$$[\hat{S}^\alpha_{\alpha,i}, \hat{S}^\beta_{\beta,j}] = \delta_{ij}(\delta^\alpha_{\alpha} \hat{S}^\beta_{\beta,i} - \delta^\beta_{\beta} \hat{S}^\alpha_{\alpha,j})$$

(1)

where $\alpha, \beta = 1, ..., N$. We adopt the definition of the Cartan algebra [32] of the SU($N$) group $\{H_{ij}\} = S_{ij}$ similar
Fig. 1. Rectangular Young tableau to denote a $\text{SU}(N)$ representation (a), single column tableau corresponding to $n_c = 1$ (b) and single row tableau standing for spin $S = n_c/2$ representation of $\text{SU}(2)$ group (c).

To the one used in [17], noting that the diagonal generators $S^a_\alpha$ are not traceless. To ensure a vanishing trace, the diagonal generators should only appear in combinations

$$\sum_{\alpha=1}^N s_\alpha S^a_\alpha \quad \text{with} \quad \sum_{\alpha=1}^N s_\alpha = 0$$

which effectively reduces the number of independent diagonal generators to $N-1$ and the total number of $\text{SU}(N)$ generators to $N^2 - 1$.

For $\text{SU}(2)$ one recognizes the usual spin operators

$$S^1_1 = S^+, \quad S^1_2 = S^- \quad \text{and} \quad S^2_1 - S^1_2 = 2S^z$$

with the usual commutation relations \[2\] and the Pauli matrices as generators of the $\text{SU}(2)$ group. We shall not confine ourself to some special type of Hamiltonian. Nevertheless, it’s worthwhile to mention that the $\text{SU}(N)$ generalization of the Heisenberg model is given by the following expression \[17, 20, 21\]

$$H = \frac{J}{N} \sum_{<\alpha, \beta>} \sum_{\alpha, \beta} \hat{S}_\beta^\alpha(i) \hat{S}_\beta(j)$$

On each site, there may exist many particles, whose symmetry properties define a specific representation of $\text{SU}(N)$. The most transparent way to visualize an irreducible $\text{SU}(N)$ representation are Young tableaux \[34, 35\]. Instead of the general Young tableau, specified by $N-1$ integers, for example the lengths of the rows, we restrict us for the main part of the paper to rectangular tableaux, with $1 \leq m \leq N$ rows and $n_c \geq 1$ columns, illustrated in Fig. 1.

The familiar spin is given by $N = 2, m = 1, n_c = 2S$, so the Young tableau contains one row of $2S$ length, with only one box for $S = 1/2$. Also of special importance are the tableaux with $n_c = 1$, giving the $N - 1$ fundamental representations of $\text{SU}(N)$.

The $\hat{S}_\beta^\alpha$ generator may be written as biquadratic form in terms of Schwinger boson operators \[22, 33\]:

$$\hat{S}_\beta^\alpha = b_{a\beta}^\dagger b^a \quad (5)$$

and a constraint as follows

$$\sum_{\alpha=1}^N b_{a\beta}^\dagger b^a \alpha \delta^\alpha_\beta n_c = m$$

where $p = 1, ..., m$ is the number of "colors".

The equivalent fermionic representation of the generators of $\text{SU}(N)$ \[17\] is given by

$$\hat{S}_\beta^\alpha = \sum_a c^\dagger_{aa} c^{\beta a}$$

where the "color" index $a, b = 1, ..., n_c$ and the $n_c(n_c+1)/2$ constraints

$$\sum_{a=1}^N c_{aa}^\dagger c^{ab} \delta^a_\beta m$$

restrict the Hilbert space to the states with $m\times n_c$ particles and ensure the characteristic symmetry in the color index $a$. The antisymmetric behavior with respect to $\alpha$ is a direct consequence of the fermionic representation.

Let us consider the partition function for the Hamiltonian, expressed in terms of $\text{SU}(N)$ generators

$$Z_S = \text{Tr} \exp(-\beta H_S)$$

For $\text{SU}(2) S = 1/2$ and $S = 1$ it is possible to map the spin partition function onto a fermionic partition function where the chemical potential of fermions is purely imaginary \[25\]

$$Z_S = A \text{Tr} \exp(-\beta (H_F - \mu N_F)) = AZ_F$$

with $\mu = -i\pi T/2$ and $A = i^{n_{\text{site}}}$ for $S = 1/2$ and $\mu = -i\pi T/3$ and $A = (i/\sqrt{3})^{n_{\text{site}}}$ for $S = 1$, $n_{\text{site}}$ denotes the number of sites in a lattice. This results in usual Feynman-like diagram technique built up with the help of auxiliary Fermi (Grassmann) fields. The corresponding Matsubara frequencies for Popov-Fedotov (PF) fermions after applying the generalized Grassmann boundary conditions \[25\] read as $\omega_n = 2\pi T(n+1/4)$ for $S = 1/2$ and $\omega_n = 2\pi T(n+1/3)$ for $S = 1$. The imaginary chemical potentials are important for the realization of an exclusion principle providing the fulfillment of the general identity

$$Z_S = \text{Tr} \exp(-\beta H_S) = \text{Tr} \exp(-\beta H_F) \delta_{n_F,1}$$

The Popov-Fedotov representation has been generalized for arbitrary values of spin $S$ for the $\text{SU}(2)$ group in \[40\] by introducing the distribution of discrete chemical potentials $\mu(j)$, with $j$ being the site index, for PF fermions:

$$Z_S = \prod_j \frac{d \mu(j) P(\mu(j)) Z_F(\mu(j))}{Z_F(\mu(j)) \mu(j) n_F}$$

For the $\text{SU}(N)$ algebra we shall try to find the partition function in a similar manner

$$Z_S = \int \prod_j d \mu(j) P(\mu(j)) \text{Tr} \exp(-\beta (H_F - \mu(j) n_F)) =$$
\[
= \int \prod_j d\mu(j)P(\mu(j))Z_F(\mu(j))
\]
(13)

We use the path integral representation of the partition function

\[
Z_S/Z_S^0 = \int \prod_j d\mu(j)P(\mu(j))\exp(A)/\int \prod_j d\mu(j)P(\mu(j))\exp(A_0)
\]
(14)

where the action \(A\) and \(A_0\) are determined by

\[
A = A_0 - \int_0^\beta d\tau H_F(\tau),
\]
and the fermionic representation of SU(N) generators \(\hat{a}_k, \hat{a}_k^\dagger\) is applied.

To begin with we confine ourselves to two particular cases of SU(N) with \(n_c = 1\) corresponding to an effective "spin size" \(S = 1/2\) and in the language of Young tableaux described by one column) and SU(2) for arbitrary value of \(n_c = 2S\) (one row Young tableau).

Let us first consider \(n_c = 1\). We denote the corresponding distribution by \(P_{N,m}(\mu(j))\), where \(m\) is the number of particles in the SU(N) orbital, or in other words, \(1 \leq m < N\) labels the different fundamental representations of SU(N),

\[
n_j = \sum_{k=1}^N \bar{a}_k(j)a_k(j) = m
\]
(16)

To satisfy this requirement, the minimal set of chemical potentials and the corresponding form of \(P_{N,m}(\mu(j))\) are to be derived.

Let us classify the states in Fock and spin spaces. We note that the dimension of the Fock space is \(\dim H_F = 2^N\) and spurious states should be excluded. Thus, there are \(\nu(N,m) = C_m^N = N!/(m!(N-m)!))\) physical states which can be obtained from the vacuum state \(\Phi_0 = [0, ..., 0]_N\) as follows

\[
\Phi_{phys}^{(\nu)} = \prod_{i=1}^m a_i^\dagger \Phi_0
\]
(17)
or from the \([1, ..., 0, ..., 0]_m\) state by transferring the occupied states from left to the right side using the group generators.

To derive the distribution function we use the following identity for constraint \([14]\) expressed in terms of Grassmann variables

\[
\delta_{n_j,m} = \frac{1}{N} \sin(\pi(n_j - m)) / \sin(\pi(n_j - m)/N)
\]
(18)

Substituting this identity into \([13]\) and comparing with \([12]\) on gets

\[
P_{N,m}(\mu(j)) = \frac{1}{N} \sum_{k=1}^N \exp\left(\frac{i\pi m}{N}(2k - 1)\right) \delta(\mu(j) - \mu_k)
\]
(19)

where

\[
\mu_k = -\frac{i\pi T}{N}(2k - 1)
\]
(20)

Since the Hamiltonian is symmetric under exchange of particles and holes if the sign of the chemical potential is changed simultaneously, we can simplify \([14]\) to

\[
P_{N,m}(\mu(j)) = \frac{2i}{N} \sum_{k=1}^{\lfloor N/2\rfloor} \sin\left(\frac{\pi m (2k - 1)}{N}\right) \delta(\mu(j) - \mu_k)
\]
(21)

where \(\lfloor N/2\rfloor\) denotes the integer part of \(N/2\). As the discussion below will show, this is the minimal representation of the distribution function corresponding to the minimal set of the discrete imaginary chemical potentials. Another distributions function different from \([21]\) can be constructed when the sum is taken from \(k = \lfloor N/2\rfloor + 1\) to \(N\). Nevertheless, this DF is different from \([21]\) only by the sign of imaginary chemical potentials \(\mu_k = \mu_k = -\mu_k\) and thus is supplementary to \([21]\).

Particularly interesting for even \(N\) is the case when the SU(N) orbital is half–filled, \(m = N/2\). Then all chemical potentials are weighted with equal weight

\[
P_{N,N/2}(\mu(j)) = \frac{2i}{N} \sum_{k=1}^{N/2} (-1)^{k+1} \delta(\mu(j) - \mu_k)
\]
(22)

Taking the limit \(N \to \infty\) one may replace the summation in expression \([22]\) in a suitable way by integration. Note, that taking \(N \to \infty\) and \(m \to \infty\) we nevertheless keep the ratio \(m/N = 1/2\) fixed. Then, the following limiting distribution function can be obtained:

\[
P_{N,N/2}(\mu(j)) \to \frac{2\beta}{\pi N} \exp\left(-\beta \mu(j) \frac{N}{2}\right)
\]
(23)

resulting in the usual continuous representation of the local constraint for the simplest case \(n_c = 1\) (compare it with \([14]\))

\[
Z_S = Tr(\exp(-\beta H_F) \delta(n_j - \frac{N}{2}))
\]
(24)

We note the obvious similarity of the limiting DF \(23\) with the Wick rotation from the imaginary axis of the chemical potential \(\mu\) to the real axis of energies \(E\) is performed and thus \(\mu(j)N/2\) has a meaning of energy.

Up to now the representation we discussed was purely fermionic and expressed in terms of usual Grassmann variables when the path integral formalism is applied. The only difference from slave fermionic approach is that imaginary chemical potentials are introduced to fulfill the constraint. Nevertheless, by making the replacement

\[
a_k(j, \tau) \to a_k(j, \tau) \exp\left(i\pi T \frac{2k - 1}{N}\right)
\]
\[
\bar{a}_k(j, \tau) \rightarrow \bar{a}_k(j, \tau) \exp \left(-i\frac{\pi}{\beta} \frac{2k - 1}{N} \right) \tag{25}
\]
we are coming to generalized Grassmann (semi-fermionic) boundary conditions

\[
a_k(j, \beta) = a_k(j, 0) \exp \left(i\frac{2k - 1}{N} \right)
\]
\[
\bar{a}_k(j, \beta) = \bar{a}_k(j, 0) \exp \left(-i\frac{2k - 1}{N} \right) \tag{26}
\]
This leads to a temperature diagram technique for Green functions

\[
\mathcal{G}^{\alpha\beta}(j, \tau) = -\langle T_\tau a_\alpha(j, \tau)\bar{a}_\beta(j, 0) \rangle \tag{27}
\]
of semi-fermons with Matsubara frequencies different from both Fermi and Bose representations.

The minimal set of Matsubara frequencies \(\omega_n/(2\pi T)\) forms for SU(N) with even \(N\) the triangle table shown in Fig.3.

![Fig. 2. The minimal set of Matsubara frequencies for SU(N) representation with even N.](image)

The exclusion principle for this case is illustrated on Fig.4, where the first two groups SU(2) and SU(4) are shown. The first point to observe is that the spin Hamiltonian does not distinguish the \(n\) and the \(n+1/2\) hole (or \(N-n\) particle) subspace. Due to Eq. (25) the two phase factors \(\exp(\beta\mu n)\) and \(\exp(\beta\mu(N-n))\) accompanying these subspaces in Eq. (26) add up to a purely imaginary value within the same chemical potential, and the empty and the fully occupied states are always canceled. In the case of \(N \geq 4\), where we have multiple chemical potentials, the distribution function \(P(\mu)\) linearly combines these imaginary prefactors to select out the desired physical subspace with particle number \(n = m\).

In Fig.4 we note that on each picture the empty and fully occupied states are canceled in their own unit circle. For SU(2) there is a unique chemical potential \(\mu = \pm i\pi T/2\) which results in the survival of single occupied states. For SU(4) there are two chemical potentials (see also Fig.4). The cancellation of single and triple occupied states is achieved with the help of proper weights for these states in the distribution function whereas the states with the occupation number 2 are doubled according to the expression (22). In general, for SU(N) group with \(n_c = 1\) there exists \(N/2\) circles providing the realization of the exclusion principle.

We consider now the generalization of the SU(2) algebra for the case of a large moment \(S\) with \(2S + 1\) projections. Here, the most convenient fermionic representation is constructed with the help of a \(2S + 1\) component Fermi field \(a_k(j)\) provided that the generators of SU(2) satisfy the following equations

\[
S^+ = \sum_{k=-S}^{S-1} \sqrt{S(S+1)-k(k+1)}a_{k+1}^\dagger(j)a_k(j)
\]
\[
S^- = \sum_{k=-S+1}^{S} \sqrt{S(S+1)-k(k-1)}a_k^\dagger(j)a_{k-1}(j)
\]
\[
S^z = \sum_{k=-S}^{S} ka_k^\dagger(j)a_k(j) \tag{28}
\]
such that \(\text{dim} H_F = 2^{2S+1}\) whereas the constraint reads as follows

\[
n_j = \sum_{k=-S}^{k=S} a_k^\dagger(j)a_k(j) = l = 1 \tag{29}
\]

We consider the distribution function for arbitrary \(l\) for the sake of generality. It describes the orbital part of an atomic subshell with orbital quantum number \(S\), with \(l\) particles present. We denote the corresponding distribution function of the chemical potential by \(P_{2S+1,l}(\mu(j))\). Following the same routine as for SU(N) generators and using the occupancy condition to have \(l\) (or \(2S + 1 - l\)) states from the \(2S + 1\) states filled, one gets the following
distribution function, after using the particle–hole symmetry of $H_S$:

$$P_{2S+1,1}(\mu(j)) = \frac{2i}{2S+1} \sum_{k=1}^{(S+1)/2} \sin \left( \frac{\pi l (2k-1)}{2S+1} \right) \delta(\mu(j)-\mu_k)$$

where the chemical potentials are $\mu_k = -\pi T (2k-1)/(2S+1)$ and $k = 1, \ldots, [S+1/2]$, similarly to Eq. (21).

In the particular case of the SU(2) model with $l = 1$ for some chosen values of spin $S$ the distribution functions are determined by the following expressions

$$P_{2,1}(\mu(j)) = i \delta(\mu(j) + \frac{i\pi T}{2})$$

for $S = 1/2$

$$P_{3,1}(\mu(j)) = P_{3,2}(\mu(j)) = \frac{i}{\sqrt{3}} \delta(\mu(j) + \frac{i\pi T}{3})$$

for $S = 1$.

This result corresponds to the original Popov-Fedotov description restricted to the $S = 1/2$ and $S = 1$ cases. We present as an example some other distribution functions obtained according to general scheme considered above:

$$P_{4,1}(\mu) = P_{4,3}(\mu) =$$

$$\frac{i\sqrt{2}}{4} \left( \delta(\mu + \frac{i\pi T}{4}) + \delta(\mu + \frac{3i\pi T}{4}) \right)$$

for $S = 3/2$, SU(2) and

$$P_{4,2}(\mu) = \frac{i}{2} \left( \delta(\mu + \frac{i\pi T}{4}) - \delta(\mu + \frac{3i\pi T}{4}) \right)$$

for effective spin "$S = 1/2"$, SU(4),

$$P_{5,1}(\mu) = P_{5,4}(\mu) =$$

$$\frac{i}{\sqrt{10}} \left( \frac{1}{\sqrt{5}} \delta(\mu + \frac{i\pi T}{5}) + \frac{1}{\sqrt{5}} \delta(\mu + \frac{3i\pi T}{5}) \right)$$

for $S = 2$, SU(2) etc.

A limiting distribution function corresponding to Eq. (23) for the constraint condition with arbitrary $l$ is given by

$$P_{\infty,l}(\mu(j)) \xrightarrow{s \to \infty} \frac{\beta}{2\pi i} \exp(-\beta \mu(j))$$

For the case $l = m = N/2 \to \infty$ and $S = (N-1)/2 \to \infty$ the expression for the limiting DF $P_{\infty,l}(\mu(j))$ coincides with (23). We note that in $S \to \infty$ (or $N \to \infty$) limit continuum chemical potentials play role of additional U(1) fluctuating field whereas for finite $S$ and $N$ they are characterized by fixed and discrete values.

When $S$ assumes integer values, the minimal fundamental set of Matsubara frequencies is given by the table in Fig. 4.

The exclusion principle for SU(2) in the large spin limit can be also understood with the help of Fig 3 and Fig. 5.

One can see that empty and fully occupied states are canceled in each given circle similarly to even-$N$ SU(N) algebra. The particle-hole (PH) symmetry of the representation results in an equivalence of single occupied and 2 $S$ occupied states whereas all the other states are canceled due to proper weights in the distribution function (30). In accordance with PH symmetry being preserved for each value of the chemical potential all circle diagrams (see Fig. 3, Fig. 5) are invariant with respect to simultaneous change $\mu \leftrightarrow -\mu$ and $n_{\text{particle}} \leftrightarrow n_{\text{holes}}$.

Let us make few comments concerning the general rectangular Young tableau of size $n_c * m$. The fermionic representation (31) is characterized by an $N* n_c$ component field with $n_c$ identical diagonal constraints and $n_c (n_c - 1)/2$ offdiagonal constraints (20). The effective "filling" determining the number of fermions on each site is $mn_c$. However, not all of these $(n_c N)!(n_c)!((N-m)n_c)!$ states are representing proper physical states. One should take
into account the constraints Eq. (8) to obtain the complete set. The number of physical states of a rectangular Young tableau is given by the expression:

$$\nu(N, m, n_c) = \frac{C_{N-m-1}^{m+n_c-1}C_{N-m}^{m+n_c-2}\cdots C_{N}^{m}}{C_{N-1}^{m}C_{N-2}^{m}\cdots C_{N-m}^{m}} = \frac{C_{n_c}^{m+n_c-1}C_{m+n_c-2}\cdots C_{m}}{C_{n_c}^{m}}$$

(37)

While the diagonal part of Eq. (5) could be satisfied with color-dependent chemical potentials $$\mu_\alpha(j)$$, coupling only to $$\sum a_\alpha e^{\mu_\alpha}$$, an exclusion procedure for the off-diagonal constraints needs either projection operators or an a priori restriction on the trace, using e.g., coherent states $$|\Theta\rangle$$.

Another generalization is applicable for a broader range of cases. The general Young tableau (not necessarily rectangular), representing any irreducible representation $$(p)$$, can be described in the context of our approach in the following way. The generators $$S_{\alpha}^{(p)}$$ are expressed as matrices

$$S_{\alpha}^{(p)} = \langle \psi_{\alpha}^{(p)} | T_{m}^{(k)} \times (l) | \psi_{\alpha}^{(p)} \rangle$$

(38)

with $$T_{m}^{(k)} \times (l) = T_{m}^{(k)} + T_{m}^{(l)}$$ being the generators in a suitable direct product of representations (k) and (l) and the states $$|\psi_{\alpha}^{(p)}\rangle$$ are obtained in terms of Clebsch–Gordan coefficients

$$|\psi_{\alpha}^{(p)}\rangle = \sum_{\mu,\nu} \langle k, l; \mu, \nu | p; \alpha \rangle |\psi_{\mu}^{(k)}\rangle \times |\psi_{\nu}^{(l)}\rangle$$

(39)

This procedure can be iterated until (k) and (l) are fundamental irreducible representations of SU(N). The size of the matrices $$S_{\alpha}^{(p)}$$ is equal to the dimension of the representation, $${\nu}^{(p)}$$. The trace is now easily expressed in terms of $${\nu}^{(p)}$$ fermionic fields, enforcing the constraint $${\delta}^{(l)}_{m,1}$$ with the distribution of chemical potentials (see Eq. (21))

$$P_{\nu^{(p)},1}(\mu(j)) = \frac{2i}{\nu^{(p)}} \sum_{k=1}^{\nu^{(p)}/2} \sin \left( \frac{2k-1}{\nu^{(p)}} \pi \right) \delta(\mu(j) - \mu_k)$$

(40)

For the simple case of SU(2), which yields only single-row tableaux, this procedure gives the fermionic representation described in Eqs. (23)-(30). In the case of single-column tableaux for SU(N), however, and in the general case of mixed symmetry, it does not fully use the fermionic commutation properties. Therefore, it is in general not the representation with the minimal number of fermions and the minimal number of chemical potentials in $$P(\mu)$$.

We discuss finally the real-time formalism based on the semi-fermionic representation of SU(N) generators. This approach is necessary for treating the systems being out of equilibrium, especially for many component systems describing Fermi (Bose) quasiparticles interacting with spins. The real-time formalism is also an alternative approach for the analytical continuation method for equilibrium problems allowing direct calculations of correlations whose analytical properties as function of many complex arguments can be quite cumbersome.

A long time ago Keldysh [28] and Schwinger [29] have proposed a novel approach for the description of kinetic phenomena in metals. This approach was found especially fruitful for normal metals [30], and, in many recent applications, for superconductors [31], for disordered interacting (normal or superconducting) electron liquids [32] for example. The previous application of the real-time formalism to the quantum theory of Bose-Einstein condensation (BEC) [33] allowed the derivation of a Fokker-Planck equation, which describes both kinetic and coherent stages of BEC. Moreover [34] developed the closed-time path integral formalism for aging effects in quantum disordered systems being in contact with an environment. The Keldysh technique in application to disordered systems (see [34]-[36] and [37]-[38]) has also been recently applied to develop a field theory alternative to the previously used replica technique.

To derive the real-time formalism for SU(N) generators we use the path integral representation along the closed-time contour (see Fig. 6). Following the standard route [39] we can express the partition function of the problem containing SU(N) generators as a path integral over Grassmann variables $$\psi_{\alpha} = (a_{0,1}(j), ..., a_{l,N}(j))^T$$ where $$l = 1, 2$$ stands for upper and lower parts of the Keldysh contour, respectively,

$$Z / Z_0 = \int D\bar{\psi} D\psi \exp(iA)/ \int D\bar{\psi} D\psi \exp(iA_0)$$

(41)

where the actions $$A$$ and $$A_0$$ are taken as an integral along the closed-time contour $$C_t + C_T$$ which is shown in Fig. 6. The contour is closed at $$t = -\infty + i\tau$$ since $$\exp(-\beta H_0) = T_T \exp(-\int_0^\beta H_0 d\tau)$$. We denote the $$\psi$$ fields on upper and lower sides of the contour $$C_t$$ as $$\psi_1$$ and $$\psi_2$$ respectively. The fields $$\Psi$$ stand for the contour $$C_T$$. These fields provide matching conditions for $$\psi_{1,2}$$ and are excluded from final expressions. Taking into account the semi-fermionic boundary conditions for generalized Grassmann fields [20],
one gets the matching conditions for $\psi_{1,2}$ at $t = \pm \infty$,

$$\psi^{\mu}_{1,\alpha}(k)(-\infty) = \exp \left( i \frac{2k - 1}{N} \right) \psi^{\mu}_{2,\alpha}(k)(-\infty)$$

$$\psi^{\mu}_{1,\alpha}(k)(+\infty) = \psi^{\mu}_{2,\alpha}(k)(+\infty)$$

(42)

for $k = 1, \ldots, [N/2]$ and $\alpha = 1, \ldots, N$. The correlation functions can be represented as functional derivatives of the generating functional

$$Z[\eta] = \mathcal{Z}^{-1}_{0} \int D\bar{\psi} D\psi \exp \left( iA + i \int d\tau (\bar{\eta} \sigma^{z} \psi + \bar{\psi} \sigma^{z} \eta) \right)$$

(43)

where $\eta$ represents sources and the $\sigma^{z}$ matrix stands for "causal" and "anti-causal" orderings along the contour.

The on-site Green’s functions (GF) which are matrices of size $2N \times 2N$ with respect to both Keldysh (lower) and spin-color (upper) indices are given by

$$G_{\mu \nu}^{(R,A)}(t, t') = -i \frac{\delta}{i \delta \eta^{\mu}_{\alpha}(t) / \delta \eta^{\nu}_{\beta}(t')} \mathcal{Z}[\eta]_{\eta \to 0}$$

(44)

To distinguish between imaginary-time ($\mathcal{Z}^{-1}_{0}$) and real-time ($\mathcal{Z}^{-1}$) GF’s we use different notations for Green’s functions in these representations.

After a standard shift-transformation of fields $\psi$ the Keldysh GF of free semi-fermions assumes the form

$$G_{0}^{(R)}(\epsilon) = G_{0}^{(R,\alpha)} \left( 1 - f_{k} - f_{-k} \right) - G_{0}^{(A,\alpha)} \left( 1 - f_{-k} - f_{k} \right)$$

(45)

where the retarded and advanced GF’s are

$$G_{0}^{(R,A)}(\epsilon) = (\epsilon \pm i \delta)^{-1}, \quad f_{k} = f_{(N,k)}(\epsilon)$$

(46)

A straightforward calculation of $f_{(N,k)}$ for the case of even $N$ leads to the following expression

$$f_{(N,k)}(\epsilon) = \frac{1}{N} \sum_{n} \frac{e^{i\omega_{nk}T + \delta}}{i\omega_{nk} - \epsilon}$$

(47)

for $k = 1, \ldots, [S + 1/2]$. Particularly simple are the cases of $S = 1/2$ and $S = 1$,

$$f_{(2,1)}^{(2)}(\epsilon) = n_{F}(2\epsilon) = \frac{1}{2} \frac{1}{\cosh(\beta \epsilon)}$$

$$f_{(3,1)}^{(3)}(\epsilon) = \frac{1}{2} n_{B}(\epsilon)^{-3} \frac{3}{2} n_{B}(3\epsilon) - i \frac{\sqrt{3}}{\sinh(3\beta\epsilon/2)}$$

(48)

Here, standard notations for Fermi/Bose distribution functions $n_{F/B}(\epsilon) = [\exp(\beta \epsilon) \pm 1]^{-1}$ are used.

In general the EDF for half-integer and integer spins can be expressed in terms of Fermi and Bose EDF respectively. We note that since auxiliary Fermi fields introduced for the representation of SU($N$) generators do not represent the true quasiparticles of the problem, helping only to treat properly the constraint condition, the distribution functions for these objects in general do not have to be real functions. Nevertheless, one can prove that the imaginary part of the EDF does not affect the physical correlators and can be eliminated by introducing an infinitesimally small real part for the chemical potential. In spin problems, a uniform/staggered magnetic field usually plays the role of such real chemical potential for semi-fermions.

Let us illustrate the application of the semi-fermionic formalism for spin Hamiltonians. As an example we consider the SU(2) Heisenberg model for $S = 1/2$ with the nearest neighbor interaction

$$H_{int} = - \sum_{\langle ij \rangle} J_{ij} S_{i} S_{j}$$

(50)

We start with imaginary-time semi-fermionic description of the ferromagnetic (FM) state of the Heisenberg model ($J > 0$). We follow the standard procedure developed in the original paper of Popov and Fedotov. After applying the Hubbard-Stratonovich transformation to decouple the four-semi-fermion term in (50) by the local vector field $\Phi_{i}(\tau)$ the effective action is obtained:

$$\mathcal{A}^{FM}_{eff}[\psi, \Phi] = \bar{\Phi}_{0}[\psi, \Phi] - \frac{1}{4} \int_{0}^{\beta} d\tau \sum_{q} (I_{FM}(q))^{-1} \Phi_{q}(\tau) \Phi_{q}^{*}(\tau)$$

(51)

where $\bar{\psi} = (\psi_{1}, \psi_{2})$ - fields denoting the semi-fermions in SU(2) representation of the $S = 1/2$ spin operators,

$$I_{FM}(q) = I_{FM/AFM}(q) = \frac{1}{N} \sum_{r_{ij}} J_{r_{ij}} e^{iqr}$$

(52)

and $I_{FM}(q) = ZJ > 0$ for the FM instability (here $Z$ denotes the number of the nearest neighbors, $N$ stands for the number of unit cells). The FM phase transition corresponds to appearance at $T_{c}$ of the nonzero average $\langle \Phi^{2}(q,0) \rangle$ which stands for nonzero uniform magnetization, or by another words, corresponds to the Bose condensation of the field $\Phi^{2}$.

Splitting the field $\Phi^{2}$ on the time-independent spatially homogeneous (uniform) part and the fluctuating field $\Phi^{2}$

$$\Phi^{2}(k, \omega) = M(\beta N)^{1/2} \delta_{k,0} \delta_{\omega,0} + \Phi^{2}(k, \omega)$$

(53)
Fig. 7. First few graphs for the free energy expanded with respect to local molecular magnetic field. Solid line stands for semi-fermions. Zig-zag line denotes the "condensate" field.

make it possible to integrate over all semi-fermionic fields. As a result, the nonpolynomial effective action can be derived for the FM Heisenberg model

$$A_{eff} = A_0[\Phi] + \text{Tr} \ln (G^{-1}_\sigma(\Phi^z, \Phi^\pm))$$

(54)

where $G_\sigma = -\langle T_\tau \psi_\sigma(j, \tau) \bar{\psi}_\sigma(j, 0) \rangle$ stands for the local Green’s function of semi-fermions. The expansion of the $\text{Tr} \ln G^{-1}_\sigma$ with respect to $\Phi$ fields results in standard Ginzburg-Landau functional (see Fig. 7). The effects of molecular field are included into zero approximation for $G$:

$$G_\sigma(i\omega_n) = [i\omega_n + \sigma^z_{\sigma\sigma}, M/2]^{-1}.$$  

In one loop approximation the standard molecular field equation can be reproduced

$$\mathcal{M} = I_{FM}(0) \tanh(\beta M/2)$$

(55)

The saddle point (mean-field) effective action is given by well-known expression

$$A_0[\mathcal{M}] = -N \left[ \frac{\beta M^2}{4I_M(0)} - \ln \left( 2 \cosh \left( \frac{\beta M}{2} \right) \right) \right]$$

(56)

and the free energy per spin $f_0$ (see Fig. 7) is determined by standard equation:

$$\beta f_0 = -\ln Z_S = \frac{\beta M^2}{4I_M(0)} - \ln \left( 2 \cosh \left( \frac{\beta M}{2} \right) \right)$$

(57)

Calculation of the second variation of $A_{eff}$ gives rise to the following expression

$$\delta A_{eff} = -\frac{1}{4} \sum_k \Phi^z(k, 0) \left[ I^{-1}_M(k) - \frac{\beta}{2 \cosh^2(\beta \Omega)} \right] \Phi^z(k, 0) -$$

$$-\frac{1}{4} \sum_{k, \omega \neq 0} I^{-1}_M(k) \Phi^z(k, \omega) \Phi^z(k, \omega) -$$

$$-\sum_{k, \omega} \Phi^z(k, \omega) \left[ I^{-1}_M(k) - \frac{\tanh(\beta \Omega)}{2 \Omega - i \omega} \right] \Phi^z(k, \omega)$$

(58)

where $\Omega = (g_\mu_B H + \mathcal{M})/2$. For $T > T_c$ one easily obtains the effective static spin-spin interaction equivalent to those given by the Random Phase Approximation (RPA)

$$\Gamma(q, 0) = (\Phi(q, 0) \Phi(-q, 0)) = 2 I(q)/(1 - 2 \chi_0 I(q))$$

where $\chi_0^+(q, 0) = 2 \chi_0^z(q, 0) = 2 \chi_0 = 2S(S + 1)\beta/3$ stands for the on-site spin susceptibility in paramagnetic state.

Let us now consider the Heisenberg model with antiferromagnetic (AFM) sign of the exchange integral ($J < 0$).

$$A_{eff}^{AFM}[\psi, \Phi] = \tilde{A}_0[\psi, \Phi] +$$

$$+ \frac{1}{4} \int_0^\beta d\tau \sum_q (I_{AFM}(q))^{-1} \Phi(q) \Phi(q)$$

(59)

and $I_M(Q) = ZJ < 0$ for the AFM instability corresponding to vector $Q = (..., \pi)$ (we consider the hypercubic lattice for simplicity). In contrast to the FM case, we can now represent the longitudinal component of the field $\Phi^z$ as a superposition of the staggered time-independent part ("staggered condensate") and a fluctuating field

$$\Phi^z(k, \omega) = N(\beta N)^{1/2} \delta_{kQ} \delta_{\omega, 0} + \tilde{\Phi}^z(k, \omega)$$

(60)

As a result, the integration over semi-fermionic fields can be done explicitly. Introducing two sublattices for $\psi$ fields one gets $4 \times 4$ matrix structure for the semi-fermionic Green’s functions. Since the AFM instability is associated with appearance of a nonzero staggered magnetization $\mathcal{N}$, it is necessary to take into account both "normal" and "anomalous" $\Phi$ determined as follows:

$$\tilde{G}_\sigma^0(i\omega_n) = -\int_0^\beta d\tau e^{i\omega_n \tau} \langle T_\tau \psi_\sigma(k, \tau) \bar{\psi}_\sigma(k, 0) \rangle =$$

$$= -\frac{i\omega_n}{\omega_n^2 + \Omega^2}$$

(61)

and

$$\mathcal{F}_\sigma^0(i\omega_n) = -\int_0^\beta d\tau e^{i\omega_n \tau} \langle T_\tau \psi_\sigma(k, \tau) \bar{\psi}_\sigma(k + Q, 0) \rangle =$$

$$= -\frac{i\Omega}{\omega_n^2 + \Omega^2}$$

(62)

where $\Omega = (\mathcal{N} + g_\mu_B h)/2$. Integrating over all semi-fermions one obtains the mean-field equation for the staggered magnetization:

$$\mathcal{N} = -I_{AFM}(Q) \tanh(\beta \mathcal{N}/2)$$

(63)

and

$$A_0[\mathcal{N}] = N \left[ \frac{\beta N^2}{4I_M(Q)} + \ln \left( 2 \cosh \left( \frac{\beta \mathcal{N}}{2} \right) \right) \right]$$

(64)

After taking into account the second variation of $A_{eff}$ the following expression for the effective action is obtained (see e.g. [36, 51]):

$$\delta A_{eff} = \frac{1}{4} \sum_k \Phi^z(k, 0) \left[ I^{-1}_M(k) + \frac{\beta}{2 \cosh^2(\beta \Omega)} \right] \Phi^z(k, 0) +$$

$$+ \frac{1}{4} \sum_{k, \omega \neq 0} I^{-1}_M(k) \Phi^z(k, \omega) \Phi^z(k, \omega) +$$

$$-\sum_k \Phi^z(k, \omega) \left[ I^{-1}_M(k) - \frac{\tanh(\beta \Omega)}{2 \Omega - i \omega} \right] \Phi^z(k, \omega)$$

(65)
\[ + \sum_{\mathbf{k}, \omega} \Phi^+(\mathbf{k}, \omega) \left[ I_M^{-1}(\mathbf{k}) + \frac{2i\Omega \tanh(\beta \Omega)}{4\Omega^2 + \omega^2} \right] \Phi^-(\mathbf{k}, \omega) - \sum_{\mathbf{k}, \omega} \Phi^+(\mathbf{k} + \mathbf{Q}, \omega) i\omega \frac{i\omega}{4\Omega^2 + \omega^2} \Phi^-(\mathbf{k}, \omega). \]  

(65)

The application of the Schwinger-Keldysh formalism for the Heisenberg model is straightforward. Applying the semi-fermionic transformation to the partition function one obtains the action as an integral along the closed-time Keldysh contour.

\[ \mathcal{A} = \mathcal{A}_0 + \mathcal{A}_{int} = \mathcal{A}_0 + \oint_C dt \sum_{\mathbf{q}} \mathcal{J}(\mathbf{q}) \mathcal{S}(\mathbf{q}, t) \mathcal{S}(-\mathbf{q}, t) \]  

(66)

where \( \mathcal{A}_0 \) corresponds to noninteracting semi-fermions.

\[ \mathcal{A}_0 = \oint_C dt \sum_i \dot{\psi}_i \left( \begin{array}{cc} (G_0^{R,\alpha})^{-1} & 0 \\ 0 & (G_0^{A,\alpha})^{-1} \end{array} \right) \psi_i \]  

(67)

We denote \( J_q = \sum_{\kappa} e^{i\mathbf{q}\cdot\mathbf{\kappa}} \nu_q = J_q/J_0 \) and apply four-component semi-fermionic representation for FM case and eight-component representation with \( \psi^T = (\psi^T \psi^T) \) for the AFM case. Performing the standard Hubbard-Stratonovich transformation along the Keldysh contour with the help of the two-Keldysh-component vector (Bose) field \( \Phi \), one gets

\[ \mathcal{A}_{int} = -\frac{1}{2} Tr(\Phi^T q^{-1}_1 \sigma^x \Phi q^+_1) + Tr(\dot{\psi}_i \Phi^i \sigma^\gamma^\mu \psi) \]  

(68)

Now we integrate out \( \psi \) fields and express the effective action in terms of \( \Phi \) fields

\[ \mathcal{A}_{eff} = -\frac{1}{2} Tr(\Phi^T q^{-1}_1 \sigma^x \Phi q^+_1) + Tr \ln(G_0^{-1} + \Phi^i \sigma^\gamma^\mu \Phi) \]  

where \( \gamma^\mu = (\sigma^2 \pm 1)/2 \) acts in Keldysh space. Since in general \( \Phi \) is a time- and space-dependent fluctuating field the partition function cannot be evaluated exactly. Nevertheless, when a magnetic instability occurs, we can represent the longitudinal component of this field as a superposition of a uniform (FM) or staggered (AFM) time-independent part and a fluctuating field

\[ \Phi^\mu_0(\mathbf{q}, \omega) = \text{condensate} + \Phi^\mu_0(\mathbf{q}, \omega), \]  

(69)

where \( \Phi^\mu_0(\mathbf{q}, \omega) = \phi^\mu_q(\mathbf{q}, \omega) \) with the matching conditions at \( t = \pm \infty \)

\[ \phi_1^\mu(-\infty) = \phi_2^\mu(-\infty), \quad \phi_1^\mu(+\infty) = \phi_2^\mu(+\infty). \]  

(70)

We expand \( Tr \ln(G_0^{-1} + \phi_\mu \sigma^\gamma^\mu) \) in accordance with

\[ Tr \ln(...) = Tr \ln G_0^{-1} + Tr \sum_{n=1}^\infty \frac{(-1)^{n+1}}{n} (G_0 \phi_\mu \sigma^\gamma^\mu)^n \]  

(71)

The spectrum of the excitations (FM or AFM magnons) can be defined as poles of the transverse GF

\[ D^{\pm}_{x,t} = D(x, t) = -i(T_C \phi^+_1(x, t) \phi^+_1(0, 0)). \]  

The procedure of the calculation of this GF is similar to that for a “fermionic” GF. Introducing the sources and evaluating \( [\hat{D}] \) one gets

\[ D_0(\omega) = \frac{1}{2} Tr(1 + N_\omega N_\omega) - \frac{1}{2} Tr(1 + N_\omega 1 + N_\omega) \]  

(72)

for FM magnons and

\[ \omega_q = |J_0| N \sqrt{1 - \nu_q^2} \Rightarrow \epsilon q, \]  

(73)

for AFM magnons. The uniform and staggered magnetization are given by equations (65) and (63) correspondingly.

The magnon damping is defined by four-magnon processes \( \Pi^{+-+} \), shown in Fig.8.b. The derivation of the kinetic equation and calculation of magnon damping is reserved here for a detailed publication.

We consider now the second possibility to decouple the four-fermion term in the Heisenberg model with the antiferromagnetic sign of spin-spin interaction which can be written in a form equivalent to \( [\hat{D}] \):

\[ H_{int} = \frac{1}{2} \sum_{<ij>} J_{ij} \psi_i^+ \psi_j^+ \psi_j^T \psi_i^+ + \frac{1}{4} \sum_{<ij>} J_{ij} \rho_i \rho_j \]  

(74)

Last term in the Hamiltonian \( [\hat{D}] \) describes the fluctuations of semi-fermionic density \( \rho_i = \psi_i^+ \psi_i \) and therefore is irrelevant for our calculations. In contrast to description of the local correlations achieved with the help of the local vector bosonic field \( A_{ij} \) depending on two sites and responsible for inter-site semi-fermionic correlations. Defining new coordinates \( R = (\mathbf{R}_i + \mathbf{R}_j)/2, r = \mathbf{R}_i - \mathbf{R}_j \) and applying a Fourier transformation we obtain the effective action

\[ \mathcal{A}_{eff} = -\frac{1}{2} Tr(A_{Pq}^T J_{q1}^{-1} q_2^2 \sigma^2 A_{Pq}) + Tr \ln(G_0^{-1} - A_{\mu} \gamma^\mu) \]  

Fig. 8. Feynman diagrams contributing to dispersion (a) and damping (b) of magnons. Solid line denotes semi-fermions.
This effective action describes the nonequilibrium quantum spin-liquid (SL). We confine ourselves to consider the uniform phase of Resonant Valence Bonds (RVB) in 2D antiferromagnets. It is suitable to rewrite the functional in new variables, namely the amplitude $\Delta$ and the phase $\Theta = r A_\mu(R)$, according to formula
\[
A^{\alpha\beta}_\mu(R, \mathbf{r}) = \Delta(r) \eta^{\mu\nu} \exp(i r A_\mu(R))
\] (75)
The exponent in (75) stands for gauge fluctuations to be taken in eikonal approximation. As a result, the effective action can be written in continuum limit in terms of the gauge fields $A_\alpha$ as follows:
\[
A_{eff} = \frac{1}{C} \int dt \int dV A_\alpha(k, t) \pi^{\alpha\beta} A_\beta(k, t)
\] (76)
The spectrum of excitations in the uniform SL is defined by the zeros of current-current correlation function $G_{\pi}$
\[
\pi^{\alpha\beta}_{q, \omega} = Tr(p^{\alpha} p^{\beta}(G_{p+q}^{K} + G_{p}^{K} G_{p}^{A} + \delta_{\alpha\beta} f(J \Delta)))
\]
in equilibrium and is purely diffusive (see e.g. [50]). The main advantage of the semi-fermionic representation in applications to the strongly correlated systems in comparison with another methods is that the local constraint is taken into account exactly and the usual Feynman diagrammatic codex for the composite itinerant-local compound is applicable.

Summarizing, we constructed a general scheme for the semi-fermionic representation for generators of the SU(N) algebra. A representation for the partition function is found both in imaginary and real time. The approach developed leads to the standard diagram technique for Fermi operators, although the constraint is taken into account rigorously. The method proposed allows to treat SU(N) generators on the same footing as Fermi and Bose systems. The technique derived can be helpful for the description of quantum systems in the vicinity of a quantum phase transition point and for nonequilibrium systems.

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