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SOLUTION OF THE KADANOFF-BAYM EQUATIONS BY ITERATED EXPANSIONS

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Abstract. In this paper, we will show how the general nonlinear Kadanoff-Baym equations can be solved with iterated series expansion. In this regard, we will neglect vertex corrections. Further, we will obtain a formal solution in terms of colored tree graphs. The iteration procedure will show that after proper discretization, well-structured matrix equations would be obtained which are easy to implement in numerical simulation.

1. Introduction

Quantum field theory is a very successful physical theory which has proven to be very successful in the description of the fundamental forces of nature [1]. Also, this theory is frequently used in condensed matter physics [2]. Frequently, this theory is formulated in a background where besides the (few) particles on interest, no other surrounding particles are considered. Thus, effects of an ensemble of particles, e.g. effects of finite temperature are not included in the theoretical description [3]. Ordinary (zero-point) Quantum field theory is formulated theoretically on a single time contour, while the finite temperature formalism allows to use Quantum statistical density matrices [4]. Two time branches instead of one time branch is used in the finite temperature formalism. In the case for which the correlation with an initial density matrix, a third time branch that analytically continues the time integration contour to the imaginary time axis is also included [5, 6].

We neglect the occurrence of initial correlations and therefore, imaginary time (Matsubara) contour is also omitted. This paper gives the solution structure of the two-time Kadanoff-Baym equation that has the general form

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$$\frac{\partial}{\partial t_1} G(1,2) = H(1)G(1,2) + \int d3\Sigma(1,3)G(3,2) \tag{0}$$

where 1, 2 and 3 are shorthand for spacetime points on Schwinger-Keldysh contour (t_1, x_1), (t_2, x_2), (t_3, x_3) and $G(1,2)$ is the Green function between spacetime points 1 and 2 on Schwinger-Keldysh contour, $H(1)$ is the kinetic part of the Hamiltonian at the spacetime point 1 and $\Sigma(1,3)$ is the self-energy function between the spacetime points 1 and 3 on the contour. Note that the above equation is very general. Indeed, there can occur situations with several types of Green functions if there are multiple kinds of elementary particles and /or force carrying bosons. One can also express different kinds of green functions, i.e. retarded, advanced, greater and lesser functions can be defined.

2. Theoretical considerations

This can be performed by discretization which is out of the scope of this paper. With discrete matrices, i.e. the transition from $G(1,2)$ to G_{12} (having discrete, not continuous variables), we have a better possibility to study mathematical details. Clearly, we can do some mathematical operations with this Green functions. Simple numbers of some ring $\Re$ can be added or multiplied. However, in this paper, the ring of matrices will have two different multiplication operators. We will call one operator the sandwhiching which is defined for the set of 2×2-matrices M (with entries in the ring $\Re$) as

$$M \times M \to M : A_{ik} \times B_{ik} \to (AB)_{ik} \tag{1}$$

This equation is just an element-wise multiplication. The second operator id the well-known matrix multiplication (in continuum: the convolution) that is defined as

$$M \times M \to M : A_{ik} \times B_{ik} \to \Sigma_j A_{ij} B_{jk} \tag{2}$$

Together with addition and substraction, polynomials over the ring of matrices can be formulated. We introduce the category of matrices with polynomial-forming operations including (1) and (2). We denote it with $C(M)$. The well-known operations in nonequilibrium Green function theory like making a Green function a greater, lesser, advanced or retarded one, we will formulate in terms of homomorphisms. The following Langreth rules for advanced and retarded propagator are known:

$$(A \star B)_{r,a} = (A)_{r,a} \star (B)_{r,a} \tag{3}$$

Here, A, B are matrices, $\star$ denotes the convolution product and subscripts r, a correspond to taking the retarded or advanced part of the Green function. We will use the star as the convolution operation (2) and ordinary product symbol for the sandwhiching operation (1). Another Langreth rule for greater and lesser operations is given by

$$(AB)_{<,>} = (A)_{<,>}(B)_{<,>} \tag{4}$$

From the equations (3) and (4) we can see that there exists homomorphisms for sandwhiching and convolution operations; the corresponding homomorphism for operation (2) is taking retarded and advanced parts according to (3) and the corresponding homomorphisms for operation (1) is taking greater and lesser parts according to (4). Thus, the matrix homomorphism

$$h_{r,a,<,>} : M \to M : A_{ik} \to (A_{ik})_{r,a,<,>} \tag{5}$$

can transform the basic objects of $C(M)$ to specified objects (i.e. whether these are retarded, advanced, greater or lesser) that lie in the category $C'(M)$ such that there exists a homomorphism

$$h_{r,a,<,>} : C(M) \to C'(M) \tag{6}$$

that preserves either convolution or sandwhiching operation. More precisely, we can introduce the convolution-preserving homomorphism $h_{C;\alpha}$ that we call Î±-homomorphism and a sandwhiching-preserving homomorphism $h_{C;\beta}$ that we will call β-homomorphism. For the polynomials that can be formed, the variables are labelled as being Î±-homomorphism invariant (retarded and advanced objects) or β-homomorphism invariant (greater and lesser objects).

General Kadanoff-Baym equations in the form of (0) can be understood as polynomials with basic variable properties as given above. Because one nonequilibrium Green functions is expressed in terms of the others in form of a polynomial, we have an equivalence relation. The equivalence class of all Kadanoff-Baym equations we will denote by $E(M)$. The space of all Nonequilibrium Green functions that satisfy the Kadanoff-Baym equations will be the following space:

$$\Gamma(M) = \frac{C(M)}{E(M)} \tag{7}$$

In a similar way, we can define solution spaces for the homomorphic images of the space $C(M)$. Summarizing all these, we have a short exact sequence that shows the solution structure for Kadanoff-Baym equations:

$$0 \to E(M) \to C(M) \to \Gamma(M) \to 0 \tag{7'}$$

Homomorphisms can be also applied to the exact sequence (7'). This can be done generally in terms of a functor Hom that maps one category either by the operation (5) or (6). We can write down exact sequences for the abelian group of homomorphisms $Hom(C(M), C'(M))$ by using the rules of homological algebra. By applying the contravariant functors $Ext^n(-, C'(M))$ with $(n = 0,\ 1,\ 2, \cdots)$ on (7'), we will obtain a long exact sequence. Here, obviously, $Ext^0(-, C'(M)) = Hom(-, C'(M))$. There will also occur elements in the sets $Ext^{(n)}(C(M), C'(M))$ with $(n = 1,\ 2, \cdots)$, and hence, we will have the long exact sequence

$$\begin{aligned}
(8)\quad 0 \quad &\to \quad Hom(\Gamma(M), C'(M)) \xrightarrow{\alpha} Hom(C(M), C'(M)) \xrightarrow{\beta} Hom(E(M), C'(M)) \\
&\to \quad Ext^1(\Gamma(M), C'(M)) \to Ext^1(C(M), C'(M)) \to Ext^1(E(M), C'(M)) \\
&\to \quad Ext^2(\Gamma(M), C'(M)) \to \cdots
\end{aligned}$$

In duality, another long exact sequence can be formed by reversing the arrows. This can be obtained by applying on (7') the covariant functors $Ext^n(C'(M), -)$ with $(n =$

$0,\ 1,\ 2, \cdots)$. Once again, $Ext^0(C'(M), -) = Hom(C'(M), -)$, we get the long exact sequence

$$\begin{aligned}(8') \qquad &\to \quad Ext^2(C'(M), \Gamma(M)) \to Ext^1(C'(M), E(M)) \to Ext^1(C'(M), C(M)) \\ &\to \quad Ext^1(C'(M), \Gamma(M)) \to Hom(C'(M), E(M)) \stackrel{\beta_*}{\to} Hom(C'(M), C(M)) \\ &\qquad \stackrel{\alpha_*}{\to} Hom(C'(M), \Gamma(M)) \to 0\end{aligned}$$

Further investigations will be discussed within these representations.

The above exact sequence can offer information to the solution of Kadanoff-Baym equations in terms of the nonequilibrium Green functions; it is more precise than the quite general solution sequence (7'). For the zero-point Quantum field theory, it is enough to consider (7), but when going to Finite temperature formalism, a functorial morphism to the type of Green function must be performed. In finite temperature theory, the above exact sequence still holds.

In the sequence (8) the map

$$0 \to Hom(\Gamma(M), C'(M)) \stackrel{\alpha}{\to} Hom(C(M), C'(M)),$$

is monic but the map

$$Hom(C(M), C'(M)) \stackrel{\beta}{\to} Hom(E(M), C'(M))$$

may not epic, so the factor space $Hom(C(M), C'(M))/\alpha(Hom(\Gamma(M), C'(M)))$ may not be isomorphic to $Hom(E(M), C'(M))$.

On the other hand, in the sequence (8') the map

$$Hom(C'(M), C(M)) \stackrel{\alpha_*}{\to} Hom(C'(M), \Gamma(M)) \to 0$$

is surjective but the map

$$Hom(C'(M), E(M)) \stackrel{\beta_*}{\to} Hom(C'(M), C(M))$$

may not be monic. This means that $\ker(\alpha_*)$ may not be the $Im(\beta_*)$. So, the factor $Hom(C'(M), C(M))/\beta_*(Hom(C'(M), E(M)))$ may not be isomorphic to $Hom(C'(M), \Gamma(M))$.

This is a special difference that occurs not at ordinary zero-point quantum field theory. In graph theory, colored tree graphs that lie generally in the category T, can be formed from any colored graph in the category of Λ, while cancelling out the set of loops Ω. We have the isomorphism $T \cong \Lambda/\Omega$ and can represent it in terms of the short exact sequence

$$0 \to \Omega \to \Lambda \to T \to 0 \tag{9}$$

By applying a functor P that preserves the exactness (9), we will arrive to (7') and see that the matrix polynomials solving Kadanoff-Baym equations without the projection to a certain nonequilibrium Green function can be expressed in terms of colored tree graph expansions via $P(T) = \Gamma(M)$. However, to obtain the solutions for a retarded, advanced, greater or lesser Green function, we have to alter the functor applied to (9). We can further apply a functor that lets forget preserving exactness denoted by Q. The injectivity between Ω and Λ is still preserved, when Q is applied. Finally, we will arrive at the result

$$Hom(\Gamma(M), C'(M)) = (Q \circ P)(T) \tag{10}$$

We will have some extension groups Ext where we are left with, when Q is applied. This extension can be seen as additional terms that are coming from e.g. identifying self-energies with interaction of an ensemble besides the (1-loop) quantum self-energy known from zero-point quantum field theory.

3. Conclusions and Discussion

Tree graphs can be made isomorphic to algebras of matrices by defining a functor that preserves exactness of short exact sequences. This will be the case for zero-point Quantum field theory. In the case of finite temperature, we will not have exactness preserving structures; since there are also statistical ensembles where interactions can take place, we have to extend the morphisms between general colored graphs to colored tree graphs. We have found out that in finite temperature formalism, there will occur some non-surjectiveness that is measured by the set $Ext(E(M), C'(M))$. That will give us some deeper structure in the iteration schemes of Kadanoff-Baym equations in future research.

4. Background to the theory

Formally, Kadanoff-Baym equations are solved by performing a fixed point iteration. Fixed point iterations are used frequently in the numerical solution of algebraic equations, supposed that the iteration converges. For example, let X be a ring and $x \in X$ a variable in that ring. Then, suppose $f : X \to Y$ is a ring morphism from X to the ring Y. A fixed point equation in that ring has the general form $x = f(x)$, for all $x \in X$, i.e. f is a ring automorphism. If the function f is analytic, we can make the power series expansion

$$x = \Sigma_{k=0}^{\infty} a_k x^k \tag{11}$$

For some coefficients $a_k \in X$ such that the sum (11) converges. Formally, if the values for x substituted into the series (11), we obtain the nested power series expansion

$$x = \Sigma_{k=0}^{\infty} a_k (\Sigma_{l=0}^{\infty} a_l x^l)^k = \Sigma_{k=0}^{\infty} b_k x^k. \tag{12}$$

To compute the new coefficients b_k one can depict the iteration as a tree of length L that is equal to the number of iterations. The power of the exponent in the sum (12) is equal to the number of leaves at the top of the tree that has length L. There are different tree topologies that have the number of leaves k after L iterations. All these topologies are summed up when computing b_k. All branches of the tree that result in a bundle of k subsequent branches are colored with values a_k. There are L times, the branches continue in a generation of other branches. For each tree topology we can assign a value equal to the product of the values a_k. As an example, consider $L = 2$. Then we have two factors for the a_k and trees which have l leaves at their top, have, when summed over all topologies, the value $b_l = \Sigma_{k=0}^{\infty} a_{l-k} a_k$, i.e. the well-known power series multiplication rule.

In the same manner as depicted above, Kadanoff-Baym equations can be seen as a system of fixed point equations. Solutions are then sums over different topologies. However, some topologies are excluded due to the structure of Kadanoff-Baym equations and invariance laws with respect to sandwhiching and convolution. With the tools of homological algebras, it is possible to rule out topologies that have not e.g. above invariance relations. We have done the restrictions by applications of functors on the category of graphs. Additional mathematical structures like that exactness of an exact sequence is not preserved in presence of thermal fields arise in the fixed point equations.

These results can alternatively derived by considering a contravariant functor that generates a long exact sequence.

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