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GENERALIZED ALLOY ANALOGY FOR THE HUBBARD MODEL

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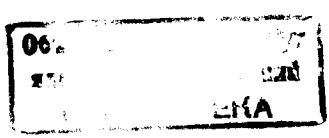

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Обобщенная аналогия сплава для модели Хаббарда

При помощи функциональных методов проблема Хаббарда точно преобразуется в проблему электронов проводимости, взаимодействующих с временно-зависящими стохастическими потенциалами. Выведенная самосогласованная схема рассмотрена в одноузельном приближении когерентного потенциала. Использование статических потенциалов в этой схеме в первом приближении приводит к результатам расщепления типа сплава.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

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Generalized Alloy Analogy for the Hubbard Model

By means of functional methods the Hubbard problem is transformed exactly into a problem of band electrons interacting with time-dependent stochastic potentials. The derived self-consistent scheme is treated in the single-site coherent potential approximation. In this scheme the alloy analogy using static potentials appears as a first approximation.

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

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1. INTRODUCTION

In the alloy analogy approximation[1] for the Hubbard model the motion of an electron with spin σ is treated by substituting the particle number operators $n_{i,-\sigma}$ of the $(-\sigma)$ electrons by *static* ramdom c - numbers $\nu_{i,-\sigma}$. According to the eigenvalues of the n, the ν take the values 0 or 1 with probabilities determined by the average number $\langle n_{i,-\sigma} \rangle$ of electrons.

Using functional Fourier transformation for the Green function with respect to a Schwinger source field we transform the Hubbard problem exactly into a problem of band electrons interacting with time-dependent stochastic potentials $U\nu_{i,-\sigma}(t)$. Like in the alloy analogy the ν take the values 0 or 1 only. The correlation functions of the ν have to be determined self-consistently. The single-site coherent potential approximation generalized to time dependent stochastic variables is applied to the derived set of equations.

2. TRANSFORMATION OF THE HUBBARD PROBLEM

The Hamiltonian of the Hubbard model is

$$H = \sum_{\substack{ij \\ \sigma}} t_{ij} \, a^{+}_{i\sigma} a_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow} \qquad (2.1)$$

with

$$t_{ij} = \tilde{t}_{ij} - \mu \delta_{ij} \, . \qquad (2.2)$$

The $\tilde{t}_{ij}$ characterize the Hartree-Fock band $(\tilde{t}_{ii} = 0)$.

We define the Green function by

$$G_{\substack{ij\\ \sigma}}(tt';\lambda) = \frac{1}{i}<T\{\gamma_\sigma a_{i\sigma}(t) a^+_{j\sigma}(t')\}> \qquad (2.3)$$

$$\gamma_\sigma = \exp\{-i\int_0^{-i\beta} d\bar{t} \sum_k \lambda_{k\sigma}(\bar{t}) n_{k,-\sigma}(\bar{t})\} \qquad (2.4)$$

$\lambda_{k\sigma}(t)$ is a c-number Schwinger source field. In solving the Hubbard model the identity for Fermion operators

$$n^2_{k,-\sigma}(\bar{t}) = n_{k,-\sigma}(\bar{t}) \qquad (2.5)$$

has to be satisfied. Here it takes the form

$$(i\frac{\delta}{\delta\lambda_{k\sigma}(\bar{t})})^2 G_{\substack{ij\\ \sigma}}(tt';\lambda) = i\frac{\delta}{\delta\lambda_{k\sigma}(\bar{t})} G_{\substack{ij\\ \sigma}}(tt';\lambda)\ . \qquad (2.6)$$

We write the functional Fourier transformation for the Green function in the following way convenient for physical interpretation:

$$G_{\substack{ij\\ \sigma}}(tt';\lambda) = <G_{\substack{ij\\ \sigma}}(tt';\nu)\exp\{-i\int_0^{-i\beta} d\bar{t} \sum_k \lambda_{k\sigma}(\bar{t})\nu_{k,-\sigma}(\bar{t})\}>_\nu\ . \qquad (2.7)$$

The Fourier coefficient is $P(\nu)\, G(\ \ ;\nu)$,

$$<\ldots>_\nu = \sum_{\substack{\text{all functions}\\ \nu_{i,-\sigma}(t)}} P(\nu)\ldots \qquad (2.8)$$

with

$$\sum_\nu P(\nu) = 1\ . \qquad (2.9)$$

Thus $G(\ \ ;\lambda=0)$ is given as the average of $G(\ \ ;\nu)$ with probabilities $P(\nu)$. From the identity (2.6) it follows that the $P(\nu)$ can be different from zero only for

$$\nu_{i,-\sigma}(t) = 0 \quad \text{or} \quad 1\ . \qquad (2.10)$$

The ν have to satisfy the Bose periodicity.

The Fourier coefficients are determined from the equation of motion for the Green function (2.3). The decomposition into the product PG allows a determination in two steps. The ν-dependent Green functions are chosen as solutions of the equation of motion

$$i\frac{\partial}{\partial t} G_{\substack{ij\\ \sigma}}(tt';\nu) - \sum_k t_{ik} G_{\substack{kj\\ \sigma}}(tt';\nu) - \qquad (2.11)$$

$$-U(\nu_{i,-\sigma}(t)\, G_{\substack{ij\\ \sigma}}(tt';\nu) = \delta_{ij}\,\delta(t-t'),$$

and the probabilities $P(\nu)$ are determined self-consistently by

$$<\exp\{-i\int_0^{-i\beta} d\bar{t} \sum_k \lambda_{k\sigma}(\bar{t})\nu_{k,-\sigma}(\bar{t})\}>_\nu =$$

$$= <T\exp\{-i\int_0^{-i\beta} d\bar{t} \sum_k \lambda_{k\sigma}(\bar{t}) n_{k,-\sigma}(\bar{t})\}> \qquad (2.12a)$$

or

$$<\nu_{i,-\sigma}(t)>_\nu = <n_{i,-\sigma}(t)>,$$

$$<\nu_{i,-\sigma}(t)\nu_{j,-\sigma}(t')>_\nu = <T\, n_{i,-\sigma}(t) n_{j,-\sigma}(t')>, \qquad (2.12b)$$

(2.12) defines the stochastic process ν.

Eqs. (2.7 to 2.12) are equivalent to the Hubbard problem. Restricting ourselves to static ν we obtain the alloy analogy. In the atomic limit the n are constants of motion so that the problem is exactly solved by static ν. From this point of view Eq. (2.10) is the essential relation. Static approximations differing from the alloy analogy (compare /2/) appear as approximation modelling the time-dependence of the ν.

3. *SINGLE-SITE COHERENT POTENTIAL APPROXIMATION*

Like in the case of the (static) alloy analogy the average (2.7) for $\lambda = 0$ can be calculated by means of the

single-site CPA. We use the locator formulation /3/ generalized to time-dependent stochastic variables. Because of this time-dependence it is convenient to remain in the t -representation. Then we have to solve the equations

$$i\frac{\partial}{\partial t}\langle G_{\substack{ij\\\sigma}}(tt';\nu)\rangle_{\nu} - \sum_{k}\tilde{t}_{ik}\langle G_{\substack{kj\\\sigma}}(tt';\nu)\rangle_{\nu} -$$

$$-\int_{0}^{-i\beta} d\bar{t}\,\Sigma(t-\bar{t})\langle G_{\substack{ij\\\sigma}}(\bar{t}t';\nu)\rangle_{\nu} = \delta_{ij}\delta(t-t'),$$

$$\Big\{i\frac{\partial}{\partial t} - [U\nu_{0,-\sigma}(t)-\mu]\Big\}\langle G_{\substack{00\\\sigma}}(tt';\nu)\rangle_{\nu,(0)} -$$

$$-\int_{0}^{-i\beta} d\bar{t}\,J(t-\bar{t})\langle G_{\substack{00\\\sigma}}(\bar{t}t';\nu)\rangle_{\nu,(0)} = \delta(t-t'), \tag{3.1}$$

$$i\frac{\partial}{\partial t}\langle G_{\substack{00\\\sigma}}(tt';\nu)\rangle_{\nu} -$$

$$-\int_{0}^{-i\beta} d\bar{t}\,[J(t-\bar{t}) + \Sigma(t-\bar{t})]\langle G_{\substack{00\\\sigma}}(\bar{t}t';\nu)\rangle_{\nu} =$$

$$= \delta(t-t'), \tag{3.2}$$

$$\ll G_{\substack{00\\\sigma}}(tt';\nu)\rangle_{\nu,(0)}\rangle_{\nu_{0,-\sigma}} = \langle G_{\substack{00\\\sigma}}(tt';\nu)\rangle_{\nu}, \tag{3.3}$$

and the self-consistency condition

$$\ll G_{\substack{00\\\sigma}}(tt';\nu)\rangle_{\nu,(0)}\rangle_{\nu_{0,-\sigma}} = \langle G_{\substack{00\\\sigma}}(tt';\nu)\rangle_{\nu}, \tag{3.4}$$

$\langle\ldots\rangle_{\nu,(0)}$ means the conditional average with fixed $\nu_{0,-\sigma}$; J and Σ are the interactor and the coherent potential, respectively.

We solve Eq. (3.2) in a simple way. First we restrict ourselves to $n=1$ (n number of electrons per site), to $\tilde{t}_{ij}\neq 0$ only for i,j nearest neighbours and to an alternating lattice. Then, because of the electron-hole symmetry

$$\mu = \frac{U}{2}. \tag{3.5}$$

Further we restrict ourselves to the paramagnetic phase. Introducing

$$\tilde{\nu}(t) = \nu_{0,-\sigma}(t) - \frac{1}{2} = \pm\frac{1}{2}, \tag{3.6}$$

$$\tilde{G}(tt',\tilde{\nu}) = \langle G_{\substack{00\\\sigma}}(tt';\nu)\rangle, \tag{3.7}$$

we write (3.2) in the form

$$\tilde{G}(tt',\nu) = \tilde{G}^{(0)}(t-t') +$$

$$+\int_{0}^{-i\beta} d\bar{t}\,\tilde{G}^{(0)}(t-\bar{t})\,U\tilde{\nu}(\bar{t})\,\tilde{G}(\bar{t}t';\tilde{\nu}). \tag{3.8}$$

$\tilde{G}^{(0)}$ is the solution of (3.2) if the term $[U\nu_{0,-\sigma}(t)-\mu] = U\tilde{\nu}(t)$ is omitted. Iterating (3.8) and averaging approximately, we obtain

$$\langle\tilde{G}(tt';\tilde{\nu})\rangle_{\tilde{\nu}} = \tilde{G}^{(0)}(t-t') +$$

$$+\int_{0}^{-i\beta} d\bar{t}\,d\bar{\bar{t}}\,\tilde{G}^{(0)}(t-\bar{t})\,\tilde{G}^{(0)}(\bar{t}-\bar{\bar{t}})\,U^{2}\langle\tilde{\nu}(\bar{t})\,\tilde{\nu}(\bar{\bar{t}})\rangle_{\tilde{\nu}}\langle\tilde{G}(\bar{\bar{t}}t';\tilde{\nu})\rangle_{\tilde{\nu}}. \tag{3.9}$$

In the last term the average splits into the product of the averages. This is in view of (3.6) exact in the static case. ($\langle\tilde{\nu}\rangle_{\tilde{\nu}} = 0$ in the paramagnetic phase). From (3.9) we get the simple result

$$\Sigma(t-t') = \tilde{G}^{(0)}(t-t')\,U^{2}\langle\tilde{\nu}(t)\tilde{\nu}(t')\rangle_{\tilde{\nu}}. \tag{3.10}$$

The ν -correlation function has to be determined self-consistently. This can be approached by an ansatz for this correlation function containing a free parameter determined by

$$i\frac{\partial}{\partial t}<\tilde{\nu}(t)\tilde{\nu}(0)>|_{t=+0} = i\frac{\partial}{\partial t}<T\, n_{0,-\sigma}(t)\, n_{0,-\sigma}(0)>|_{t=+0}$$

$$= \frac{1}{N}\sum_{\vec{k}} \epsilon_{\vec{k}} <n_{\vec{k},-\sigma}>. \qquad (3.11)$$

The right-hand side of (3.11) can be expressed by the one-electron Green function.

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