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Pseudo-fermion formalism applied to nonequilibrium Kondo-type problems

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Summary. — A straightforward limit procedure is developed for evaluating the expectation value of a generic many-particle operator defined in the Abrikosov-Coleman's pseudo-fermion formalism. It can be useful for the study of nonequilibrium Kondo-type problems.

PACS 72.10.Fk – Scattering by point defects, dislocations, surfaces, and other imperfections (including Kondo effect).

1. - Introduction

Diagrammatic expansion of the time-dependent Green's function is a powerful and systematic technique for evaluating high-order many-body interaction contributions to the time evolution of strongly correlated systems. Furthermore, the well-established development of various renormalization procedures gives the possibility of studying nonperturbative effects and to treat singular interactions. From the pioneering work by Kondo of the anomalous resistivity at low temperature in metal doped with very few magnetic impurities [1,2], diagrammatic expansion of the exchange interaction between the magnetic species and the conduction electrons has been a tool of primary importance for understanding the microscopical processes underlying the observed phenomenon. The apparently simple spin-spin exchange interaction postulated by Kondo has revealed a great source of difficulty both from a mathematical and a physical interpretation point of view. While the original approach followed by Kondo (which is based on a direct second-order expansion of the exchange interaction) was able to exhibit the primary role played by the spin interaction in the scattering processes between the magnetic impurities and the conduction electrons, the appearance of various divergent terms in the resistivity expansion has early revealed the limits of this approach. Since then, in spite of the great theoretical effort which has been devoted to overcome the technical difficulties and obtain a clear understanding of the thermodynamical properties of a gas of itinerant fermions interacting with well spatially localized spins, at present, little is known about the dynamical aspects of such systems. With the availability of ultrashort and intense optical sources operating in the femtosecond time-scale it is nowadays possible to induce and to investigate nonequilibrium regimes in Kondo-like systems such as, for example, demagnetization processes in diluted magnetic semiconductors [3]. Various theoretical studies have been addressed to quantify the effect of dynamical spin correlations in such systems [4-7]. It is well known that many-body correlations effects between localized magnetic ions and itinerant charge carriers play an important role for the ground-state properties of the system. The lack of simple properties of the commutation relations of the magnetic ion spin operators prevents the use of a systematic expansion procedure such as Feynman's diagram expansion to obtain high-order interaction terms. In order to circumvent this technical difficulty, a theoretical study of the Kondo-type interaction needs a special treatment of the many-body properties of the system. In particular it is well known that, in the second quantization formalism, almost all the standard theorems concerning the many-particle expansion of the contour-ordered operators like Wick's theorem for the Green's function of the system, are based on elementary commutation rules for the creation and annihilation operators. This problem was already known in the early study of the anomalous resistivity at low temperature. Abrikosov proposed an alternative approach based on the use of fictitious particles (pseudo-fermions) which formally preserves the standard commutation rules for spin-(1/2) particles [8]. Unfortunately, this formalism introduces non-physical states in the Hilbert space of the magnetic ions for which the impurity sites allows multiple occupation. Therefore, a suitable limit procedure is required in order to recover the correct physical description of the magnetic species.

In this work we present a systematic asymptotic procedure able to recover the correct expression of the mean magnetic ion spin density in the *physical Hilbert space*. Our approach is based on the use of Coleman's limit procedure [9] applied to the diagrammatic expansion of the exchange interaction. We show that it is well suited for the evaluation of the time-dependent Green's functions of both the magnetic ions and the delocalized charge carriers.

2. - Pseudo-fermion formalism

In this section, we describe the time-evolution of two different populations of particles (hereafter the symbols h and M are used to represent, respectively, the delocalized charge carriers $(cc)(^1)$ and the magnetic ions) in the second quantization formalism. We denote by $a_{k,s}^{\dagger}$ $(a_{k,s})$ and $b_{\eta,m}^{\dagger}$ $(b_{\eta,m})$ the creation (annihilation) operators of a cc having a spin s and a quasi-momentum k and a pseudo-fermion ion with spin m and spatial position R_{η} , respectively. The annihilation and creation operators respect the usual commutation relations $\{a_{k,s}^{\dagger},a_{k',s'}\}=\hbar$ $\delta_{s,s'}\delta_{k,k'}$, $\{a_{k,s},a_{k',s'}\}=\{a_{k,s}^{\dagger},a_{k',s'}^{\dagger}\}=0$, $\{b_{\eta,m}^{\dagger},b_{\eta',m'},b_{\eta',m'}\}=\hbar$ $\delta_{m,m'}\delta_{\eta,\eta'}$, $\{b_{\eta,m},b_{\eta',m'}\}=\{b_{\eta',m'}^{\dagger},b_{\eta',m'}^{\dagger},b_{\eta',m'}^{\dagger}\}=0$ and $[a_{k,s},b_{\eta,m}]=[a_{k,s},b_{\eta,m}^{\dagger}]=0$. In particular, the b operator denotes Abrikosov's pseudo-fermion operator which gives the correct physical states provided that one and only one particle can be found in each ion site, i.e. $\hat{n}_{\eta}^{m}=b_{\eta,m}^{\dagger}b_{\eta,m}$, $\hat{n}_{\eta}=\sum_{m=-S^{M}}^{S^{M}}\hat{n}_{\eta}^{m}=1$. To ensure this constraint we have followed the procedure outlined in [8,9]. Let us denote $|\Psi\otimes\Upsilon\rangle$ the many-particle wave function containing both the holes (Υ) and the ions (Ψ) degrees of freedom. In particular

 $^(^1)$ In the original Kondo problem, the charge carriers are electrons while in diluted magnetic semiconductors they are holes.

for $|\Psi\rangle$ we have

$$\mathcal{H}\Psi_{i} = E_{i}\Psi_{i},$$

$$\mathcal{H}_{0}\Phi_{i} = E_{i}^{0}\Phi_{i},$$

$$\mathcal{H} = \mathcal{H}_{0} + \mathcal{H}_{ex},$$

$$\mathcal{H}_{0} = \sum_{\eta,m} \lambda_{\eta} b_{\eta,m}^{\dagger} b_{\eta,m} + \sum_{k,s} \varepsilon_{k,s} a_{k,s}^{\dagger} a_{k,s},$$

where Ψ_0 (Φ_0) denotes the interacting (non-interacting) ground state and Ψ_i (Φ_i) the i-th excited many-particle state in the interacting (non-interacting) case, respectively. The unperturbed Hamiltonian takes into account the kinetic energy of the delocalized particles having a dispersion relation $\varepsilon_{k,s}$. Furthermore, an artificial ion contribution to the total energy which is defined by the pseudo-chemical parameters λ_{η} is added. The physical meaning of this term is to assign a higher energy to the multiply occupied states. Their contribution to the ion spin density is removed in the limit $\lambda_{\eta} \to \infty$, and the correct ion dynamics is recovered. In particular, the wave function Φ describes a generic many-particle state with r ion sites each of them can contain up to $(2S^M + 1)$ pseudo-particles (the subscript recalls that the basis states are diagonal with respect to the hamiltonian \mathcal{H}_0) and explicitly reads

$$|\Phi\rangle = \left|n_1^1, \dots n_1^{(2S^M+1)}; \dots; n_\eta^1, \dots n_\eta^{(2S^M+1)}; \dots; n_r^1, \dots n_r^{(2S^M+1)}\right\rangle \equiv \left|n_{\overline{\eta}}^{\overline{m}}\right\rangle,$$

where $n_{\eta}^{m}(=0,1)$ are the occupation numbers related to the m-th spin projection at position R_{η} and \overline{m} ($\overline{\eta}$) denotes the set spanned by index m (η). Abrikosov-Coleman's procedure allows us to extract the correct physical states, for which there exists for each ion position R_{η} one and only one m such as $n_{\eta}^{m}=1$ and $n_{\eta}^{m'\neq m}=0$ ($\langle \Phi | \hat{n}_{\eta} | \Phi \rangle = n_{\eta}=1 \forall \eta$). The Kondo-like exchange interaction $\mathcal{H}_{\rm ex}$ is given by

(1)
$$\mathcal{H}_{\text{ex}} = \frac{\gamma}{V} \sum \left(b_{\eta,m'}^{\dagger} b_{\eta,m} a_{k',s'}^{\dagger} a_{k,s} \right) \mathbf{J}_{m',m} \cdot \boldsymbol{\sigma}_{s',s} \ e^{i(k'-k)R_{\eta}},$$

where the sum is extended over all indices, γ is the coupling constant, V is the volume of the system, and σ , J are the spin matrices related to the cc and the magnetic ions, respectively.

2.1. Coleman's procedure applied to the fermionic limit. – We focus here on the general properties of the ion expectation value and for the sake of simplicity we will discard the cc degrees of freedom since they do not play a role in the limit procedure. The grand-canonical expectation value of a generic operator \mathcal{A} in the pseudo-fermion space is defined in the usual way

(2)
$$\langle \mathcal{A} \rangle_{\lambda}^{\text{PF}} = \frac{1}{\mathcal{Z}_{\lambda}^{\text{PF}}} \operatorname{Tr} \left\{ \rho_{\mathcal{H}} e^{-\beta \sum_{\eta} \lambda_{\eta} \hat{n}_{\eta}} \mathcal{A} \right\} = \frac{1}{\mathcal{Z}_{\lambda}^{\text{PF}}} \sum_{\{n_{\eta}^{m}\}_{r}} \left\langle n_{\eta}^{m} \middle| \rho_{\mathcal{H}} e^{-\beta \sum_{\eta} \lambda_{\eta} \hat{n}_{\eta}} \mathcal{A} \middle| n_{\eta}^{m} \right\rangle,$$

where $\mathcal{Z}_{\lambda}^{\mathrm{PF}}=\mathrm{Tr}\{\rho_{\mathcal{H}}e^{-\beta\sum_{\eta}\lambda_{\eta}\hat{n}_{\eta}}\}$. The operator $\hat{n}_{\eta}=\sum_{m=-S^{M}}^{S^{M}}b_{\eta,m}^{\dagger}b_{\eta,m}$ and $\{n_{\overline{\eta}}^{\overline{m}}\}_{r}=\{n_{1}^{m},\ldots,n_{r}^{m}\}$ denotes all possible occupation numbers n_{η}^{k} with r ion sites. Since each ion site has $(2S^{M}+1)$ available pseudo-fermion states, the system will contain a maximum

number of pseudo-particles equal to $(2S^M+1)r$. The sum in (2) is explicitly given by $\sum_{\{n_{\eta}^m\}_r} = \sum_{\eta=1}^r \sum_{n_{\eta}=1}^{2S^M+1} \sum_{(\{n_{\eta}^m\}_r:\sum_m n_{\eta}^m=n_{\eta})}$. Furthermore, $\rho_{\mathcal{H}} = e^{-\beta\mathcal{H}}$ and $\beta = 1/k_BT$, with k_B Boltzmann's constant and T the temperature. The expectation value of \mathcal{A} in the physical fermionic Hilbert space is denoted by $\langle \mathcal{A} \rangle^{\mathrm{F}}$ and reads

$$\langle \mathcal{A} \rangle^{\mathrm{F}} \equiv \frac{1}{\mathcal{Z}^{\mathrm{F}}} \operatorname{Tr}^{\mathrm{F}} \{ \rho_{\mathcal{H}} \mathcal{A} \} = \frac{1}{\mathcal{Z}^{\mathrm{F}}} \sum_{\{n_{n}^{m}\}_{r}; n_{\eta} = 1} \left\langle n_{\overline{\eta}}^{\overline{m}} \middle| \rho_{\mathcal{H}} \mathcal{A} \middle| n_{\overline{\eta}}^{\overline{m}} \right\rangle$$

with $\mathcal{Z}^{\mathrm{F}} = \sum_{\{n_n^m\}_r ; n_n=1} \langle n_{\overline{\eta}}^{\overline{m}} | \rho_{\mathcal{H}} | n_{\overline{\eta}}^{\overline{m}} \rangle$. It can be obtained by using the limit

(3)
$$\left\langle \widetilde{\mathcal{A}} \right\rangle^{\mathrm{F}} = \lim_{\{z_{\eta}\} \to 0} \frac{\partial^{r} \left\langle \widetilde{\mathcal{A}} \right\rangle_{\lambda}^{\mathrm{PF}}}{\partial z_{1} \cdots \partial z_{r}},$$

where we have defined $z_{\eta} = e^{-\beta\lambda_{\eta}}$ and $\langle \widetilde{\mathcal{A}} \rangle^{\mathrm{F}} \equiv \langle \mathcal{A} \rangle^{\mathrm{F}} \mathcal{Z}^{\mathrm{F}}$, $\langle \widetilde{\mathcal{A}} \rangle^{\mathrm{PF}} \equiv \langle \mathcal{A} \rangle^{\mathrm{PF}} \mathcal{Z}^{\mathrm{F}}$. Indeed, we have

$$\frac{\partial^{r} \left\langle \widetilde{\mathcal{A}} \right\rangle_{\lambda}^{\text{PF}}}{\partial z_{1} \cdots \partial z_{r}} = \sum_{\{n_{\eta}^{m}\}_{r}} \left\langle n_{\overline{\eta}}^{\overline{m}} \middle| \rho_{\mathcal{H}} \mathcal{A} \frac{\partial^{r}}{\partial z_{1} \cdots \partial z_{r}} \prod_{\eta}^{r} z_{\eta}^{\hat{n}_{\eta}} \middle| n_{\overline{\eta}}^{\overline{m}} \right\rangle
= \sum_{\{n_{\eta}^{m}\}_{r}; n_{\eta} > 0} \prod_{\eta}^{r} n_{\eta} z_{\eta}^{n_{\eta} - 1} \left\langle n_{\overline{\eta}}^{\overline{m}} \middle| \rho_{\mathcal{H}} \mathcal{A} \middle| n_{\overline{\eta}}^{\overline{m}} \right\rangle.$$

In the limit $\{z_{\eta}\} \to 0$ the only non-vanishing contribution to the sum comes from the states with just one particle per site and therefore eq. (3) is satisfied. By using the same argument one can immediately prove that

(4)
$$\mathcal{Z}^{F} = \left. \frac{\partial^{r} \mathcal{Z}_{\lambda}^{PF}}{\partial z_{1} \cdots \partial z_{r}} \right|_{\{z_{n}\}=0}$$

which follows from the previous formula with the substitution $\rho_{\mathcal{H}} \mathcal{A} = 1$.

2'2. Fermionic limit in the many-particle expansion: general case. – For future considerations it is convenient to consider a generic operator \mathcal{O}_{η_0} where the subscript η_0

means that \mathcal{O} contains only $b_{\eta_0,m}^{\dagger}$ $(b_{\eta_0,m})$ operators acting on the R_{η_0} ion site. We have

$$\begin{split} \langle \widetilde{\mathcal{O}}_{\eta_0} \rangle_{\lambda}^{\mathrm{PF}} &= \sum_{\{n_{\overline{\eta}}^{\overline{m}}\}_r} \langle n_{\overline{\eta}}^{\overline{m}} \big| \, \rho_{\mathbf{H}} e^{-\beta \sum_{\eta} \lambda_{\eta} \hat{n}_{\eta}} \mathcal{O}_{\eta_0} \, \big| n_{\overline{\eta}}^{\overline{m}} \, \big\rangle \\ &= \sum_{\{n_{\overline{\eta}}^{\overline{m}}\}_r} \prod_{\eta} z_{\eta}^{n_{\eta}} \langle n_{\overline{\eta}}^{\overline{m}} \big| \, \rho_{\mathbf{H}} \mathcal{O}_{\eta_0} \, \big| n_{\overline{\eta}}^{\overline{m}} \, \big\rangle \\ &= \sum_{n_{\eta}=0}^{\infty} \sum_{n_{\eta}^{m}=0}^{n_{\eta}} \prod_{\eta,\eta'=1}^{r} z_{\eta}^{n_{\eta}} e^{-\beta \sum_{m} \mathbf{H}(\eta',m)n_{\eta'}^{m}} \langle n_{\overline{\eta}}^{\overline{m}} \big| \, \mathcal{O}_{\eta_0} \, \big| n_{\overline{\eta}}^{\overline{m}} \, \big\rangle \\ &= \sum_{n_{\eta}=0}^{\infty} \sum_{\binom{n_{\eta'}=0}{\eta'\neq\eta}}^{\infty} \sum_{n_{\eta'}=0}^{n_{\eta'}} \prod_{\binom{\eta,\eta'=1}{\eta,\eta'\neq\eta_0}}^{r} z_{\eta}^{n_{\eta}} e^{-\beta \sum_{m} \mathbf{H}(\eta',m)n_{\eta'}^{m}} \\ &\times \langle n_{\overline{\eta}}^{\overline{m}} \big| \, \mathcal{O}_{\eta_0} \, \big| n_{\overline{\eta}}^{\overline{m}} \, \big\rangle \, z_{\eta_0}^{n_{\eta_0}} e^{-\beta \sum_{m} \mathbf{H}(\eta_0,m)n_{\eta_0}^{m}}, \end{split}$$

where the sum over n_{η}^{m} is restricted to all possible configuration occupations n_{η}^{m} such that $\sum_{m} n_{\eta}^{m} = n_{\eta}$. In particular, we have separated the thermal occupation probability related to the pseudo-chemical potentials from all the other statistical contributions which can be described by an effective Hamiltonian of the form $\mathbf{H} = \sum_{\eta,m} \mathbf{H}(\eta,m) \hat{n}_{\eta}^{m}$. Typically \mathbf{H} takes into account the simplest part of the particle-particle interaction that in our case is represented by the terms of $\mathcal{H}_{\rm ex}$ of eq. (1) with m'=m. For example, for the Kondo exchange interaction it is convenient to extract the mean-field contribution from the other more complex many-particle interactions. In the spirit of the Hartree approximation, \mathbf{H} takes into account the mean magnetic field S^{z} generated by the delocalized charge carriers which constitutes the first-order contribution to the magnetic ion polarization. Explicitly, it is given by $\mathbf{H}_{\rm MF} = \frac{\gamma}{V} S^{z} \sum_{\eta,m} m \, \hat{n}_{\eta}^{m}$. Since the expectation value $\langle n_{\overline{\eta}}^{\overline{m}} | \mathcal{O}_{\eta_0} | n_{\overline{\eta}}^{\overline{m}} \rangle$ does not depend on the occupation numbers n_{η} with $\eta \neq \eta_0$, the previous formula simplifies to

(5)
$$\left\langle \widetilde{\mathcal{O}}_{\eta_0} \right\rangle_{\lambda}^{\mathrm{PF}} = \left(\sum_{n_{\eta}=0}^{\infty} \sum_{\substack{\eta \neq \eta_0 \\ \eta \neq \eta_0}}^{n_{\eta}} \sum_{\substack{n_{\eta}'=1 \\ \eta, \eta' \neq \eta_0}}^{r} z_{\eta}^{n_{\eta}} e^{-\beta \sum_{m} \mathrm{H}(\eta', m) n_{\eta'}^{m}} \right) \mathfrak{O}_{\eta_0, \lambda_{\eta_0}},$$

(6)
$$\mathfrak{O}_{\eta_0,\lambda_{\eta_0}} = \sum_{n_{\eta_0}=0}^{\infty} \sum_{n_{\eta_0}=0}^{n_{\eta_0}} \left\langle n_{\overline{\eta}}^{\overline{m}} \right| \mathcal{O}_{\eta_0} \left| n_{\overline{\eta}}^{\overline{m}} \right\rangle z_{\eta_0}^{n_{\eta_0}} e^{-\beta \sum_m H(\eta_0,m) n_{\eta_0}^m},$$

where we have factorized out the contribution of the R_{η_0} site. In the limit $\{z_{\eta}\}$ goes to zero we have

$$(7) \lim_{\{z_{\eta}\} \to 0} \left\langle \widetilde{\mathcal{O}}_{\eta_{0}} \right\rangle_{\lambda}^{\text{PF}} = \left(\sum_{n_{\eta}=0}^{\infty} \sum_{\eta \neq \eta_{0}}^{n_{\eta}} \prod_{\substack{n_{\eta}=1 \\ (\eta, \eta' \neq \eta_{0})}}^{r} \delta_{n_{\eta}, 0} e^{-\beta \sum_{m} \mathbf{H}(\eta', m) n_{\eta'}^{m}} \right) \lim_{z_{\eta_{0}} \to 0} \mathfrak{O}_{\eta_{0}, \lambda_{\eta_{0}}},$$

$$= \lim_{z_{\eta_{0}} \to 0} \mathfrak{O}_{\eta_{0}, \lambda_{\eta_{0}}},$$

$$\lim_{z_{\eta_{0}} \to 0} \mathfrak{O}_{\eta_{0}, \lambda_{\eta_{0}}} = \langle 0 | \mathcal{O}_{\eta_{0}} | 0 \rangle$$

and

$$\begin{split} \lim_{\{z_{\eta}\}\to 0} \frac{\partial^{r} \left\langle \widetilde{\mathcal{O}}_{\eta_{0}} \right\rangle_{\lambda}^{\text{PF}}}{\partial z_{1} \cdots \partial z_{r}} &= \lim_{\{z_{\eta}\}\to 0} \left(\sum_{n_{\eta}=0 \eta \neq \eta_{0}}^{\infty} \sum_{n_{\eta}^{m}=0}^{n_{\eta}} \prod_{\substack{\eta, \eta'=1 \\ (\eta, \eta' \neq \eta_{0})}}^{r} n_{\eta} z_{\eta}^{n_{\eta}-1} e^{-\beta \sum_{m} \mathbf{H}(\eta', m) n_{\eta'}^{m}} \right) \frac{\partial \mathfrak{O}_{\eta_{0}, \lambda_{\eta_{0}}}}{\partial z_{\eta_{0}}} \\ &= \left(\sum_{n_{\eta}^{m}; \sum_{m} n_{\eta}^{m}=1}^{r} \prod_{\eta'=1; \eta' \neq \eta_{0}}^{r} e^{-\beta \sum_{m} \mathbf{H}(\eta', m) n_{\eta'}^{m}} \right) \lim_{z_{\eta_{0}} \to 0} \frac{\partial \mathfrak{O}_{\eta_{0}, \lambda_{\eta_{0}}}}{\partial z_{\eta_{0}}} \\ &= \left(\sum_{m} e^{-\beta \mathbf{H}(\eta', m)} \right)^{r-1} \lim_{z_{\eta_{0}} \to 0} \frac{\partial \mathfrak{O}_{\eta_{0}, \lambda_{\eta_{0}}}}{\partial z_{\eta_{0}}} \,. \end{split}$$

Since the sum runs over all the possible states with only one particle in the η site, the possible values of $\{n_{\eta}^m\}_r$ are $n_{\eta}^m = \underbrace{(1,0,\ldots,0)}_{2S^M+1}$; $(0,1,\ldots,0)$; $(0,0,\ldots,1)$ $\forall \eta$ and therefore

only the vector with 1 at the m-th position contributes to the sum. Finally one gets

$$\begin{split} \lim_{z_{\eta_0} \to 0} \frac{\partial \mathfrak{O}_{\eta_0, \lambda_{\eta_0}}}{\partial z_{\eta_0}} &= \sum_{n_{\eta_0}^m : \sum_m n_{\eta_0}^m = 1} \left\langle n_{\overline{\eta}}^{\overline{m}} \right| \mathcal{O}_{\eta_0} \left| n_{\overline{\eta}}^{\overline{m}} \right\rangle^{\mathrm{F}} e^{-\beta \sum_m \mathrm{H}(\eta_0, m) n_{\eta_0}^m} \\ &= \sum_m \left\langle n_{\overline{\eta}}^{\overline{m}} \right| \mathcal{O}_{\eta_0} \left| n_{\overline{\eta}}^{\overline{m}} \right\rangle^{\mathrm{F}} e^{-\beta \mathrm{H}(\eta_0, m)} = \sum_m \left\langle n_{\eta_0}^{\overline{m}} \right| \mathcal{O}_{\eta_0} \left| n_{\eta_0}^{\overline{m}} \right\rangle^{\mathrm{SP}} e^{-\beta \mathrm{H}(\eta_0, m)}, \end{split}$$

where for sake of clarity we have defined

$$\left| n_{\overline{\eta}}^{\overline{m}} \right\rangle^{\mathcal{F}} = \left| n_{1}^{1}, \dots n_{1}^{(2S^{M}+1)}; \dots; \underbrace{0, \dots n_{\eta}^{m} = 1, \dots, 0}_{\eta}; \dots; n_{r}^{1}, \dots n_{r}^{(2S^{M}+1)} \right\rangle,
\left| n_{\eta_{0}}^{\overline{m}} \right\rangle^{\mathcal{SP}} = \left| 0, \dots n_{\eta_{0}}^{m} = 1, \dots, 0 \right\rangle.$$

The superfix SP indicates single-particle states and we have used the fact that the operator \mathcal{O}_{η_0} acts only on the R_{η_0} site. As a particular case, the less-than $\mathcal{G}^{<}_{\eta_0}$ (greater-than $\mathcal{G}^{>}_{\eta_0}$) Green's function and the partition function $\mathcal{Z}^{\mathrm{PF}}_{\lambda}$ are obtained by using the previous formula with the substitution $\mathcal{O}_{\eta_0} = b^{\dagger}_{\eta_0,m}b_{\eta_0,m}$ ($\mathcal{O}_{\eta_0} = b_{\eta_0,m}b^{\dagger}_{\eta_0,m}$) and $\mathcal{O}_{\eta_0} = 1$, respectively. We have applied the previous formulae for recovering the correct n-th-order expansion contribution to the expectation value of \mathcal{A} . The expectation value of a generic operator defined on Abrikosov's pseudo-fermion space can be expanded in the usual way by means of Wick's theorem. As a final result, Langreth's theorem for the time-ordered product ensures that the time-dependent expectation value can be expressed as a product of simpler single-particle Green's functions and which will be denoted \mathcal{A}_w . \mathcal{A}_w reads

$$\begin{split} \langle \mathcal{A}_w \rangle_{\lambda}^{\mathrm{PF}} &= \sum_{\xi} \langle \mathcal{A}_w^{\xi} \rangle_{\lambda}^{\mathrm{PF}}, \\ \langle \mathcal{A}_w^{\xi} \rangle_{\lambda}^{\mathrm{PF}} &\equiv \prod_{\eta \in X} \mathbf{A}_{\eta}^{\xi} (\mathcal{G}_{\eta}^{>})^{g_{\eta}^{\xi}} (\mathcal{G}_{\eta}^{<})^{l_{\eta}^{\xi}} = \prod_{\eta \in X} \mathbf{A}_{\eta}^{\xi} \left(\frac{\widetilde{\mathcal{G}}_{\eta}^{>}}{\mathcal{Z}_{\lambda}} \right)^{g_{\eta}^{\xi}} \left(\frac{\widetilde{\mathcal{G}}_{\eta}^{<}}{\mathcal{Z}_{\lambda}} \right)^{l_{\eta}^{\xi}}. \end{split}$$

Here, the pseudo-fermion Green's function $\mathcal{G}_{\eta}^{<}(\mathcal{G}_{\eta}^{>})$ is defined as in eq. (2) with $\mathcal{A} = b_{\eta,m}b_{\eta,m}$ ($\mathcal{A} = b_{\eta,m}b_{\eta,m}^{\dagger}$) and $\mathcal{H} = \mathbf{H}$. \mathbf{A}_{η}^{ξ} are the expansion coefficients of $\langle \mathcal{A}_w \rangle_{\lambda}^{\mathrm{PF}}$ on the monomial $\mathcal{G}_{\eta}^{>}\mathcal{G}_{\eta}^{<}$ for a given couple of the exponents g_{η}^{ξ} , l_{η}^{ξ} , and whose explicit form depends on the detail of the interaction. For the sake of simplicity, the index m in the Green's functions is not explicitly mentioned. By using eqs. (5), (6) we obtain

(8)
$$\langle \mathcal{A}_w \rangle_{\lambda}^{\mathrm{PF}} = \sum_{\varepsilon} \prod_{\eta \in X} \mathbf{A}_{\eta}^{\xi} \left(\frac{\widetilde{\mathcal{G}}_{\eta, \lambda_{\eta}}^{>}}{\mathcal{Z}_{\eta, \lambda_{\eta}}} \right)^{g_{\eta}^{\xi}} \left(\frac{\widetilde{\mathcal{G}}_{\eta, \lambda_{\eta}}^{<}}{\mathcal{Z}_{\eta, \lambda_{\eta}}} \right)^{l_{\eta}^{\xi}},$$

where $\widetilde{\mathcal{G}}_{\eta,\lambda_{\eta}}^{<}$ ($\widetilde{\mathcal{G}}_{\eta,\lambda_{\eta}}^{>}$) and $\mathcal{Z}_{\eta,\lambda_{\eta}}$ are defined in the same way as in eq. (6) with $\mathcal{O}_{\eta_{0}} = b_{\eta_{0},m}^{\dagger}b_{\eta_{0},m}$ ($\mathcal{O}_{\eta_{0}} = b_{\eta_{0},m}b_{\eta_{0},m}^{\dagger}$) and $\mathcal{O}_{\eta_{0}} = 1$. X denotes the different ion sites appearing in the \mathcal{A}_{v}^{ξ} expansion. We have the following limits:

(9)
$$\lim_{\{z_{\eta}^{\text{PF}}\}\to 0} \mathcal{Z}_{\lambda} = \sum_{\{n_{\overline{\eta}}^{\overline{m}}\}_r} e^{-\beta \mathbf{H}} \prod_{\eta'}^r \lim_{\{z_{\eta'}\}\to 0} z_{\eta'}^{n_{\eta'}} = \sum_{\{n_{\overline{\eta}}^{\overline{m}}\}_r: n_{\eta} = 0} e^{-\beta \mathbf{H}} = e^{-\beta \mathbf{H}} \Big|_{\{n_{\overline{\eta}}^{\overline{m}}\}_r = 0} = 1$$

and by using eq. (8)

(10)
$$\lim_{z_{\eta} \to 0} \mathcal{Z}_{\eta, \lambda_{\eta}} = 1; \qquad \lim_{z_{\eta} \to 0} \widetilde{\mathcal{G}}_{\eta, \lambda_{\eta}}^{<} = 0; \qquad \lim_{z_{\eta} \to 0} \widetilde{\mathcal{G}}_{\eta, \lambda_{\eta}}^{>} = 1.$$

We recover the true many-particle expansion in the limit

(11)
$$\langle \mathcal{A}_w \rangle^{\mathrm{F}} = \frac{1}{\mathcal{Z}^{\mathrm{F}}} \lim_{\{z_n\} \to 0} \frac{\partial^r \left[\langle \mathcal{A}_w \rangle_{\lambda}^{\mathrm{PF}} \mathcal{Z}_{\lambda}^{\mathrm{PF}} \right]}{\partial z_1 \cdots \partial z_r} .$$

If we insert eq. (8) in the previous expression and use the limits of eqs. (9), (10), it is clear that, in the limit $\{z_{\eta}\} \to 0$, eq. (11) vanishes unless the derivative acts on the less-than operator. We have

$$\begin{split} \langle \mathcal{A}_{w} \rangle^{\mathrm{F}} &= \frac{1}{\mathcal{Z}^{\mathrm{F}}} \sum_{\xi} \lim_{\{z_{\eta}\} \to 0} \frac{\partial^{r} \left[\prod_{\eta \in X} \mathbf{A}_{\eta}^{\xi} \left(\frac{\widetilde{g}_{\eta, \lambda_{\eta}}^{>}}{Z_{\eta, \lambda_{\eta}}} \right)^{g_{\eta}^{\xi}} \left(\frac{\widetilde{g}_{\eta, \lambda_{\eta}}^{<}}{Z_{\eta, \lambda_{\eta}}} \right)^{l_{\eta}^{\xi}} \mathcal{Z}_{\lambda}^{\mathrm{PF}} \right] \\ &= \frac{1}{\mathcal{Z}^{\mathrm{F}}} \sum_{\xi} \lim_{\{z_{\eta}\} \to 0} \left[\prod_{\eta \in X} \mathbf{A}_{\eta}^{\xi} \frac{\partial}{\partial z_{\eta}} \left[\left(\frac{\widetilde{g}_{\eta, \lambda_{\eta}}^{>}}{Z_{\eta, \lambda_{\eta}}} \right)^{g_{\eta}^{\xi}} \left(\frac{\widetilde{g}_{\eta, \lambda_{\eta}}^{<}}{Z_{\eta, \lambda_{\eta}}} \right)^{l_{\eta}^{\xi}} \right] \right] \left[\left(\prod_{\eta' \notin X} \frac{\partial}{\partial z_{\eta'}} \right) \mathcal{Z}_{\lambda}^{\mathrm{PF}} \right] \\ &= \frac{1}{\mathcal{Z}^{\mathrm{F}}} \sum_{\xi} \prod_{\eta \in X} \mathbf{A}_{\eta}^{\xi} \delta_{l_{\eta}^{\xi}, 1} \lim_{z_{\eta} \to 0} \frac{\partial \widetilde{g}_{\eta, \lambda_{\eta}}^{<}}{\partial z_{\eta}} \lim_{\{z_{\eta'}\}_{\eta' \notin X} \to 0} \left[\left(\prod_{\eta' \notin X} \frac{\partial}{\partial z_{\eta'}} \right) \mathcal{Z}_{\lambda}^{\mathrm{PF}} \right] \\ &= \sum_{\xi} \prod_{\eta \in X} \mathbf{A}_{\eta}^{\xi} \delta_{l_{\eta}^{\xi}, 1} \lim_{z_{\eta} \to 0} \frac{\partial \widetilde{g}_{\eta, \lambda_{\eta}}^{<}}{\partial z_{\eta}} \left[\frac{\partial \mathcal{Z}_{z_{\eta}, \lambda_{\eta}}}{\partial z_{\eta}} \right]^{-1} \\ &= \sum_{\xi} \prod_{\eta \in X} \mathbf{A}_{\eta}^{\xi} \delta_{l_{\eta}^{\xi}, 1} \mathcal{G}_{\eta}^{\zeta}, \end{split}$$

where $\mathfrak{G}_{\eta} = \frac{1}{Z^{\mathrm{F}}} \lim_{\{z_{\eta}\} \to 0} \frac{\partial^{r} [\mathcal{G}_{\gamma}^{c} Z_{\lambda}^{\mathrm{PF}}]}{\partial z_{1} \cdots \partial z_{r}}$ is the physically correct Green's function in the fermionic limit. The above expression shows that in Abrikosov-Coleman's formalism the fermionic limit can be easily recovered through the usual many-particle expansion applied to the pseudo-fermion Green's ion propagator. In particular, Feynman's diagram containing more than one single less-than Green's function for each ion site vanish in the pseudo-fermion limit and the greater-than Green's functions reduce to the identity. Differing from the original Abrikosov's approach, Coleman's limit procedure allows to recover the expression of the many-particle expansion in the physical space directly in terms of the corresponding Green's functions \mathfrak{G} , their explicit expressions being not needed. Therefore, this procedure may be successfully applied to describe dynamical properties of Kondo-type systems, for which non-equilibrium Green's functions cannot be approximated by multi-pole functions in the energy representation.

2.3. Example. As an example, we have applied our procedure to a system of localized magnetic ions interacting with the mean magnetic field generated by a hole gas (here a charge carrier is a hole). In this case $\mathbf{H} = \mathbf{H}_{\mathrm{MF}}$ and we have considered the following operator $\mathcal{A} = (\hat{n}_n^m)^2$. A direct calculation shows that

(12)
$$\langle (\hat{n}_{\eta}^{m})^{2} \rangle^{F} = \langle \hat{n}_{\eta}^{m} \rangle^{F} = \langle b_{\eta,m}^{\dagger} b_{\eta,m} \rangle^{F} = \frac{e^{-\beta \frac{\gamma}{V} m S_{z}}}{\sum_{m} e^{-\beta \frac{\gamma}{V} m S_{z}}} ,$$

where, in the last equality, we have assumed that the system is at equilibrium. In order to apply our procedure the operator must be expanded in Abrikosov's pseudo-fermion space (where $\langle n_{n,m}^2 \rangle \neq \langle n_{\eta,m} \rangle$)

$$\left\langle (\hat{n}_{\eta}^{m})^{2} \right\rangle_{\lambda}^{\mathrm{PF}} = \left\langle b_{\eta,m}^{\dagger} b_{\eta,m} b_{\eta,m}^{\dagger} b_{\eta,m} \right\rangle_{\lambda}^{\mathrm{PF}} = \lim_{t' \to t} \left\langle T \left[b_{\eta,m}^{\dagger}(t^{+}) b_{\eta,m}(t) b_{\eta,m}^{\dagger}(t'^{+}) b_{\eta,m}(t') \right] \right\rangle_{\lambda}^{\mathrm{PF}}$$

and if we apply Wick's theorem one gets

$$\begin{split} \left\langle (\hat{n}_{\eta}^{m})^{2} \right\rangle_{\lambda}^{\mathrm{PF}} &= \lim_{t' \to t^{-}} [\mathcal{G}_{\eta,m}(t,t)\mathcal{G}_{\eta,m}(t',t') - \mathcal{G}_{\eta,m}(t,t')\mathcal{G}_{\eta,m}(t',t)] \\ &= [\mathcal{G}_{\eta,m}^{<}(t,t)\mathcal{G}_{\eta,m}^{<}(t,t) + \mathcal{G}_{\eta,m}^{>}(t,t)\mathcal{G}_{\eta,m}^{<}(t,t)]. \end{split}$$

Using the previous prescription, in the limit λ goes to infinity, the first contribution vanishes and one recovers eq. (12).

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