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ON FUNCTIONAL INTEGRAL REPRESENTATIONS IN THE LOWER HUBBARD BAND BASED ON GENERALIZED COHERENT STATES

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1. INTRODUCTION

We consider a high-T_c superconductor as a strongly correlated system [1] with a small concentration of holes. For simplicity we restrict here to a one-band Hubbard Hamiltonian. However, the described methods are without essential changes applicable to more realistic Hamiltonians taking into account, e.g. (i) the anisotropy of the coupled Cu-O planes, (ii) two bands corresponding to Cu and O respectively (see, however, also [2]), and (if necessary) (iii) electron-phonon interaction. Thus we start from the Hamiltonian

$$H = -|t| \sum_{\substack{<ij> \\ \sigma}} c^{+}_{i\sigma} c_{j\sigma} - \mu \sum_{i\sigma} n_{i\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow} \, . \tag{1}$$

Eliminating (in first order in t/U) from the first term in (1) the transitions between singly and doubly occupied states [3] we obtain

$$H_{eff} = -|t| \sum_{\substack{<ij> \\ \sigma}} c^{+}_{i\sigma} c_{j\sigma} - \mu \sum_{i\sigma} n_{i\sigma} + \frac{4t^2}{U} \sum_{<ij>} \{ \vec{S}_i \vec{S}_j - \frac{1}{4} n_i n_j \} , \tag{2}$$

($n_i = n_{i\uparrow} + n_{i\downarrow}$). For simplicity, in (2) we left out a 3-sites term, small for small hole concentration. H_{eff} has to be used only in the restricted Hilbert space *without double occupation!* (The kinetic term in (2) should be better written in terms of the Hubbard operators: $c^{+}_{i\sigma} \to \chi_i^{\sigma 0}$, $c_{j\sigma} \to \chi_j^{0\sigma}$).

The exclusion of double occupation can be done in several ways. (i) The simplest method is explicit projection, i.e. to substitute in the kinetic energy in (2)

$$c^{+}_{i\sigma} c_{j\sigma} \to (1 - c^{+}_{i,-\sigma} c_{i,-\sigma}) \, c^{+}_{i\sigma} c_{j\sigma} \, (1 - c^{+}_{j,-\sigma} c_{j,-\sigma}) \, . \tag{3}$$

This leads to a complicated 3-Fermion interaction. (ii) A second possibility is the slave boson technique [4]. This method, like the representation of the c-operators used by Anderson and coworkers (see, e.g. [5], and also [10]), has some similarity with the method used here. However, besides the not very clear statistical nature of the introduced "bosons", too much fields are used (note that additionally a Lagrange multiplier for the constraint is needed). (iii) Anderson and coworkers [6] used the Lagrange multipliers of three constraints as the time components of an SU(2) gauge field. (iv) A fourth possibility, considered here, is based on the idea to derive a functional integral representation by introducing (after each infinitesimal time interval) a "restricted" unity, $\hat{1}$, i.e. a projection onto the restricted Hilbert space.

In a special representation that fourth possibility was already used by Wiegmann /7/. It is the aim of this work to investigate systemically such representation with the smallest possible number of fields corresponding to the restricted number of degrees of freedom.

2. RESTRICTED UNITY BY MEANS OF COHERENT STATE

From generalized coherent states /8/, $T(\alpha)|\,)$, where the operator $T(\alpha)$, giving an irreducible unitary representation of the Lie group (α characterizes the group element), acts on a reference state $|\,)$, one can construct projection operators

$$P(\alpha) = T(\alpha)\,\chi\, T^{+}(\alpha)\,; \tag{4}$$

$\chi = |\,)(\,|$ is the projection operator onto the reference state. Integration over α with respect to an invariant measure $d_\mu(\alpha)$ provides then a resolution of the (restricted) unity $\hat{1}$:

$$\int d_\mu(\alpha)\, P(\alpha) = \hat{1}\,. \tag{5}$$

This restricted unity is used for the derivation of a functional integral representation by inserting $\hat{1}$ after each infinitesimal time interval (see Appendix). Strictly, what is really necessary for the construction of the functional integral is an operator $T(\alpha)$ satisfying

$$(\,|T^{+}(\alpha)T(\alpha)|\,) = 1\,, \tag{6}$$

and a measure satisfying (5).

For illustration let us consider a spinless "fermion" characterized by the operators c, c^{+} (one degree of freedom):

$$P(\psi, \psi^{+}) = e^{i(\psi c^{+} + c\psi^{+})}|0)(0|\,e^{-i(\psi c^{+} + c\psi^{+})}. \tag{7}$$

Here the vacuum is used as reference state, the exponents contain the element of the Lie algebra spanned by c, c^{+} (and unity, not necessary), and (correspondingly) the ψ, ψ^{+} are Grassmann variables /9/. The resolution (here of the unrestricted) unity is given by

$$\int d\psi\, d\psi^{+}\, P(\psi, \psi^{+}) = |0)(0| + |1)(1| = \hat{1}\,. \tag{8}$$

In the case of the lower Hubbard band the super Lie algebra is spanned by the Hubbard projection operators /10/ χ^{00}, $\chi^{\uparrow\uparrow}$, $\chi^{\downarrow\downarrow}$, $\chi^{\uparrow\downarrow} = |\uparrow)(\downarrow|$, $\chi^{\downarrow\uparrow}$, $\chi^{0\uparrow}$, $\chi^{0\downarrow}$, $\chi^{\uparrow 0}$, $\chi^{\downarrow 0}$ and unity, instead of the much simpler algebra of $c_\uparrow$, $c_\downarrow$, $c^{+}_\uparrow$, $c^{+}_\downarrow$ (and unity) characterizing the unrestricted Hilbert space.

In the following we introduce only one pair of Grassmann variables ψ, ψ^{+} (for each lattice site and each time) in contrast to Wiegmann /7/, who introduced $\psi_\uparrow, \psi^{+}_\uparrow, \psi_\downarrow, \psi^{+}_\downarrow$ (and thereafter a constraint). Our physical reasoning for the minimal possible number of fields is as follows: The electron is either present or absent (at given site and time), this should be described by one Grassmann pair; then we have to fix its spin direction, this should be described by one c-number with at least two values. We write down the most general expression for T with only one Grassmann variable ψ:

$$\begin{aligned} T = {} & 1 + \alpha_0\chi^{00} + \alpha_\uparrow\chi^{\uparrow\uparrow} + \alpha_\downarrow\chi^{\downarrow\downarrow} + \gamma\chi^{\uparrow\downarrow} + \tilde{\gamma}\chi^{\downarrow\uparrow} + \\ & + \beta_\uparrow\psi\chi^{\uparrow 0} + \chi^{0\uparrow}\psi^{+}\tilde{\beta}_\uparrow + \beta_\downarrow\psi\chi^{\downarrow 0} + \chi^{0\downarrow}\psi^{+}\tilde{\beta}_\downarrow\,; \end{aligned} \tag{9}$$

$$\begin{aligned} \alpha_0 &= a_0 + b_0\psi\psi^{+}, & \gamma &= g + d\psi\psi^{+}, \\ \alpha_{\uparrow\downarrow} &= a_{\uparrow\downarrow} + b_{\uparrow\downarrow}\psi\psi^{+}, & \tilde{\gamma} &= \tilde{g} + \tilde{d}\psi\psi^{+}. \end{aligned} \tag{10}$$

For the c-number coefficients a_0, b_0, $a_{\uparrow\downarrow}$, $b_{\uparrow\downarrow}$, g, d, $\tilde{g}$, $\tilde{d}$, $\beta_{\uparrow\downarrow}$, $\tilde{\beta}_{\uparrow\downarrow}$ we obtain conditions by the unitarity requirement for T and the requirement of the resolution of unity (5).

Out of the large family of representations we concentrate in the following on special representations by specifying the reference state as the vacuum, $|\,) = |0)$. We think that this reference state corresponds better to the (magnetically not ordered) superconducting phase than the antiferromagnetic reference state used in /7/. However it is clear from the general theory /8/ that the chosen reference state does not play any physical role. Then we obtain for the projection operator (4) the special solution (among other solutions)

$$\begin{aligned} P = {} & T\chi^{00}T^{+} = \\ & [1 + \psi\psi^{+} + \beta_\uparrow\psi\chi^{\uparrow 0} + \beta_\downarrow\psi\chi^{\downarrow 0}]\,\chi^{00}\,[1 + \psi\psi^{+} + \beta^{+}_\uparrow\chi^{0\uparrow}\psi^{+} + \beta^{+}_\downarrow\chi^{0\downarrow}\psi^{+}] \end{aligned} \tag{11}$$

for each site and each time. For β the following two representations can be used

$$\text{(i)}\quad \beta_\uparrow = \beta^{+}_\downarrow = e^{i\varphi}\,. \tag{12a}$$

with the resolution of the restricted unity

$$\int d\psi^{+} d\psi\, e^{-\psi\psi^{+}} \int_{0}^{\pi} \frac{d\phi}{\pi} P = \chi^{00} + \chi^{\uparrow\uparrow} + \chi^{\downarrow\downarrow} =: \hat{1},$$

or

$$\text{(ii)}\quad \beta_{\uparrow} = 1, \quad \beta_{\downarrow} = \pm 1, \tag{12b}$$

with

$$\int d\psi^{+} d\psi\, e^{-\psi\psi^{+}} \frac{1}{2} \sum_{\beta_{\downarrow} = \pm 1} P = \chi^{00} + \chi^{\uparrow\uparrow} + \chi^{\downarrow\downarrow} =: \hat{1}.$$

The second case precisely corresponds to the physical reasoning given above.

Finally we write down the substitutions transforming the original operators into the fields of the functional integral (for details see the Appendix):

$$\begin{aligned} c_{j\sigma} &\to \chi_j^{0\sigma} + \psi_j \beta_{j\sigma}, \\ c^{+}_{j\sigma} &\to \chi_j^{\sigma 0} + \psi_j^{+} \beta^{*}_{j\sigma}. \end{aligned} \tag{13}$$

3. DISCUSSION

We constructed a functional integral representation in the lower Hubbard band (after taking into account virtual transitions to the upper Hubbard band by the usual canonical transformation) based on one Grassmann field and one two-valued c-number field. At least for evaluation by a computer this minimal possible range of the field configurations in our scheme seems to be an advantage. The description with only one Grassmann field was formulated without introducing a constraint between Grassmann fields for the two spin directions. The connection of our scheme with a gauge field theory is to be studied.

In some sense the Grassmann field ψ reminds Anderson's spinon, the phase ϕ of β has some similarity with the transformed phase in the slave boson technique [11].

In the action the kinematical part Λ_{00} and the term coming from H''_{eff} are bilinear in the Grassmann field. The part Λ_{AF} of the action coming from the antiferromagnetic term in H_{eff} can be bilinearized with respect to the Grassmann field in the usual way by means of a Hubbard Stratonovich transformation. After evalution of the Grassmann integral a purely bosonic theory remains, where the constraints (exclusion of double occupation) are exactly taken into account.

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APPENDIX

We consider the generating functional (Matsubara technique) and introduce a time lattice:

$$Z[\eta, \eta^{+}] = \mathrm{Tr}\,\{T \exp[-i \int_{0}^{-i\beta} dt (H_{eff} + \sum_{j\sigma} \eta^{+}_{j\sigma}(t)\, \chi_j^{0\sigma} + \sum_{j\sigma} \chi_j^{\sigma 0}\, \eta_{j\sigma}(t))]\} =$$

$$= \int \prod_{\substack{n=0 \\ j}}^{N-1} \{ d\psi_j^{+}(t_n)\, d\psi_j(t_n)\, e^{-\psi_j(t_n)\psi_j^{+}(t_n)} \frac{1}{2} \sum_{\beta_{j\downarrow}(t_n) = \pm 1} \} \times$$

$$\times \mathrm{Tr}\{[1 - iH_{eff}\Delta t][1 - i \sum_{j\sigma} (\eta^{+}_{j\sigma}(t_{N-1})\, \chi_j^{0\sigma} + \chi_j^{\sigma 0}\, \eta_{j\sigma}(t_{N-1}))\Delta t] \times \tag{A1}$$

$$\times T(t_{N-1})\, \chi^{00}\, T^{+}(t_{N-1}) \cdot \ldots [1 - iH_{eff}\Delta t][1 - i \sum_{j\sigma} (\eta^{+}_{j\sigma}(t_0)\, \chi^{0\sigma} + \text{h.c.})\Delta t]\, T(t_0)\, \chi^{00}\, T^{+}(t_0)\} =$$

$$= \int \prod_{\substack{n=0 \\ j}}^{N-1} \{ d\psi_j^{+}(t_n)\, d\psi_j(t_n)\, e^{-\psi_j(t_n)\psi_j^{+}(t_n)} \frac{1}{2} \sum_{\beta_{j\downarrow}(t_n)} \}\, e^{\Lambda_{00} + \Lambda_{kin} + \Lambda_{\mu} + \Lambda_{AF} + \Lambda_{source}}$$

$\eta, \eta^{(+)}$ are Grassmann sources; $n = 0, 1, \ldots, N-1$; $\Delta t = -i\beta/N$, $N \to \infty$. The "kinematic" term Λ_{00} is given by

$$\Lambda_{00} = \sum_{\substack{n=0 \\ j}}^{N-1} \psi_j^{+}(t_n)\, \{\psi_j(t_{n-1})[1 + \beta_{j\downarrow}(t_n)\, \beta_{j\downarrow}(t_{n-1})] - \psi_j(t_n)\}; \tag{A2}$$

the representation (12b) was used in (A1, A2). The kinetic energy in (2) gives rise to

$$\Lambda_{kin} = i(-|t|) \sum_{\substack{n=0 \\ \langle ij \rangle \\ \sigma}}^{N-1} \psi_i^{+}(t_n)\, \beta^{*}_{i\sigma}(t_n)\, \psi_j(t_{n-1})\, \beta_{j\sigma}(t_{n-1})\, \Delta t, \tag{A3}$$

and analogous expressions for the other terms of the action.

Because of the T-ordering in (A1) the sources have to satisfy the boundary condition

$$\eta_{j\sigma}(t_N) = -\eta_{j\sigma}(t_0 = 0)\,, \tag{A4}$$

leading to (as one would expect)

$$\begin{aligned} \psi_{j\sigma}(t_N) &= -\psi_{j\sigma}(t_0)\,, \\ \beta_{j_\downarrow^\uparrow}(t_N) &= \beta_{j_\downarrow^\uparrow}(t_0)\,. \end{aligned} \tag{A5}$$

We have to mention that in (A2, A3) terms (coming from (A1, A5)) anomalous at the lower boundary of the time interval (at $t_o = 0$) are not written down. It has to be investigated in detail whether such terms and other (time) lattice effects are essential in the sense of Klauder [12] or whether one can immediately go to a simpler continuum version.

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Веллер В. E17-88-510

О функционально-интегральных представлениях для нижней хаббардовской зоны с использованием обобщенных когерентных состояний

Изучался однозонный гамильтониан Хаббарда в пределе сильного взаимодействия. С помощью канонического преобразования (в первом порядке по t/U) в этом гамильтониане исключались переходы между состояниями с одним электроном и двумя электронами на узле. При использовании обобщенных когерентных состояний исследовались представления в виде функционального интеграла, которые исключают дважды заполненные состояния. Предложено специальное представление, в котором требуется только одно грассманово поле ψ и одно c-числовое поле β (в простейшем виде $\beta = \pm 1$) в точном соответствии с ограничением на число степеней свободы.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

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Weller W. E17-88-510

On Functional Integral Representations in the Lower Hubbard Band Based on Generalized Coherent States

The Hubbard Hamiltonian is considered after the elimination (to first order in t/U) of transitions between singly and doubly occupied sites by means of a canonical transformation. Using generalized coherent states we investigate functional integral representations excluding double occupation. A special representation is constructed, which needs only one Grassmann field ψ and one c-number field β (in the simplest form $\beta = \pm 1$) in exact correspondence to the restricted number of degrees of freedom.

The investigation has been performed at the Laboratory of Theoretical Physics, JINR.

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