TRANSFORMATIONS OF THE HUBBARD INTERACTION TO QUADRATIC FORMS

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Various transformations of the Hubbard interaction to quadratic forms used for functional integral techniques are discussed. A generalised quadratic form in terms of both spins and quasispins is given which contains one free parameter.

Starting with Hubbard's famous paper [1] functional integral techniques have developed to a powerful tool for handling many-particle systems in condensed matter physics. Especially in dealing with the Hubbard model and its generalisations great progress has been achieved during the last 20 years [2] culminating in the so-called "unified picture of magnetism" [3]. Nevertheless, some points are not completely clarified, since for different functional integral techniques arising from the possibility of rewriting the Hubbard interaction by means of the fermion annihilation and creation operator commutation rules different answers to the same physical questions result. Macedo et al. [4] have in particular solved some of the problems by starting from a generalised quadratic form in terms of spin and charge densities. Although the transformation introduced in ref. [4] includes almost all biquadratic forms of the interaction used in the literature until now it is not the most general form, since it is restricted to the spin algebra only. The most general form has to be constructed from combinations of nonvanishing single-particle fermion operators. There are only six such operators:

$$c_\uparrow^+ c_\uparrow;\quad c_\downarrow^+ c_\downarrow;\quad c_\uparrow^+ c_\downarrow;\quad c_\downarrow^+ c_\uparrow;\quad c_\uparrow^+ c_\downarrow^+;\quad c_\uparrow c_\downarrow\,. \qquad (1)$$

This set together with the unity operator has the structure of two isomorphic SU(2) algebras. The spins are as usual

$$S_x=\tfrac{1}{2}(c_\uparrow^+ c_\downarrow+c_\downarrow^+ c_\uparrow)\,,$$

$$S_y=\frac{1}{2\mathrm{i}}(c_\uparrow^+ c_\downarrow-c_\downarrow^+ c_\uparrow),$$

$$S_z=\tfrac{1}{2}(n_\uparrow-n_\downarrow)\,, \qquad (2)$$

with

$$S_xS_y=\tfrac{1}{2}\mathrm{i}S_z\,,$$

$$\mathrm{i}[S_x,S_y]_-=-S_z \quad \text{and cycl. perm.} \qquad (3)$$

Furthermore the quasispins are

$$R_x=\tfrac{1}{2}(c_\uparrow^+ c_\downarrow^+ +c_\downarrow c_\uparrow)\,,$$

$$R_y=\frac{1}{2\mathrm{i}}(c_\uparrow^+ c_\downarrow-c_\downarrow c_\uparrow)\,,$$

$$R_z=\tfrac{1}{2}(n_\uparrow+n_\downarrow-1)\,, \qquad (4)$$

with

$$R_xR_y=\tfrac{1}{2}\mathrm{i}R_z\,,$$

$$\mathrm{i}[R_x,R_y]_-=-R_z \quad \text{and cycl. perm.} \qquad (5)$$

Spins and quasispins are connected by a canonical transformation [5] and commute with each other, because of

$$R_iS_j=S_iR_j=0 \quad \text{for} \quad i,j=x,y,z\,. \qquad (6)$$

Whereas a lot of authors employed the spin algebra

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to rewrite $n_\uparrow n_\downarrow$, only few authors [5,6] treat quasispin algebra descriptions but not in the context of the functional integration procedure. There is no a priori reason preferring one algebra. The most general ansatz for a quadratic form both in spin and quasispin is

$$n_\uparrow n_\downarrow = c_0 + \sum_{i,j=1}^{6} \lambda_{ij} S_i S_j , \tag{7}$$

where $S_4 ... S_6$ stands for $R_1 ... R_3$. By means of eqs. (3), (5), and (6) and using $S_x^2 = S_y^2 = S_z^2 = \boldsymbol{S}^2/3$, $R_x^2 = R_y^2 = R_z^2 = \boldsymbol{R}^2/3$ it can be shown that without loss of generality eq. (7) reduces to

$$n_\uparrow n_\downarrow = c_0 + a_x S_x + a_y S_y + a_z S_z + A\boldsymbol{S}^2 + b_x R_x + b_y R_y + b_z R_z + B\boldsymbol{R}^2 . \tag{8}$$

Comparing the r.h.s. of eq. (8) with the l.h.s. it can be immediately seen that eq. (8) holds for the coefficients a_i, b_i, A and B determined as follows:

$$a_x = a_y = a_z ; \quad b_x = b_y = 0 ; \quad b_z = 1 ;$$
$$A = -4a_0 ; \quad B = -4a_0 + \tfrac{2}{3} . \tag{9}$$

So, at least, the most general expression contains only one free parameter. With $\alpha = -4a_0 + \frac{1}{3}$ it is designed as

$$n_\uparrow n_\downarrow = \tfrac{1}{4} - \tfrac{3}{4}\alpha + R_z + (\alpha - \tfrac{1}{3})\boldsymbol{S}^2 + (\alpha + \tfrac{1}{3})\boldsymbol{R}^2 . \tag{10}$$

From this expression with $\alpha = 0$ one finds

$$n_\uparrow n_\downarrow = \tfrac{1}{4} + R_z - \tfrac{1}{3}\boldsymbol{S}^2 + \tfrac{1}{3}\boldsymbol{R}^2 , \tag{11}$$

which would lead via the Hubbard-Stratonovič technique to two vector fields. One couples to the spin vector $\boldsymbol{S}$ and the other to the quasispin vector $\boldsymbol{R}$ producing a six-component order parameter. To our knowledge such a scheme has not been reported for the Hubbard model yet, but with $\frac{1}{3}\boldsymbol{R}^2 = R_z$ and keeping in mind $\frac{1}{4} + R_z + R_z^2 = \frac{1}{4}(n_\uparrow + n_\downarrow)^2$ one obtains the form

$$n_\uparrow n_\downarrow = \tfrac{1}{4}(n_\uparrow + n_\downarrow)^2 - \tfrac{1}{3}\boldsymbol{S}^2 . \tag{12}$$

It results in a four-component order parameter due to one scalar field coupling to the charge density and a vector field coupled to the spin. This scheme was extensively studied among others by Moriya and Hasegawa [7] with the result of a quite unified picture of magnetism including both the localised and the itinerant limits. Using $\boldsymbol{S}^2/3 = S_z$ Hamann [8] obtained the two-field scheme

$$n_\uparrow n_\downarrow = \tfrac{1}{4}(n_\uparrow + n_\downarrow)^2 - \tfrac{1}{4}(n_\uparrow - n_\downarrow)^2 , \tag{13}$$

studied well by a lot of authors, e.g. in ref. [9]. For $\alpha = -\frac{1}{3}$ follows immediately from eq. (10)

$$n_\uparrow n_\downarrow = \tfrac{1}{2}(n_\uparrow + n_\downarrow) - \tfrac{2}{3}\boldsymbol{S}^2 . \tag{14}$$

From this Heisenberg-like form studied by Moriya [10] one can get an Ising-like expression by substituting the spin vector by its z-component only. The resulting expression was first introduced by Wang, Evenson and Schrieffer [11]:

$$n_\uparrow n_\downarrow = \tfrac{1}{2}(n_\uparrow + n_\downarrow) - \tfrac{1}{2}(n_\uparrow - n_\downarrow)^2 \tag{15}$$

and produces a one-field scheme. The choice $\alpha = -\frac{1}{6}$ finally gives the representation used by Gomes and Lederer [12], so that all schemes developed so far are contained in the generalised representation (10). At this point we mention that with $\alpha = \frac{1}{3}$ the interaction is represented in terms of quasispins alone:

$$n_\uparrow n_\downarrow = R_z + \tfrac{2}{3}\boldsymbol{R}^2 . \tag{16}$$

Again $\boldsymbol{R}^2$ may be replaced by $3R_z^2$ resulting in

$$n_\uparrow n_\downarrow = R_z + 2R_z^2 . \tag{17}$$

The identities (16) and (17) may be useful in dealing with superconducting or charge ordered phases of models with a Hubbard interaction. From the representation (17) it becomes clear that a contribution to the free energy arises only if $R_z \neq 0$, i.e. if $n_\uparrow + n_\downarrow \neq 1$, which characterizes the "charged model". The latter case may be of interest if one tries to explain high T_c superconductivity within models containing Hubbard-like interactions, which may be attractive as in the BCS theory or repulsive as in the theory of magnetism. Both cases are included since the above discussion is valid for arbitrary prefactors of $n_\uparrow n_\downarrow$. We mention that Hubbard introduced a representation with a local anisotropy, i.e. he replaced S_z in eq. (13) by $\boldsymbol{e}\cdot\boldsymbol{S}$ with $\boldsymbol{e}$ being an arbitrary unit vector, and restored rotational symmetry by a final integration over all directions. This idea may be generalised by using $\boldsymbol{e}\cdot\boldsymbol{R}$ instead of R_z in eq. (17). From eq. (10) one has to calculate the thermodynamical potential in a more or less comprehensive approximation. The appropriate value of α has to be determined by min-

imizing with respect to α. If one starts from an a priori value the approximations used in the literature are known to destroy operator identities in an uncontrolled manner. Furthermore regarding thermodynamics it seems hard to justify that phases produced by quasispin operators should be avoided. This is automatically done if one restricts the considerations to a pure spin representation. A more detailed discussion of eq. (10) is in preparation.

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