



ОБЪЕДИНЕННЫЙ
ИНСТИТУТ
ЯДЕРНЫХ
ИССЛЕДОВАНИЙ
ДУБНА

538

E17-89-99

R.Schumann¹, E.Heiner²

TRANSFORMATIONS
OF THE HUBBARD INTERACTION
TO QUADRATIC FORMS

Submitted to "Physics Letters A"

¹ On leave from Hochschule fuer Verkehrswesen
"Friedrich List", WB Physik, Dresden 8072, PF 103, GDR

² On leave from Central Institute for Nuclear Research
Academy of Sciences of the GDR, Rossendorf, Dresden 8051,
PF 19, GDR

Starting with J. Hubbards famous contribution to Phys. Rev. Lett in 1959^{1/1} functional integral techniques have developed themselves to a powerful tool for handling many particle systems in condensed matter physics. Especially dealing with the Hubbard model and its generalisations great progress has been reached during the last 20 years^{2/2} culminating in the so-called "unified picture of magnetism"^{3/3}. 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 result different answers to the same physical questions. C.A. Macedo et al.^{4/4} have particularly 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.^{4/4} 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:

$$c_{\uparrow}^{\dagger}c_{\uparrow}; c_{\downarrow}^{\dagger}c_{\downarrow}; c_{\uparrow}^{\dagger}c_{\downarrow}; c_{\downarrow}^{\dagger}c_{\uparrow}; c_{\uparrow}^{\dagger}c_{\downarrow}^{\dagger}; c_{\uparrow}c_{\downarrow}. \quad (1)$$

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

$$S_x = \frac{1}{2}(c_{\uparrow}^{\dagger}c_{\downarrow} + c_{\downarrow}^{\dagger}c_{\uparrow}), S_y = \frac{1}{2i}(c_{\uparrow}^{\dagger}c_{\downarrow} - c_{\downarrow}^{\dagger}c_{\uparrow}), S_z = \frac{1}{2}(n_{\uparrow} - n_{\downarrow}) \quad (2)$$

with

$$S_x S_y = \frac{i}{2} S_z; i[S_x, S_y] = -S_z \quad \text{and cycl.} \quad (3)$$

furthermore the quasispins are

$$R_x = \frac{1}{2}(c_{\uparrow}^{\dagger}c_{\downarrow}^{\dagger} + c_{\downarrow}c_{\uparrow}), R_y = \frac{1}{2i}(c_{\uparrow}^{\dagger}c_{\downarrow}^{\dagger} - c_{\downarrow}c_{\uparrow}), \quad (4)$$

$$R_z = \frac{1}{2}(n_{\uparrow} + n_{\downarrow} - 1)$$

with

$$R_x R_y = \frac{1}{2} R_z; i[R_x, R_y] = -R_z \quad \text{and cycl.} \quad (5)$$

Spins and quasispins are connected by a canonical transformation^{5/} and commute one with the other, because of

$$R_i S_j = S_i R_j = 0 \quad \text{for } i, j = x, y, z. \quad (6)$$

Whereas a lot of authors employed the spin algebra to rewrite $n_{\uparrow} n_{\downarrow}$ only few authors^{5,6/} treat quasispin algebra descriptions but not in context with 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:

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

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

$$n_{\uparrow} n_{\downarrow} = a_0 + a_x S_x + a_y S_y + a_z S_z + A S^2 + b_x R_x + b_y R_y + b_z R_z + B R^2. \quad (8)$$

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

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

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

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

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

$$n_{\uparrow} n_{\downarrow} = \frac{1}{4} + R_z - \frac{1}{3} S^2 + \frac{1}{3} R^2 \quad (11)$$

which would lead via the Hubbard-Stratonovic technique to two vector fields. One couples to the spin vector S and the other to the quasispin vector R producing a six component order parameter. To our knowledge such a scheme has not been reported

for the Hubbard model yet, but with $R^2/3 = R_z$ and keeping in mind $1/4 + R_z + R_z^2 = (n_{\uparrow} + n_{\downarrow})^2/4$ one obtains the form

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

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 $S^2/3 = S_z$ Hamann^{8/} has obtained the two-field-scheme

$$n_{\uparrow} n_{\downarrow} = \frac{1}{4} (n_{\uparrow} + n_{\downarrow})^2 - \frac{1}{4} (n_{\uparrow} - n_{\downarrow})^2 \quad (13)$$

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

$$n_{\uparrow} n_{\downarrow} = \frac{1}{2} (n_{\uparrow} + n_{\downarrow}) - \frac{2}{3} S^2. \quad (14)$$

From this Heisenberg like form studied by Moriya and Takahashi^{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/}:

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

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

$$n_{\uparrow} n_{\downarrow} = R_z + \frac{2}{3} R^2. \quad (16)$$

Again R^2 may be substituted by $3R_z^2$ resulting in

$$n_{\uparrow} n_{\downarrow} = R_z + 2R_z^2. \quad (17)$$

The identities (16) and (17) may be usefull dealing with superconducting or charge ordered phases of models with Hubbard's interaction. From representation (17) it becomes clear that a contribution to the free energy arises only if $R_z \neq 0$, i.e. if $n_{\uparrow} + n_{\downarrow} \neq 1$ what 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. substituted S_z in eq.(13) by $(\mathbf{e}S)$ with \mathbf{e} being an arbitrary unit vector, and restored rotational symmetry by a final integration over all directions. This idea may be generalised by using $(\mathbf{e}R)$ 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 minimizing 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.

REFERENCES

1. Hubbard J. - Phys.Rev.Lett., 1959, 3, p.78.
2. Ed. Moriya T. - Electron Correlation and Magnetism in Narrow Band Systems (Springer, Berlin, 1981).
3. See for instance: T.Moriya, Spin Fluctuation in Itinerant Electron Magnetism (Springer, Berlin, 1985).
4. Macedo C.A., Continho-Filho M.D., de Morca M.A. - Phys.Rev., 1982, B26, p.5965.
5. Dichtel K., Jelitto R.J., Koppe H. - Z.Physik, 1971, 246, p. 248; 1972, 251, p.173.
6. Birman J.L., Solomon A.L. - Prog.Theor.Phys.Suppl., 1984, 80, p.62.
7. Moriya T., Hasegawa H. - J.Phys.Soc.Japan, 1980,48,p.1490.
8. Hamann D.R. - Phys.Rev.Lett., 1969, 23, p.95.
9. Lacour-Gayet P., Cyrot M. - J.Phys., 1974, C7, p.400.
10. Moriyaya T. - J.Magn.Magn.Mat., 1979, 14, p.1.
11. Wang S.Q., Evenson W.E., Schrieffer J.R. - Phys.Rev.Lett., 1969, 23, p.92.
12. Gomes A.A., Leder H.J. - J.Phys.(Paris), 1977, 38,p.231.
13. Hubbard J. - Phys.Rev., 1979, B10, p.2626; 1979, B20, p.4584.

Received by Publishing Department
on February 17, 1989.