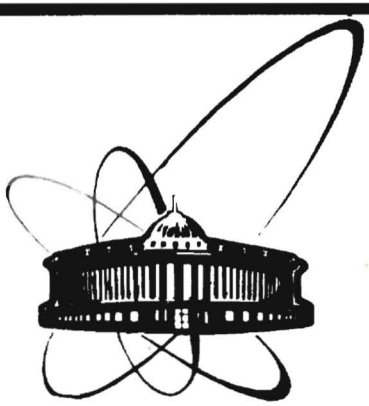

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A.L.Kuzemsky

IRREDUCIBLE GREEN FUNCTION METHOD IN THE CONDENSED MATTER THEORY

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1. The study of the excitations in many-body systems has been one of the most fascinating subjects for many years. The quantum field theoretical techniques have been widely applied to statistical treatment of a large number of interacting particles. Some powerful approaches such as Green function (GF) method, Feynman diagrams and the canonical transformation method gradually penetrated the domain of condensed matter physics. Among important influences of the quantum field theory on the conceptual development of condensed matter physics were the concepts of quasiparticles and symmetry breakdown.

The considerable progress in studying the spectrum of elementary excitations and thermodynamic properties of many-body systems has been for the most part due to the development of the temperature-dependent Green function method which has been elaborated by many authors. The method of two-time thermal (retarded or advanced) GF's in its initial form goes back almost thirty years to a paper by N.N.Bogolubov and S.V.Tyablikov[1] demonstrating that the retarded and advanced GF's can hopefully serve as a basis for studying the physical properties of many-body systems as well as the causal ones. The causal GF's which play a vital role in quantum field theory cannot be analytically continued into the complex energy plane and therefore the retarded or advanced GF's are more convenient in this sense. The method of two-time thermal GF's has been widely used in a large number of investigations[2,3], especially in the quantum theory of magnetism[4]. The exact equation of motion for the GF involves higher-order GF's and must be linearized by a certain approximation so that it can be solved for the GF. The random-phase approximation[5] is the simplest and most popular decoupling scheme for this purpose. Unfortunately the damping effects and finite lifetimes are not taken into account for an approximation of the sort.

Over the years, however, new developments have been made both in a deeper understanding of the interrelation between the quantum field theory and condensed matter physics[6] as well as the GF method itself. In the last decades a helpful reformulation of the two-time GF method has been given[7-11]. This approach is based on the introduction of "irreducible"

parts of GF's, which makes it possible, without recourse to a truncation of the hierarchy of equations for the GF's, to write down the exact Dyson equation and to obtain an exact analytical representation for the self-energy operator. Thus, this irreducible Green function (IGF) method incorporated certain advantages of the causal GF formalism, namely the Dyson equation conserving the useful analytical properties. Therefore, in contrast to the standard equation-of-motion approach the decoupling is only introduced in the self-energy operator and in a certain sense there is a possibility of controlling, in diagrammatic language, the relevant decoupling procedure in further approximative self-energy calculations. The crucial point of the whole problem is the same form of the equation of motion for all three (retarded, advanced and causal) GF's.

2. As an introduction to the concepts of IGF's let us describe the main ideas of this approach in a symbolic form. To calculate the retarded GF

$$G^r(t-t') = \ll A(t),\, A^+(t') \gg = \\ = -i\theta(t-t') \langle [A(t),\, A^+(t')]_\eta \rangle , \qquad \eta = \pm 1, \tag{1}$$

let us consider the equation of motion for (1)

$$\omega G(\omega) = \langle [A, A^+]_\eta \rangle + \ll [A, H]_- \,|\, A^+ \gg_\omega . \tag{2}$$

By definition we introduce the irreducible part (ir) of the GF

$$^{ir}\ll [A, H]_- \,|\, A^+ \gg = \ll [A, H]_- - \alpha A \,|\, A^+ \gg . \tag{3}$$

The unknown constant α is defined by the condition

$$\langle [\, [A, H]_-^{ir}, A^+ \,]_\eta \rangle = 0. \tag{4}$$

From the condition (4) one can find

$$\alpha = \frac{\langle [\, [A, H]_- A^+ \,]_\eta \rangle}{\langle [A, A^+]_\eta \rangle} = \frac{M_1}{M_0}. \tag{5}$$

The IGF's are defined so that they cannot be reduced to the low-order ones by any kind of decoupling. The irreducible correlation functions are well known in statistical mechanics. They are obviously defined as

$$K^A(x) = \langle A(x) \rangle = G^A(x),$$

$$K^{AB}(x_1, x_2) = \langle A(x_1)\, B(x_2) \rangle = G^{AB}(x_1, x_2) + G^A(x_1)\, G^B(x_2).$$

- -

In the diagrammatic approach the irreducible vertices are defined as the graphs that do not contain inner parts connected by the G°-line. With the aid of (3) the mean-field contributions are removed. This procedure extracts all relevant (for the problem under consideration) mean-field contributions and puts them into the generalized mean-field GF which has the form

$$G^\circ = \frac{\langle [A, A^+]_\eta \rangle}{(\omega - \alpha)} . \tag{6}$$

To calculate the IGF $^{ir}\ll [A, H]_-(t) \,|\, A^+(t') \gg$ in expression (3), we have to write the equation of motion after differentiation with respect to the second time variable t' [7]. The conditions (4) remove the inhomogeneous terms from this equation. If one introduces an irreducible part for the right-hand side operator as discussed above for the "left" operator, the equation of motion (2) can be exactly rewritten in the following form

$$G = G^\circ + G^\circ P G^\circ. \tag{7}$$

The scattering operator P is given by the expression

$$P = (M_0)^{-1}\, ^{ir}\ll [A, H]_- \,|\, [A, H]_-^+ \gg^{ir} (M_0)^{-1} . \tag{8}$$

From the Dyson equation

$$G = G^\circ + G^\circ M G \tag{9}$$

we get the following equation for M

$$P = M + M G^\circ P \tag{10}$$

from which it follows that we can say, in complete analogy to the diagrammatic approach, that the self-energy operator M is defined as a proper (in the diagrammatic language "connected") part of the scattering operator

$$M = (P)^{p}. \qquad (11)$$

Thus, by introducing "irreducible" parts of GF (or the "irreducible" parts of the operators, out of which the GF is constructed) the equation of motion for the GF can be exactly transformed into a Dyson equation with an exact representation of the self-energy operator which is represented by a higher order GF. It should be emphasized that for the retarded and advanced GF's the proper part (11) has only a symbolic character. However, one can use the causal instead of retarded GF at any step of calculations due to the same form of the equations for all three types of GF's. In a certain sense there is such a possibility to control, in the diagrammatic language, the relevant decoupling procedure in further approximative self-energy calculations.

3. The general philosophy of the IGF method is to try to separate and identify scattering effects which are "elastic" and "inelastic" in nature. Before going into the field of the concrete examples it will be worth while to emphasize that from a technical point of view the IGF method is a special kind of the projection-operator approach in the theory of two-time Green functions[11,12]. It turns out that there is a possibility of generalizing the scheme described above introducing the "irreducible" GF's for higher-order equations of motion. We describe briefly this point of view in order to explain that the structure of the obtained solution for one-particle GF depends strongly on the stage at which "irreducible" parts have been introduced. Let us consider equation (2) again. Instead of (3), now we introduce the IGF's in the following way

$$\begin{aligned}
\omega \ll A \mid A^{+} \gg &= M_0 + \ll [A,H]_{-} \mid A^{+} \gg_{\omega}, \\
\omega \ll [A,H]_{-} \mid A^{+} \gg &= M_1 + {}^{ir}\ll [[A,H]_{-},H]_{-} \mid A^{+} \gg_{\omega} + \\
&+ a_1 \ll A \mid A^{+} \gg_{\omega} + a_2 \ll [A,H]_{-} \mid A^{+} \gg_{\omega}.
\end{aligned} \qquad (12)$$

The unknown constants a_1 and a_2 are connected by the conditions

$$\langle [[A,H]_{-},H]^{ir}_{-}, A^{+}]_{\eta} \rangle = 0. \qquad (13)$$

As we have tried to illustrate in this article only the main ideas, consider the simplest possibility and write down the following equation

$$\omega\, {}^{ir}\ll [[A,H]_{-},H]_{-} \mid A^{+} \gg_{\omega} = {}^{ir}\ll [[A,H]_{-},H]_{-} \mid [H,A^{+}]_{-} \gg_{\omega}. \qquad (14)$$

Then by introducing the irreducible part for the "right" operator we obtain

$${}^{ir}\ll [[A,H]_{-},H]_{-} \mid A^{+} \gg_{\omega} (\omega - a_1^{+}) = {}^{ir}\ll [[A,H]_{-},H]_{-} \mid [H,A^{+}]_{-} \gg^{ir}. \qquad (15)$$

From (12)-(15) we arrive at the following set of equations

$$\begin{aligned}
&\omega \ll A \mid A^{+} \gg_{\omega} - \ll [A,H]_{-} \mid A^{+} \gg_{\omega} = M_0, \\
&a_1 \ll A \mid A^{+} \gg_{\omega} + (\omega - a_2) \ll [A,H]_{-} \mid A^{+} \gg_{\omega} = M_1 - \Phi,
\end{aligned} \qquad (16)$$

where Φ denote

$$\Phi = {}^{ir}\ll [[A,H]_{-},H]_{-} \mid [A,H]^{+}_{-} \gg^{ir}. \qquad (17)$$

The solutions of equations (16) are given by

$$\ll A \mid A^{+} \gg_{\omega} = \frac{M_0(\omega - a_2) - (M_1 - \Phi)}{\omega(\omega - a_2) + a_1}, \qquad (18)$$

$$\ll [A,H]_{-} \mid A^{+} \gg_{\omega} = \frac{\omega(M_1 - \Phi) + a_1 M_0}{\omega(\omega - a_2) + a_1}, \qquad (19)$$

$$a_1 M_0 + a_2 M_1 = M_2. \qquad (20)$$

There is a great similarity between the present approach and the moment method [13,14]. The structure of equation (18) exactly corresponds to the two-first-moment expansions[13], but differs from it by the factor Φ. But the basic idea of the present method resembles that of the Mori-Zwanzig projection method rather than the moment method as shown in paper [11] in a self-consistent manner.

4. The IGF method has been applied recently to a number of problems of condensed matter theory[9,10,15-24]. It is worth emphasizing that in a general case the mean-field renormalizations can be of a very nontrivial structure. To obtain this nontrivial structure of the mean-field renormalization cor-

rectly, one must construct the full GF built on the complete algebra of relevant operators and develop a special projection procedure for higher-order GF's in accordance with the finding algebra. The IGF method allows one to completely describe the quasiparticle spectra with damping in a very general way. To calculate the self-energy operator in a self-consistent way, we have to express it approximately by lower order GF's. Here we will restrict ourselves to mentioning a few most interesting examples.

Let us consider the famous Hubbard Hamiltonian

$$H = \sum_{ij\sigma} t_{ij} a^{+}_{i\sigma} a_{j\sigma} + \frac{U}{2} \sum_{i\sigma} n_{i\sigma} n_{i-\sigma}, \qquad (21)$$

which really gives a better understanding of the electronic correlations in solids. Two variants of the IGF theory make it possible to obtain two exact representations for the self-energy operator (11) which are used to obtain approximate solutions in the atomic ($U \gg t$) and band ($U \ll t$) limits[10]. In the atomic limit we obtain for (6)

$$G^{0}_{\sigma}(q,\omega) \cong \frac{(1-n_{-\sigma})}{\omega - E_{-} - n_{-\sigma} W^{-}_{q,-\sigma}} + \frac{n_{-\sigma}}{\omega - E_{+} - (1-n_{-\sigma}) W^{+}_{q,-\sigma}}, \qquad (22)$$

where $W^{\pm}$ are the shifts for the upper and lower bands due to the correlation of electrons:

$$W^{\pm} \sim \{ \langle a^{+}_{i-\sigma} n^{\pm}_{i\sigma} a_{j-\sigma} \rangle + \langle a_{i-\sigma} n^{\mp}_{i\sigma} a^{+}_{j-\sigma} \rangle +$$

$$+ \langle n^{\pm}_{j-\sigma} n^{\pm}_{i-\sigma} \rangle + \langle a_{i\sigma} a^{+}_{i-\sigma} a_{j-\sigma} a^{+}_{j\sigma} \rangle - \langle a_{i\sigma} a_{i-\sigma} a^{+}_{j-\sigma} a^{+}_{j\sigma} \rangle \}. \qquad (23)$$

So the GF (22) of the generalized mean-field approximation takes more accurately into account the nondiagonal matrix elements and due to this fact has a more general two-pole structure than the famous "Hubbard III" and Roth solutions. In particular, from our solution it is clear that for the atomic limit the mean fields cannot be represented by the functionals of the mean electron density $F[\langle n_{\sigma} \rangle]$. The solution (22) goes over into the "Hubbard I" solution if we make a very crude approximation

$$W^{\pm} \sim \langle n_{j-\sigma} n_{i-\sigma} \rangle \approx n^{2}_{-\sigma}.$$

Therefore, the use of the IGF method makes it possible to see clearly what correlations are omitted in the total correlation functions to obtain any particular approximation. This essentially makes it possible to construct approximate solutions systematically. The correlations due to the self-energy operator

$$\bar{M}_{q\sigma}(\omega) = \bar{\Phi}^{-1} \{ \sum_{em} t_{ie} t_{mj}\, {}^{ir}\langle\langle \bar{D}_{ie} | \bar{D}^{+}_{mj} \rangle\rangle^{ir} \}_{q} \bar{\Phi}^{-1}, \qquad (24)$$

occur in (11) as additive corrections which is very convenient for estimations of various scattering effects. Note that the "Hubbard III" solution gives the local self-energy operator. We remark that the Hubbard model in the strong correlation limit gives the archetypical example of the fact that in the general case the mean-field renormalization can have a very nontrivial structure. Under various regimes the mean-field corrections can be drastically changed and the relevant mean-field renormalizations must be considered. According to the rigorous mathematical theory of superconductivity which has been given by N.N.Bogolubov[2] the mean-fields or Hartree-Fock-Bogolubov renormalizations must contain the anomalous contributions. For example, if we consider the system with the Hamiltonian (21), equation (3) for the superconducting case takes the form

$$^{ir}\langle\langle a_{i\sigma} n_{i-\sigma} | a^{+}_{j\sigma} \rangle\rangle = \langle\langle a_{i\sigma} n_{i-\sigma} | a^{+}_{j\sigma} \rangle\rangle - \langle n_{i-\sigma} \rangle \langle\langle a_{i\sigma} | a^{+}_{j\sigma} \rangle\rangle +$$

$$+ \langle a_{i\sigma} a_{i-\sigma} \rangle \langle\langle a^{+}_{i-\sigma} | a^{+}_{j\sigma} \rangle\rangle. \qquad (25)$$

With the aid of the definition (25) the equations for the strong-coupling superconductivity in the transition metals[15,18] and their disordered alloys[17,19] have been derived.

The next very interesting many-body problem is the formation of polaron-like states in magnetic semiconductors due to the effective attraction of the electron and magnon. It is possible for the case of the antiferromagnetic coupling of the electron spin to the lattice (magnetic subsystem). Investigations of the magnetic polarons permit us to clarify the nature of the true carriers at low temperatures of the magnetic semiconductors. Let us consider the s-f model. The total Hamiltonian of this model describes the two subsystems (band electrons and localized spins) coupled by a local spin-spin exchange interaction[20]

$$H_{sf} = -2I \sum_{i\sigma\sigma'} (S_{i} \cdot \sigma)_{\sigma\sigma'} a^{+}_{i\sigma} a_{i\sigma'} \qquad (26)$$

It has already been noted[25] that the GF calculations for this problem must be provided including both spin-conserving

and spin-flip processes. Crucial differences between bound- and scattering-state[20] contributions to the electron spectral weight have been high-lighted. Using the procedure outlined in (2)-(11) for the calculation of the electronic quasiparticle spectrum of the s-f model (26) we get the equation for magnetic polaron quasiparticle energies[21]

$$E_{k\sigma} = \epsilon^{\circ}_{k\sigma} + I^2 N^{-1} \Psi_{k\sigma}(E_{k\sigma}),$$

$$\Psi_{k\sigma}(\omega) = \sum_q \{ \frac{\langle S^{-\sigma}_{-q} S^{\sigma}_{q} \rangle}{[1 - I\Lambda_{k\sigma}(\omega)](\omega + z_\sigma \omega_q - \epsilon^{\circ}_{k+q,\sigma})} + \qquad (27)$$

$$+ \frac{[1 + I\Lambda_{k\sigma}(\omega)] \langle (S^{z}_{-q})^{ir} (S^{z}_{q})^{ir} \rangle}{[1 - I\Lambda_{k\sigma}(\omega)](\omega - \epsilon^{\circ}_{k+q,\sigma})} \}.$$

The energy spectrum $E_{k\sigma}$ consists of two bands for any electron spin projection. The magnetic polaron states are formed only for antiferromagnetic s-f coupling ($I < 0$) when there is a lowering of the band electron energy due to the effective attraction of the electron and magnon. Our generalized mean-field solution is exactly reduced to the Shastry-Mattis result[25] for $T = 0K$.

5. In this paper, we have shown that the IGF method gives a unified and self-consistent formalism for the full description of the quasiparticle spectra and damping for many-particle systems. The most important conclusion to be drawn from this paper is that the mean-field renormalization can have, in general, a very nontrivial structure as in cases of the Hubbard model in the strong correlation limit and the magnetic polaron problem at finite temperatures and an arbitrary value of s-f exchange. It is important to emphasize that these self-consistent mean-field approximations can be interpreted in term of diagrams. Thus, the IGF method leads to relatively "well established" criteria underlying the approximations for the solution of the hierarchy of equations of motion for the one-particle GF of any given Hamiltonian. It is also worth noticing that on the basis of the IGF method it becomes apparent that the relevant mean-field renormalization in Eq.(3) may also be analyzed by an appropriate formulation of the broken-symmetry theory. One of the best known approaches in this field is the Bogolubov fundamental idea of quasi-averages[26]. Most successful realizations of this concept are the Bogolubov theories of superfluidity and superconductivity. Bogolubov has shown that the use of the anomalous propagators can be justified by using a source term in the Hamiltonian[2,26]. Thus the present study might be a useful reconfirmation of his results. Our recent results[24] also reveal that there is much hope that such type of a formalism would clarify a very difficult problem of the microscopic description of the antiferromagnetism. We also believe that the IGF method can be a basis of the study of more general cases than that considered in papers[15-24].

It therefore gives some real insight into the foundations of the GF method for the condensed matter theory.

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Метод неприводимых функций Грина
в теории конденсированных сред

Развит новый метод для расчета квазичастичных спектров и их затухания в системах многих взаимодействующих частиц. С помощью введения неприводимых частей для запаздывающих функций Грина выводится точное уравнение Дайсона. При этом точный массовый оператор выражается через функцию Грина высшего порядка. Показано, что для широкого круга задач теории конденсированных сред метод неприводимых функций Грина позволяет весьма просто вычислять квазичастичный спектр и затухание.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

Препринт Объединенного института ядерных исследований. Дубна 1988

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