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PROBABILISTIC INTERPRETATION
# OF QUANTUM STATISTICAL MODELS

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1. INTRODUCTION

The substitution of an operator in the interaction term by a c-number forms the basis of many approximations. In the Hartree approximation the relevant operator is substituted by its mean value. More sophisticated approximations use random c-numbers with an appropriate distribution function. The alloy analogy approximation [1] for the Hubbard model is of this type. In the equations of motion of the electron subsystem with spin up the particle number operators $n_{i\downarrow}$ are replaced by c-numbers $\nu_{i\downarrow}$ randomly distributed over the values 0 or 1 with fixed averages $\langle \nu_{i\downarrow} \rangle_{\nu} = \langle n_{i\downarrow} \rangle$. Also the treatment of the electron-phonon interaction in a disordered system by Chen et al. [2] belongs to this type. There, the linear combinations $\gamma_{si} b_s + \gamma_{si}^{*} b_s^{+}$ of phonon operators are replaced by random c-numbers with a Gaussian distribution.

Of course, such schemes are limited in approaching the exact behaviour if only time-independent c-numbers are used. To our knowledge the first who replaced an operator by a time-dependent c-number in a many body problem were Nozières and De Dominicis [3] in their treatment of x-ray absorption and emission in metals. The particle number operator of the deep hole is there substituted by a given c-number function of time. The replacement is exact, and as a consequence of the simple form of the Hamiltonian the c-number is not random (see also ref. [6]).

The application of the Hubbard-Stratonovich transformation to the Anderson model and the Hubbard model (compare, e.g., ref. [4]) leads to exact expressions for the partition function or Green functions, where operators in the interaction terms are replaced by time-dependent random c-numbers. Because the Hubbard-Stratonovich transformation applies to quadratic interactions the interaction terms first have to be rewritten identically which much complicates the situation.

In refs. [5,6] we considered the Hubbard interaction term $U \sum_i n_{i\uparrow} n_{i\downarrow}$ in its original simple form and showed that the Hubbard problem can be exactly transformed into a problem of band electrons with spin σ interacting with time-dependent random potentials $U\nu_{i,-\sigma}(t)$. The stochastic process $\nu_{i,-\sigma}(t)$ jumps between the values 0 and 1. In ref. [5] the probabilities are determined implicitly by the requirement that all $\nu_{i,-\sigma}$-correlation functions have to coincide with all T-ordered $n_{i,-\sigma}$-correlation functions; in ref. [6] an explicit, however formal, expression for the probabilities is derived.

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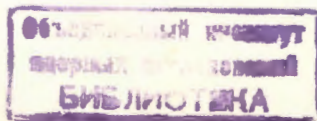
In Sec. 2 of this paper we again consider the stochastic process ν for the Hubbard model. Starting from the Green function represented as a functional integral we construct by partially evaluation of this functional integral the probability measure of the stochastic process explicitly. The (free) process is like a Binomial process in the Poisson limit, jumping between 0 and 1; however it has to be periodic because of the periodicity condition for Bose-type operators in quantum statistical thermodynamics.

In Sec. 3 we consider a simple electron-phonon interaction model using the functional integral representation to substitute the phonon operators by a stochastic process. The free process turns out to be Gaussian and periodic.

The situation in quantum statistical thermodynamics is similar to that in Euclidean quantum field theory (compare, e.g., ref. [7]). The imaginary time is even more "natural" in quantum statistics. The type of the free process depends on the unperturbed Hamiltonian and the substituted operator. However, the Markovian property known in quantum field theory is obviously destroyed here by the periodicity condition.

2. THE STOCHASTIC PROCESS FOR THE HUBBARD MODEL

The Hamiltonian of the Hubbard model is given by

$$H = \sum_{ij \atop \sigma} t_{ij} a^+_{i\sigma} a_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} , \tag{1}$$

with $t_{ii} = -\mu$ (μ chemical potential), $t_{<ij>} = t$ ($<ij>$ means nearest neighbours), and for simplifying the discussion $t_{ij} = 0$ otherwise. The thermodynamical Green function of the spin $\uparrow$ electron subsystem (interacting via the last term in (1) with the spin $\downarrow$ subsystem) can be represented as a functional integral [8-10] :

$$G_\uparrow(j\tau, j'\tau') \equiv -<T a_{j\uparrow}(\tau) a^+_{j'\uparrow}(\tau')> =$$

$$= - \frac{\int D a_\uparrow D a^+_\uparrow D a_\downarrow D a^+_\downarrow a_{j\uparrow}(\tau) a^+_{j'\uparrow}(\tau') e^S}{\int D a_\uparrow D a^+_\uparrow D a_\downarrow D a^+_\downarrow e^S} , \tag{2}$$

with the action

$$S = - \int_0^\beta d\tau \{ \sum_{i\sigma} a^+_{i\sigma} \frac{\partial}{\partial \tau} a_{i\sigma} + H \} . \tag{3}$$

We use imaginary time $t = -i\tau$, $\tau \in [0, \beta]$. The a, a^+ are Grassmann variables, totally anticommuting (including the differentials), and antiperiodic on the time interval:

$$a_{i\sigma}(0) = -a_{i\sigma}(\beta) . \tag{4}$$

For the following we define the functional integral in the simplest way as a multiple integral on the equidistant time points $\tau_\ell = \ell \Delta \tau$, $\ell = 0,1,...,L-1$, with $\tau_0 = 0$ and $\tau_L = L\Delta\tau = \beta$, $L \to \infty$. Then

$$D a_\downarrow D a^+_\downarrow = \prod_{i,\ \ell=0}^{L-1} d a_{i\downarrow}(\tau_\ell) d a^+_{i\downarrow}(\tau_\ell) , \tag{5}$$

and we use the standard integrals

$$\int d a_{i\sigma} = \int d a^+_{i\sigma} = 0 ,$$
$$\int a_{i\sigma} d a_{i\sigma} = \int a^+_{i\sigma} d a^+_{i\sigma} = 1 . \tag{6}$$

For the derivative term in S we write

$$\int_0^\beta d\tau a^+_{i\downarrow} \frac{\partial}{\partial \tau} a_{i\downarrow} = \sum_{\ell=0}^{L-1} a^+_{i\downarrow}(\tau_\ell) \frac{a_{i\downarrow}(\tau_{\ell+1}) - a_{i\downarrow}(\tau_\ell)}{\Delta\tau} \Delta\tau . \tag{7}$$

(7) could be written in a more symmetrical form, but this simpler form gives the same results.

Now we partially evaluate the functional integrals in (2) by performing the integrations $D a_\downarrow D a_\downarrow$ over the variables of the spin $\downarrow$ subsystem. We consider the integral in the denominator of (2):

$$\int D a_\downarrow D a^+_\downarrow e^S =$$

$$= \int D a_\downarrow D a^+_\downarrow \prod_{i\ell} \{ 1 - a^+_{i\downarrow}(\tau_\ell) a_{i\downarrow}(\tau_{\ell+1}) +$$

$$+ a^+_{i\downarrow}(\tau_\ell) a_{i\downarrow}(\tau_\ell)(1 + \mu\Delta\tau - U n_{i\uparrow}(\tau_\ell)\Delta\tau) \} \times$$

$$\times \{ 1 - \sum_{j(\neq i)} t_{ij} a^+_{i\downarrow}(\tau_\ell) a_{j\downarrow}(\tau_\ell) \Delta\tau \} =$$

$$= \int D a_\downarrow D a^+_\downarrow \prod_{i\ell} \{ 1 - A_{i\ell} + B_{i\ell} \exp[(\mu - U n_{i\uparrow}(\tau_\ell))\Delta\tau]\} \{ 1 - \sum_{j(\neq i)} T_{ij,\ell} \} .$$

The expansion of the exponential in the first equation of (8) is exact because of $a_{i\sigma}^2(r_\ell) = 0$. The integral is only different from zero if any a, a^+ appears once. We get 3 typical combinations:

(i) products of $B_{i\ell}$ multiplied by

$$\exp[(\mu - Un_{i\uparrow}(r_\ell))\nu_{i\downarrow}(r_\ell)\Delta r] \text{ with } \nu_{i\downarrow}(r_\ell) = 1 ;$$

(ii) products of $A_{i\ell}$ multiplied by the same exponential with $\nu_{i\downarrow}(r_\ell) = 0$.

(iii) single transfer factors $T_{ij,\ell}$ changing
$\nu_{i\downarrow}$ from 0 to 1,
$\nu_{j\downarrow}$ from 1 to 0.

The final result is the following. The Green function is represented as

$$G_\uparrow(jr, j'r') = -\frac{\int P_0[\nu_\downarrow]D\nu_\downarrow \int Da_\uparrow Da_\uparrow^+ a_{j\uparrow}(r)a_{j'\uparrow}^+(r')e^{S_\uparrow[\nu_\downarrow]}}{\int P_0[\nu_\downarrow]D\nu_\downarrow \int Da_\uparrow Da_\uparrow^+ e^{S_\uparrow[\nu_\downarrow]}}, \quad (9)$$

with

$$S_\uparrow[\nu_\downarrow] = -\int_0^\beta dr \{ \sum_i a_{i\uparrow}^+ \frac{\partial}{\partial r} a_{i\uparrow} + \sum_{ij} t_{ij} a_{i\uparrow}^+ a_{j\uparrow} +$$

$$+ \sum_i (-\mu + Ua_{i\uparrow}^+ a_{i\uparrow}(r))\nu_{i\downarrow}(r) \}. \quad (10)$$

Eqs. (9,10) describe band electrons with spin ↑ moving in stochastic potentials $U\nu_{i\downarrow}(r)$. For practical calculations it is convenient to return to the operator representation with respect to the $a_\uparrow, a_\uparrow^+$. The stochastic process $\nu_\downarrow$ defined by the probability measure P_0 has the following characteristic properties:

(i) $\nu_{i\downarrow}(r) = 0$ (11)
    $\nu_{i\downarrow}(0) = \nu_{i\downarrow}(\beta)$,   (12)

only periodic realizations are allowed,

$$\sum_i \nu_{i\downarrow}(r) = N_\downarrow, \quad (13)$$

particle number conservation for the $N_\downarrow$ electrons with spin ↓.

(ii) The process shows features analogous to a Binomial process in the Poisson limit. At any time r_ℓ the

(unnormalized) probability for no jump is equal to 1, the (unnormalized) probability for a jump is $t\Delta r$; in the Poisson limit $Lt\Delta r = t\beta = \text{const}$ for $\Delta r \to 0$. It is essential that a jump is understood as a change of two variables: a change of a $\nu_{i\downarrow}$ at a time r_ℓ and a change of a neighbouring $\nu_{j\downarrow}$ in the opposite sense at the same time. Thus, the normalized probability for an allowed trajectory $\nu_\downarrow$ (this means for an allowed set of functions $\nu_{i\downarrow}(r)$ for all i, r) with $r[\nu_\downarrow]$ jumps is

$$P_0[\nu_\downarrow] = \frac{(t\Delta r)^{r[\nu_\downarrow]}}{\int\limits_{\substack{\text{allowed} \\ \text{trajectories}}} D\nu_\downarrow (t\Delta r)^{r[\nu_\downarrow]}}. \quad (14)$$

We draw attention to the essential fact that the periodicity condition (12) excluding nonperiodic trajectories so to say "at the end $r = \beta$ of the process obviously destroys the Markovian property of the process.

3. THE STOCHASTIC PROCESS FOR THE ELECTRON-PHONON MODEL

We consider a simple Hamiltonian used for the calculation of the temperature dependence of the electrical resistivity in disordered alloys [2] :

$$H = \sum_{\substack{ij \\ \sigma}} t_{ij} a_{i\sigma}^+ a_{j\sigma} + \sum_s \omega_s b_s^+ b_s +$$
$$+ \sum_{\substack{i\sigma \\ s}} a_{i\sigma}^+ a_{i\sigma}(\gamma_{is} b_s + \gamma_{is}^* b_s^+) . \quad (15)$$

b_s, b_s^+ are the annihilation, creation operators for a phonon of mode s with energy ω_s; γ_{is} describes the electron-phonon coupling, for simplicity the interaction is restricted to terms with no transfer of electrons. We again represent the Green functions by functional integrals, and the action is now

$$S = -\int_0^\beta dr \{ \sum_{i\sigma} a_{i\sigma}^+ \frac{\partial}{\partial r} a_{i\sigma} + \sum_s \beta_s^* \frac{\partial}{\partial r} \beta_s + H \}. \quad (16)$$

The a, a^+ are Grassmann variables, the β, β^* are complex c-numbers.

The probability measure for the stochastic process β can be easily seen from (16) to be

$$P_0[\beta] = \prod_{s\ell} \exp\left\{\left[-\frac{1}{2}\frac{\beta_s^*(\tau_{\ell+1})+\beta_s^*(\tau_\ell)}{2}\frac{\beta_s(\tau_{\ell+1})-\beta_s(\tau_\ell)}{\Delta\tau}+\right.\right.$$

$$\left.\left.+\frac{1}{2}\frac{\beta_s^*(\tau_{\ell+1})-\beta_s^*(\tau_\ell)}{\Delta\tau}\frac{\beta_s(\tau_{\ell+1})+\beta_s(\tau_\ell)}{2}-\omega_s\beta_s^*(\tau_\ell)\beta_s(\tau_\ell)\right]\Delta\tau\right\}. \tag{17}$$

The process is obviously Gaussian (compare, e.g., ref.[11]). Again, this process is not Markovian because of the periodicity condition

$$\beta_s(0) = \beta_s(\beta). \tag{18}$$

To compare with the static approximation of Chen et al. (ref.[2]) we use Fourier transformation,

$$\beta_s(\tau) = \frac{1}{\beta^{1/2}}\sum_n \tilde{\beta}_s(\omega_n)e^{-i\omega_n\tau}, \quad \omega_n = 2n\pi/\beta, \tag{19}$$

and obtain for the probability

$$P_0[\beta] = \prod_{sn}\exp\{(i\omega_n-\omega_s)|\tilde{\beta}_s(\omega_n)|^2\}. \tag{20}$$

For high temperatures, $\beta\omega_s\ll 1$, the nonstatic contributions ($n\neq 0$) can be neglected, and we arrive at

$$P_0^{stat}[\beta] = \prod_s\exp\{-\beta\omega_s|\beta_s|^2\} \tag{21}$$

in accordance with ref.[2].

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