ON THE FUNCTIONAL INTEGRAL METHOD APPLIED TO MODELS WITH HUBBARD TYPE INTERACTION

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To avoid the arbitrariness of the functional integral method, originating from the numerous different ways to rewrite the Hubbard interaction, a self-consistent procedure is given based on a generalized quadratic form in terms of spins and quasispins.

The Hamiltonian

$$H=\sum_{k}\sum_{\sigma}\epsilon_k c_{k\sigma}^{+}c_{k\sigma}+U\sum_{i}n_{i\uparrow}n_{i\downarrow}\,, \tag{1}$$

with $c_{i\sigma}^{+}$ and $c_{k\sigma}^{+}$ being creation operators of fermions in a Bloch and Wannier state respectively, is usually called the Hubbard model [1], if one assumes U to be positive, since it is the on-site matrix element of the electron–electron interaction. Otherwise, if U is thought to describe a kind of effective attraction of electrons like in the simplest version of a model of superconductivity, it can be negative. Unfortunately the two cases, i.e. $u>0$ and $u<0$, are usually treated differently, due to the differing goals of describing magnetism and superconductivity [2,3]. In the following it will be shown, that by generalization of the functional integral method worked out mainly for magnetic purposes, it is possible to handle both the attractive and the repulsive version of the model (1) on the same footing.

The functional integral technique starts with rewriting the interaction term of the Hamiltonian as quadratic form. There are several different transformations known up to now within the context of magnetism, which are all operator identities and formally equivalent, when approximations are introduced. However, employing a special approximation scheme usually destroys this equivalence resulting in different results to the same physical questions. Due to the lack of criterion which transformation is to be preferred the method is often called arbitrary, since the choice of the quadratic form predetermines the results. To avoid this disadvantage the authors argued, that dealing with the model (1) one should not restrict the various possibilities to break symmetries, what is usually done by adopting a special quadratic form, rather the model should "have the choice" by minimizing its thermodynamical potential [4]. Working out this idea we start by rewriting the interaction term

$$n_{i\uparrow}n_{i\downarrow}=\tfrac{1}{4}(1-\alpha_i)+R_{iz}+\tfrac{1}{3}(\alpha_i-1)\boldsymbol{S}_i^2+\tfrac{1}{3}(\alpha_i+1)\boldsymbol{R}_i^2\,, \tag{2}$$

with $\boldsymbol{S}_i$ being the spin vector

$$S_{ix}=\tfrac{1}{2}(c_{i\uparrow}^{+}c_{i\downarrow}+c_{i\downarrow}^{+}c_{i\uparrow})\,,\quad S_{iy}=\frac{1}{2\mathrm{i}}(c_{i\uparrow}^{+}c_{i\downarrow}-c_{i\downarrow}^{+}c_{i\uparrow})\,,\quad S_{iz}=\tfrac{1}{2}(n_{i\uparrow}-n_{i\downarrow})\,, \tag{3}$$

and $\boldsymbol{R}_i$ being the quasispin vector

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$$R_{ix}=\tfrac{1}{2}(c_{i\uparrow}^{+}c_{i\downarrow}^{+}+c_{i\downarrow}c_{i\uparrow}),\quad R_{iy}=\frac{1}{2\mathrm{i}}(c_{i\uparrow}^{+}c_{i\downarrow}^{+}-c_{i\downarrow}c_{i\uparrow}),\quad R_{iz}=\tfrac{1}{2}(n_{i\uparrow}+n_{i\downarrow}-1)\,. \tag{4}$$

This transformation was shown to be a generalization of almost all quadratic forms used in the context of magnetism [4]. However, due to the containment of both spins and quasispins in (2) it is possible to look for magnetism ($\langle \boldsymbol{S}_i\rangle \neq 0$), charge ordering ($\langle R_{iz}\rangle \neq 0$), or superconduction ($\langle R_{ix}\rangle \neq 0$) in a unified manner. Inserting eq. (2) into eq. (1) and applying the time ordering trick the partition sum becomes

$$\mathscr{Z}_\alpha=\exp\Big(-\tfrac{1}{4}\beta U\sum_i(1+\alpha_i)\Big)\,\mathrm{tr}\Big\{T_\tau\exp(-\beta\mathscr{H}_0)\exp\Big(-\beta\int_0^1 \mathrm{d}\tau\, H_1(\tau)\Big)\Big\}\,, \tag{5}$$

with

$$\mathscr{H}_0=\sum_{\boldsymbol{k}}\sum_\sigma(\epsilon_{\boldsymbol{k}}-\mu+\tfrac{1}{2}U-\sigma h_{\mathrm{ex}})n_{\boldsymbol{k}\sigma}\,, \tag{6}$$

$$H_1(\tau)=-\tfrac{1}{3}U\sum_i(1-\alpha_i)\boldsymbol{S}_i^2(\tau)+\tfrac{1}{3}U\sum_i(1+\alpha_i)\boldsymbol{R}_i^2(\tau)\,, \tag{7}$$

$$A(\tau)=\exp(\tau\beta\mathscr{H}_0)\,A\exp(-\tau\beta\mathscr{H}_0)\,, \tag{8}$$

and h_{ex} the external magnetic field applied in the z-direction and measured in energy units. One can immediately see that the chemical potential μ which is known to be $U/2$ when neutrality and electron hole symmetry is assumed, acts as symmetry breaking field with respect to R_z in the same manner as h_{ex} does with respect to S_z. The latter may be of interest when (1) is applied to describe substitution effects in magnets or superconductors. Now, the Hubbard–Stratonovic transformation

$$\exp(aA^2)=\int_{-\infty}^{\infty}\mathrm{d}x\exp(-\pi x^2-2\sqrt{\pi a}\,xA) \tag{9}$$

is used at every lattice site and at each instant of "imaginary time" to rewrite the partition sum as functional integral,

$$\mathscr{Z}_\alpha=\int_{-\infty}^{\infty}\prod_{i=1}^{N}\mathscr{D}^3\boldsymbol{x}_i(\tau)\mathscr{D}^3\boldsymbol{y}_i(\tau)\exp\{-\Omega_\alpha[\ldots\boldsymbol{x}_i(\tau)\ldots,\ldots\boldsymbol{y}_i(\tau)\ldots]\}\,, \tag{10}$$

with Ω_α being the functional

$$\Omega_\alpha=\pi\sum_i\int_0^1\mathrm{d}\tau\,[\boldsymbol{x}_i^2(\tau)+\boldsymbol{y}_i^2(\tau)]+\ln Z_\alpha[\ldots\boldsymbol{x}_i(\tau)\ldots,\ldots\boldsymbol{y}_i(\tau)\ldots]\,, \tag{11}$$

where

$$Z_\alpha=\mathrm{tr}\Big\{T_\tau\exp(-\beta\mathscr{H}_0)\exp\Big(-\sqrt{\tfrac{4}{3}\pi\beta U}\sum_i\int_0^1\mathrm{d}\tau\,(\sqrt{1-\alpha_i}\,\boldsymbol{x}_i\boldsymbol{S}_i+\mathrm{i}\sqrt{1+\alpha_i}\,\boldsymbol{y}_i\boldsymbol{R}_i)\Big)\Big\}\,. \tag{12}$$

By substituting

$$\boldsymbol{X}_i(\tau)=\sqrt{1-\alpha_i}\,\boldsymbol{x}_i(\tau)\,,\quad \boldsymbol{Y}_i(\tau)=\sqrt{1+\alpha_i}\,\boldsymbol{y}_i(\tau) \tag{13}$$

one can shift the α_i-dependence to the Gaussian measure

$$\mathscr{Z}_\alpha = \int_{-\infty}^{\infty} \prod_{i=1}^{N} \frac{\mathscr{D}^3 \boldsymbol{X}_i(\tau)\, \mathscr{D}^3 \boldsymbol{Y}_i(\tau)}{(\sqrt{1-\alpha_i^2})^3} \exp\{-\Omega[\alpha; ...\boldsymbol{X}_i(\tau)..., ...\boldsymbol{Y}_i(\tau)...]\}\,, \tag{14}$$

with

$$\Omega[\alpha; ...] = \pi \sum_i \int_0^1 \mathrm{d}\tau \left(\frac{\boldsymbol{X}_i^2(\tau)}{1-\alpha_i} + \frac{\boldsymbol{Y}_i^2(\tau)}{1+\alpha_i} \right) + \ln Z[...\boldsymbol{X}_i(\tau)..., ...\boldsymbol{Y}_i(\tau)...]\,, \tag{15}$$

$$Z[...] = \mathrm{tr}\left\{ T_\tau \exp(-\beta \mathscr{H}_0) \exp\left(-\sqrt{\tfrac{4}{3}\pi\beta U} \sum_i \int_0^1 \mathrm{d}\tau\, [\boldsymbol{X}_i(\tau)\boldsymbol{S}_i(\tau) + \mathrm{i}\boldsymbol{Y}_i(\tau)\boldsymbol{R}_i(\tau)] \right) \right\}. \tag{16}$$

Therefore the functional Z is no longer explicitly dependent on the α_i. Now, one can proceed in the usual way, i.e. applying the coupling constant trick, writing down the associated Dyson equation, discuss the different approximation schemes developed to calculate Z, etc., as done e.g. in ref. [3] for the two-field scheme, which is a special case of eq. (2). Of course, the latter is outside the scope of this Letter and will be published elsewhere. However, without doing any special calculation one immediately recognizes that for each approximation the dependence of the α_i will be different. Therefore the best choice of the α_i is determined by the approximation employed to calculate the partition sum and the related thermodynamical potential. By minimizing the latter one finds the equation determining the α_i straightforwardly,

$$-\frac{1}{\beta}\frac{\partial}{\partial \alpha_i} \ln \mathscr{Z}_\alpha = 0 \quad \text{for all } \alpha_i\,. \tag{17}$$

This criterion holds independent of the method used to evaluate the functional integral (14). However, usually the partition sum is calculated by means of the saddle point approximation, i.e. only the extremizing "paths", hereafter assigned as $\boldsymbol{X}_i^{\mathrm{e}}(\tau)$ and $\boldsymbol{Y}_i^{\mathrm{e}}(\tau)$, are of interest. By minimizing the functional Ω with respect to the fields one finds

$$\boldsymbol{X}_i^{\mathrm{e}}(\tau) = \frac{1-\alpha_i}{2\pi} \frac{\delta}{\delta \boldsymbol{X}_i(\tau)} \ln Z|_{\boldsymbol{X}_i(\tau)=\boldsymbol{X}_i^{\mathrm{e}}(\tau),\, \boldsymbol{Y}_i(\tau)=\boldsymbol{Y}_i^{\mathrm{e}}(\tau)}\,, \tag{18}$$

$$\boldsymbol{Y}_i^{\mathrm{e}}(\tau) = \frac{1+\alpha_i}{2\pi} \frac{\delta}{\delta \boldsymbol{Y}_i(\tau)} \ln Z|_{\boldsymbol{X}_i(\tau)=\boldsymbol{X}_i^{\mathrm{e}}(\tau),\, \boldsymbol{Y}_i(\tau)=\boldsymbol{Y}_i^{\mathrm{e}}(\tau)}\,. \tag{19}$$

Within the saddle point approximation the thermodynamical potential becomes a functional of the extremizing paths, which are functions of the α_i via eqs. (18) and (19). One has

$$-\frac{1}{\beta} \ln \mathscr{Z}_\alpha^{\mathrm{sp}} = \tfrac{1}{4} U \sum_i (1+\alpha_i) + \frac{3}{2\beta} \sum_i \ln(1-\alpha_i^2) + \frac{1}{\beta} \Omega[\alpha; ...\boldsymbol{X}_i^{\mathrm{e}}..., ...\boldsymbol{Y}_i^{\mathrm{e}}...]\,. \tag{20}$$

From eq. (17) one finds

$$0 = \frac{1}{\beta}\frac{\partial \Omega}{\partial \alpha_i} + \frac{1}{\beta}\frac{\delta \Omega}{\delta \boldsymbol{X}_i^{\mathrm{e}}}\frac{\mathrm{d}\boldsymbol{X}_i^{\mathrm{e}}}{\mathrm{d}\alpha_i} + \frac{1}{\beta}\frac{\delta \Omega}{\delta \boldsymbol{Y}_i^{\mathrm{e}}}\frac{\mathrm{d}\boldsymbol{Y}_i^{\mathrm{e}}}{\mathrm{d}\alpha_i} - \frac{3\alpha_i}{\beta(1-\alpha_i^2)} + \tfrac{1}{4}U\,. \tag{21}$$

The second and the third term in eq. (21) vanish due to the saddle point approximation. Since Z depends not explicitly on α_i the resulting expression looks like

$$0 = \tfrac{1}{4}\beta U - \frac{3\alpha_i}{1-\alpha_i^2} + \frac{\pi}{(1-\alpha_i)^2} \int_0^1 \mathrm{d}\tau\, \boldsymbol{X}_i^{\mathrm{e}2}(\tau) - \frac{\pi}{(1+\alpha_i)^2} \int_0^1 \mathrm{d}\tau\, \boldsymbol{Y}_i^{\mathrm{e}2}(\tau)\,. \tag{22}$$

The fields can be expressed by means of the mean values of the local spins and quasispins. From variation of the functional $\ln Z$ in eqs. (18) and (19) one finds

$$\boldsymbol{X}_i^e(\tau) = -\frac{1-\alpha_i}{2\pi}\sqrt{\tfrac{4}{3}\pi\beta U}\,\langle \boldsymbol{S}_i(\tau)\rangle_e\,, \tag{23}$$

$$\boldsymbol{Y}_i^e(\tau) = -\mathrm{i}\frac{1+\alpha_i}{2\pi}\sqrt{\tfrac{4}{3}\pi\beta U}\,\langle \boldsymbol{R}_i(\tau)\rangle_e\,. \tag{24}$$

Here we introduced

$$\langle A(\tau)\rangle_e = \frac{\mathrm{tr}\{T_\tau \rho_e A(\tau)\}}{\mathrm{tr}\{T_\tau \rho_e\}} \tag{25}$$

and

$$\rho_e = \exp(-\beta\mathscr{H}_0)\exp\left(-\sqrt{\tfrac{4}{3}\pi\beta U}\sum_i \int_0^1 \mathrm{d}\tau\,[\boldsymbol{X}_i^e(\tau)\boldsymbol{S}_i(\tau) + \boldsymbol{Y}_i^e(\tau)\boldsymbol{R}_i(\tau)]\right). \tag{26}$$

Inserting eqs. (23) and (24) into eq. (22) yields

$$\frac{\alpha_i}{1-\alpha_i^2} = \tfrac{1}{12}\beta U\left(1 + \tfrac{4}{3}\int_0^1 \mathrm{d}\tau\,\langle \boldsymbol{S}_i(\tau)\rangle_e^2 + \tfrac{4}{3}\int_0^1 \mathrm{d}\tau\,\langle \boldsymbol{R}_i(\tau)\rangle_e^2\right) =: B\,, \tag{27}$$

which gives the two solutions

$$\alpha_{i1,2} = -\frac{1}{2B}\,(1 \pm \sqrt{1+4B^2})\,. \tag{28}$$

The second term in eq. (20) demands

$$1-\alpha_i^2 = \alpha_i/B > 0\,. \tag{29}$$

This selects

$$\alpha_i = -\frac{1}{2B}\,(1-\sqrt{1+4B^2})\,. \tag{30}$$

By eq. (30) the α_i are completely determined and therefore no "arbitrariness" remains. However, since the α_i depend on the mean values of the local spins and quasispins, i.e. the quadratic form itself depends on the results which should be calculated from it, one has to solve a self-consistent problem. The remaining task is to determine the functional Z in a more or less advanced approximation scheme. This is beyond the scope of this Letter and will be published elsewhere.

The idea of the method presented above can also be applied if the functional integration is carried out by expansion around the extremizing paths to the second order. Furthermore, what is said above is independent on the special kind of $\mathscr{H}_0$, since it is related to the Hubbard interaction term only, and therefore other models, e.g. the (periodic) Anderson model, may be treated in complete analogy.

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