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Non-equilibrium Green functions: generalized Wick's theorem and diagrammatic perturbation theory with initial correlations

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Abstract. Wick's theorem is combined with a cluster decomposition to derive a generalized statistical Wick's theorem for a non-equilibrium system with initial correlations. This enables a diagrammatic time-dependent perturbation theory which is a simple extension of the usual one to be developed for time-path causal statistical Green functions and their matrix equivalents. This provides a complete non-equilibrium theory. Reduction of diagrams and equations of motion for the Green functions are also discussed.

1. Introduction

The introduction of time-path and similar methods for non-equilibrium statistical Green functions (many-body propagators) has greatly facilitated their study, and their usefulness has been clearly demonstrated (Craig 1968, Korenman 1966, 1969, Mills 1969, Keldych 1965, Caroli *et al* 1971, Sandstrom 1970, Dubois 1966, Hall 1974, to be referred to as I; this list is not exhaustive but hopefully representative). However, methods used have not taken into consideration initial correlations and therefore do not give a complete non-equilibrium many-body theory. Such a complete theory is found in the Liouville operator methods of Prigogine and co-workers (eg Prigogine 1962, Mayne and Prigogine 1973) and great advances have been made in a number of general problems (eg Rosenfeld 1972) and in problems of weakly interacting systems (eg Balescu 1963, Baus 1971). However, for certain problems difficulties arise (I) and it will be useful to have a non-equilibrium theory clearly related to the main body of many-body theory as represented by the statistical Green function methods. Fujita (1969, 1971) has derived such a theory using his diagrammatic method, but this is not entirely uniform with the usual diagrammatic Green function method. In this paper the time-path method is used to study the time-path causal statistical Green function for a non-equilibrium system with initial correlations, and the matrix equivalent of this Green function.

In § 2 Wick's theorem for time-path ordered operators is combined with a cluster decomposition to derive a generalized statistical Wick's theorem for a non-equilibrium system with initial correlations. No specification of the density matrix for the total system is required except that given by the specification of initial correlations. This Wick's theorem is used to obtain a diagrammatic perturbation method including initial correlations, which is a simple extension of the usual one. This is the main purpose and result of the paper. The resulting rules are given in appendix 1. Two dentate structure theorems (proved in appendix 2) ensure that there is no contribution from unlinked graphs, where the concept of an unlinked graph is extended to include a class of graphs

having initial correlations. In § 3 the reduction of graphs is considered and the self-energy function is introduced together with three other functions which play a similar role for correlated particles; and finally the generalized equations of motion (Kadanoff and Baym equations) for non-equilibrium statistical Green functions are derived in terms of these functions.

2. Perturbation series and Wick's theorem

Definitions of notation are like those of a previous paper (I) and will only be repeated briefly where necessary for clarity. A non-relativistic momentum representation is used with the momentum–time point $\boldsymbol{p}_1 t_1$ denoted by 1. Many of the considerations are not specific to this representation and extension to the configurational space is simple. The basic contour causal statistical Green function is defined as the statistical average over a non-equilibrium density matrix of a time ordered pair of field creation and annihilation operators (I § 2, Craig 1968, Mills 1969)

$$G(11') = -\mathrm{i}\langle T_c[a(1)a^+(1')]\rangle, \tag{1}$$

T_c orders in the sense of the time path given below. In the interaction picture

$$a(1)a^+(1') = U(t_0 t_1)a_I(1)U(t_1 t_1')a_I^+(1')U(t_1' t_0) \tag{2}$$

$$U(tt') = \sum_{n=0}^{\infty} (\mathrm{i}\hbar)^{-n}(n!)^{-1} \int_{t'}^{t} \mathrm{d}t_1 \ldots \int_{t'}^{t} \mathrm{d}t_n T[V(t_1)\ldots V(t_n)]. \tag{3}$$

The T in (3) orders in the sense of the integral. In equation (2) the first U has its time arguments reversed from the usual order so that the time can be considered to run from t_0 to t_1' to t_1 and then back again to t_0; T_c orders in the sense of this path. When the U are placed in equation (1) the overall T_c will order the factors in the U correctly both internally and also with respect to the creation and annihilation operators and the other U. Thus the perturbation expansion of the statistical Green function is correctly and compactly given by

$$G(11') = -\mathrm{i} \sum_{n=0}^{\infty} (\mathrm{i}\hbar)^{-n}(n!)^{-1} \int_C \mathrm{d}t_1 \ldots \int_C \mathrm{d}t_n \langle T_c[V(t_1)\ldots V(t_n)a_I(1)a_I^+(1')]\rangle. \tag{4}$$

The integrals are over the path described above.

The zeroth order term of the series is

$$\begin{aligned} G_0(11') &= -\mathrm{i}\langle T_c[a_I(1)a_I^+(1')]\rangle \\ &= -\mathrm{i}\exp[-\mathrm{i}\epsilon_1(t_1 - t_0) + \mathrm{i}\epsilon_1'(t_1' - t_0)][\theta_c(t_1 - t_1')n_0^>(\boldsymbol{p}_1\boldsymbol{p}_1') \\ &\quad + \theta_c(t_1' - t_1)\kappa n_0(\boldsymbol{p}_1\boldsymbol{p}_1')] \\ &\quad n_0(\boldsymbol{p}_1\boldsymbol{p}_1') \equiv n(\boldsymbol{p}_1\boldsymbol{p}_1', t_0), \qquad n_0^>(\boldsymbol{p}_1\boldsymbol{p}_1') = \delta(\boldsymbol{p}_1 - \boldsymbol{p}_1') + \kappa n_0(\boldsymbol{p}_1\boldsymbol{p}_1'). \end{aligned} \tag{5}$$

The $\theta_c(t_1 - t_2)$ are step functions which act in the direction of the path; κ is $+1$ for bosons and -1 for fermions. n is the single-particle density matrix. It is convenient to separate the other reduced density matrices by the following equations into parts which

can be factorized into single-particle density matrices and correlated parts. Writing a_r for $a(\boldsymbol{p}_r t)$:

$$n(\boldsymbol{p}_1\boldsymbol{p}_2 t) = \langle a_2^+ a_1 \rangle = \Gamma_1(\boldsymbol{p}_1, \boldsymbol{p}_2 t)$$

$$\begin{aligned} n_2(\boldsymbol{p}_1\boldsymbol{p}_2\boldsymbol{p}_3\boldsymbol{p}_4 t) &= \langle a_4^+ a_3^+ a_2 a_1 \rangle \\ &= n(\boldsymbol{p}_1\boldsymbol{p}_4 t)n(\boldsymbol{p}_2\boldsymbol{p}_3 t) + \kappa n(\boldsymbol{p}_1\boldsymbol{p}_3 t)n(\boldsymbol{p}_2\boldsymbol{p}_4 t) + \Gamma_2(\boldsymbol{p}_1\boldsymbol{p}_2, \boldsymbol{p}_3\boldsymbol{p}_4 t) \end{aligned} \tag{6}$$

$$\begin{aligned} n_u(\{\boldsymbol{p}_r\}, \{\boldsymbol{p}_s\} t) &= \left\langle \prod^u a_s^+ \prod^u a_r \right\rangle \\ &= \sum_{m=0}^{u} \sum_{\text{app}} \kappa^P \prod^m n(\boldsymbol{p}_r\boldsymbol{p}_s t)\Gamma_{u-m}(\{\boldsymbol{p}_r\}', \{\boldsymbol{p}_s\}' t). \end{aligned}$$

P is the parity of the permutation of the operators needed to obtain the order of the arguments on the right from the order on the left. The sum app is over all possible ways of picking m pairs one from each of the sets $\{\boldsymbol{p}_r\}$ $\{\boldsymbol{p}_s\}$ the remaining $u-m$ members of the sets $\{\ldots\}$ being the sets $\{\ldots\}'$ which give the arguments of the correlation matrix Γ_{u-m} of $u-m$ particles. The correlation matrices are related to a cluster decomposition below.

The potential in the interaction representation (not including exchange) is

$$V(t) = (2\Omega)^{-1} \sum_{\substack{12 \\ 1'2'}} V(121'2') a_I^+(1) a_I^+(2) a_I(2') a_I(1') \qquad t_1 = t_1' = t_2 = t_2'. \tag{7}$$

Any higher-order contribution to the perturbation series consists of potential factors, exponential factors as in equation (5), and statistical averages of ordered products of creation and annihilation operators which can be evaluated at time t_0. Although all the operators in these products can be referred to the same time t_0 their order is predetermined by the T_c of equation (4). It is useful therefore to keep T_c to signify the ordering. The T_c-ordered products in the perturbation expansion are related to the normal (N) ordered products occurring in the definitions (6) of the reduced density matrices by Wick's theorem in its original form (Wick 1950, Brown 1972). Denoting both creation and annihilation operators by b

$$\begin{aligned} T_c[b_1 b_2 \ldots b_{n-1} b_n] &= N[b_1 b_2 \ldots b_{n-1} b_n] + N[\dot{b}_1 \dot{b}_2 \ldots b_{n-1} b_n] + \ldots + N[b_1 \dot{b}_2 \ldots \dot{b}_{n-1} b_n] \\ &\quad + \ldots + N[\dot{b}_1 \dot{b}_2 \ldots \dot{b}_{n-1} \dot{b}_n] + \ldots \end{aligned} \tag{8}$$

$$T_c[b_i b_j] = N[b_i b_j] + \dot{b}_i \dot{b}_j. \tag{9}$$

All contractions (denoted by superscript dots) are zero except for those of pairs T_c-ordered as $a_r a_s^+$ whose contraction is $\delta(\boldsymbol{p}_r - \boldsymbol{p}_s)$. The statistical averages of both sides of equation (8) are taken and the correlation decompositions (6) of averages of normal products substituted. The contractions then combine with averages of normal ordered pairs to give averages of time-ordered pairs. Hence a generalized statistical Wick's theorem with all operators evaluated at the same time is

$$\langle T_c[b_1 b_2 \ldots b_{2u}] \rangle = \sum_{m=0}^{u} \sum_{\text{app}} \kappa^P \prod^m \langle T_c[b_r b_s] \rangle \kappa^{u-m} \Gamma_{u-m}(\ldots \boldsymbol{p}_q \ldots t). \tag{10}$$

The averages of time ordered pairs are either n, $n^>$ or zero, this latter if the pair does not

contain one annihilation and one creation operator. Replacing the time dependence in the operators gives

$$\langle T_c[b(1)b(2)\dots b(2u)]\rangle = \sum_{m=0}^{u} \sum_{\text{app}} \kappa^p \prod^{m} iG_0(rs)\kappa^{u-m}\Gamma^0_{u-m}(\dots q \dots t) \tag{11}$$

$$\Gamma^0_m(1\dots m, m'\dots 1') = \prod_{j=1}^{m} \exp[-i\epsilon_j(t_j - t_0) + i\epsilon'_j(t_j - t_0)]\Gamma_m(\boldsymbol{p}_1 \dots \boldsymbol{p}_m, \boldsymbol{p}'_m \dots \boldsymbol{p}'_1 t). \tag{12}$$

This is still not quite convenient for developing a diagrammatic perturbation theory because of the problem of the ordering of the arguments in the correlation matrices. The argument in the Γ are paired in the sense that the jth argument from the left is associated with the jth argument from the right. From equation (6) interchange of arguments leads to a Γ differing only by κ^p, and such an interchange is only different if it leads to a different pairing (otherwise two operators must have been moved in similar ways giving an even number of interchanges). To generate all possible pairings it is only necessary to carry out the m permutations of one of the sets of m arguments. Hence introducing

$$\gamma_m = (m!)^{-1}\Gamma_m \tag{13}$$

the statistical Wick's theorem becomes

$$\langle T_c[b(1)b(2)\dots b(2u)]\rangle = \sum_{m=0}^{u} \sum_{\text{app}} \kappa^p \prod^{m} iG_0(rs)\kappa^{u-m}\gamma^0_{u-m}(\dots q \dots). \tag{14}$$

The sum app now extends over all possible pairings of labels including those within γ.

The diagrammatic perturbation formalism is constructed in the usual way (Mills 1969, Brown 1972) leading to the rules for Green functions as given by previous workers (Craig 1968, Mills 1969, I) but now it also includes initial correlations. It is convenient to represent $\gamma^0_m(1\dots m, m'\dots 1')$ as in figure 1 by m directed lines running from j' to j where j and j' are paired labels, and these directed lines joined by a double line called a correlation bond.

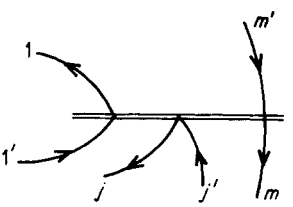

Figure 1.

The directed lines and labelling associated with the γ have the same combinational properties as those associated with the Green functions. Thus the overall κ^p is taken care of by the usual fermion loop rule as long as lines running through γ are taken into account. Topological indistinguishability has its usual effects in reducing the number of graphs required.

Using matrix representations (I § 2, Craig 1968, Mills 1969) for the contour causal Green functions simplifies the time integration to a single part from t_0 to t_p the latest of

t_1 and t_1'. The time path from t_0 to t_p is C_1 and from t_p to t_0 it is C_2; then

$$\mathcal{G}_{ab}(11') = G(11')\sigma_b, \qquad t_1 \in C_a \text{ and } t_2 \in C_b$$
$$\sigma = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \qquad \sigma_b = \sigma_{bb}. \tag{15}$$

Other matrix functions are similarly denoted by script letters. The appropriate matrix form for the correlation parts is

$$\mathcal{g}^0(1 \ldots m, m' \ldots 1)$$
$$= \prod_{j=1}^{m} \exp[-i\epsilon_j(t_j - t_0)]\mu(-i\kappa)^m \gamma_m(\boldsymbol{p}_1 \ldots \boldsymbol{p}_m, \boldsymbol{p}_m' \ldots \boldsymbol{p}_1' t) \exp[i\epsilon_j'(t_j' - t_0)]\bar{\mu} \tag{16}$$
$$\mu = \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \qquad \bar{\mu} = (1, -1).$$

The real-time matrix Green functions generate real-time ordered matrix Green functions (I, §2). However, the correlation parts are the same no matter what the time ordering of the arguments. For convenience rules for the diagrams and their interpretation are given in appendix 1.

The separation of the correlation matrices in equation (6) is the first step in a cluster decomposition which can be defined in the usual way (Kahn and Uhlenbeck 1938). Introducing the cluster matrices $\mathrm{X}_m(\boldsymbol{p}_1 \ldots \boldsymbol{p}_m, \boldsymbol{p}_m' \ldots \boldsymbol{p}_1', t)$ these preserve the same pairings of arguments as in the density matrices from which they are derived. The cluster decomposition is symbolically

$$n_u = \sum_{\mathrm{ac}} \kappa^P \prod_{(\Sigma m = u)} \mathrm{X}_m. \tag{17}$$

The sum ac is over all clusters of m pairs of arguments such that the total number of arguments is $2u$. In order to allow for all pairings of arguments further cluster matrices are introduced by

$$\chi_m = (m!)^{-1}\mathrm{X}_m$$
$$\chi_1 = n, \qquad \chi_2 = \gamma_2. \tag{18}$$

The statistical Wick's theorem is

$$\langle T_c[b(1)b(2) \ldots b(2u)]\rangle = \sum_{\mathrm{ac}} \sum_{\mathrm{app}} \kappa^P \prod^{n} iG_0(rs) \prod_{(\Sigma m = u - n)} \kappa^m \chi_m^0(\ldots q \ldots). \tag{19}$$

Diagrammatic rules are easily developed and are given in appendix 1. χ_m^0 can be represented in a similar way to γ_m^0, thus giving rise to a cluster bond. However, in view of the possibility of a number of clusters it may be more convenient to simply place a distinctive mark through each line belonging to a separate cluster. In figure 2 all lines with an a on them belong to one cluster as distinct from the other clusters labelled by b etc.

The cluster decomposition and therefore also the correlation decomposition is analytically valid only in the bulk limit (Kahn and Uhlenbeck 1938). However, this should not restrict the use of this formalism as the decomposition will be numerically valid even for small numbers of particles and small volumes.

There are two useful theorems which limit the number of diagrams which contribute. These are the left dentate structure (LDS) and correlation dentate structure (CDS) theorems

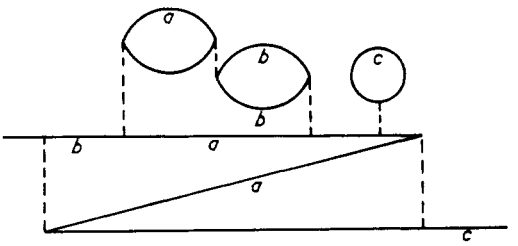

Figure 2.

discussed in appendix 2. If a diagram has an unlinked part this part must have an LDS and therefore the contribution from such a diagram is zero. Because a diagram with a CDS also contributes nothing the definition of the unlinked part can be extended to any part not joined to the main diagram by a potential bond or a Green function line. The LDS theorem has the effect of a causality principle ensuring that there is no contribution from times later than the latest time of interest t_p and this enables the maximum real time to be taken at any later time including $+\infty$. Then if the effects of initial correlations are not being studied the initial time t_0 can be taken as $-\infty$, so that the real time integral can run from $-\infty$ to $+\infty$.

3. Reduction of diagrams, self-energies and Kadanoff–Baym equations

A self-energy part M is an insertion in a line as in figure 3. If the lines on either side of M are taken into consideration then the whole of the structure containing M can replace a line in a diagram giving another valid diagram. Other line replacements contain similar structures denoted by C, E, D but the central graph is joined as in figure 3 to the ingoing, outgoing or both lines respectively by a cluster bond

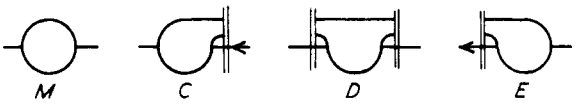

Figure 3.

Conversely if these structures occur in a graph then if they are replaced by a line the resulting graph is still valid. Such structures are therefore *line-replaceable*. The statistical Green function G is the sum of all permutations to all orders of all line-replaceable parts. The definition of a proper graph can be generalized: a *proper graph* has no two portions which are connected by less than two lines or one line and one cluster bond. The self-energy function M corresponds to the sum of all proper graphs having no cluster bond to ingoing or outgoing lines. Similarly a function D corresponds to the sum of all proper graphs with cluster bonds to ingoing and outgoing lines and including these lines. Convenient functions C and E are obtained by first defining C^p and E^p corresponding to sums of all proper graphs having the correct cluster bond; then symbolically

$$C = \sum_{n=0}^{\infty} (C^p)^n, \qquad E = \sum_{n=0}^{\infty} (E^p)^n. \tag{20}$$

The interative equations for the matrix forms $\mathscr{C}$ are $\mathscr{E}$

$$\begin{aligned}\mathscr{C}(11') &= \Delta(1-1') + \int_{t_0}^{t_p} dt_2 \sum_2 \mathscr{C}^p(12)\mathscr{C}(21') \\ \mathscr{E}(11') &= \Delta(1-1') + \int_{t_0}^{t_p} dt_2 \sum_2 \mathscr{E}^p(12)\mathscr{E}(21')\end{aligned} \tag{21}$$

$$\Delta(1-1') = \delta(\boldsymbol{p}_1 - \boldsymbol{p}_1')\delta(t_1 - t_1')\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}. \tag{22}$$

Now G_0 and D can be joined on the right by M and C and on the left by M and E. C can be joined on the right by M and C and on the left by G_0, D and C. E can be joined on the right by G_0, D and E and on the left by M and E. Thus the line-replaceable elements can only be joined together in certain ways. Taking this into consideration the iterative equation for G in symbolic form is

$$G = E(G_0 + D)C + E(G_0 + D)CMG. \tag{23}$$

Line replacements for lines running to and from cluster bonds will contain the graphs of figures 4 (*a* and *b*) respectively

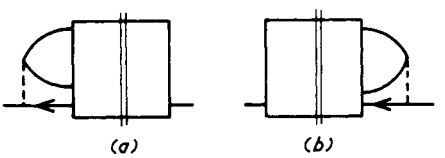

Figure 4.

In figure 4(*a*) the initial structure may represent either M or C and in figure 4(*b*) the final structure may represent either M or E. These structures therefore represent the functions written symbolically as

$$\begin{aligned}&(C-1)+CMG\\ &GME+(E-1).\end{aligned} \tag{24}$$

The sums of all possible line-replaceable parts for lines running to and from cluster bonds are in matrix form

$$\begin{aligned}\mathscr{F}(11') = \int_{t_0}^{t_p} dt_2\, dt_3 \sum_{23} \delta(\boldsymbol{p}_1 - \boldsymbol{p}_2)\exp[-i\epsilon_1(t_1 - t_2)]\bar{\mu}\mathscr{C}(23) \\ \times\left(\Delta(31') + \int_{t_0}^{t_p} dt_4 \sum_4 \mathscr{M}(34)\mathscr{G}(41')\right) \\ \mathscr{H}(11') = \int_{t_0}^{t_p} dt_2\, dt_3 \sum_{23}\left(\Delta(12) + \int_{t_0}^{t_p} dt_4 \sum_4 \mathscr{G}(14)\mathscr{M}(42)\right) \\ \times \mathscr{E}(23)\mu\delta(\boldsymbol{p}_3 - \boldsymbol{p}_1')\exp[-i\epsilon_1'(t_3 - t_1')].\end{aligned} \tag{25}$$

$\mathscr{F}$ is a row matrix and $\mathscr{H}$ a column matrix. The corresponding equations for non-matrix F and H are obvious from inspection of equations (25).

The usual definition of an irreducible graph can be generalized to: an *irreducible graph* contains no line-replaceable parts. The rules in appendix 1 can now be amended so that only irreducible graphs are used and all lines represent G, F or H ($\mathscr{G}$, $\mathscr{F}$, $\mathscr{H}$) respectively.

Previous approaches to non-equilibrium Green functions have used equation-of-motion and functional-integration methods which usually start from an equation for the Green function and proceed via a self-energy function. A familiar version is the method studied by Kadanoff and Baym (1962). Since these methods neglect initial correlations it is of interest to derive the generalized Kadanoff and Baym equations for a system with initial correlations. This has been done previously by Fujita (1969, 1971); however, the time-path method gives a more compact and explicit derivation and result, and establishes the equations in the matrix form. The equations of motion for the statistical Green functions are derived in the usual way (Kadanoff and Baym 1962) by differentiating definition (1) and using the equations of motion for the creation and annihilation operators.

$$\left(\mathrm{i}\frac{\partial}{\partial t_1}-\epsilon_1\right)G(11') = \delta(\boldsymbol{p}_1-\boldsymbol{p}_1')\delta_c(t_1-t_1')+\frac{\mathrm{i}\kappa}{2\Omega\hbar}\sum_{2\bar{2}}(V(12\bar{1}\bar{2})+\kappa V(12\bar{2}\bar{1}))G^{(2)}(\bar{1}\bar{2}21'),$$

$$t_1 = t_2 = \bar{t}_2 = \bar{t}_1 \tag{26}$$

$$G^{(2)}(1234) = -\langle T_c[a(1)a(2)a^+(4)a^+(3)]\rangle. \tag{27}$$

The delta function on the time path, $\delta_c(t_1-t_1')$, arises from differentiation of the time-path step function $\theta_c(t_1-t_1')$. On C_2 this step function acts in the reverse direction of physical time. Hence

$$\delta_c(t_1-t_1') = \begin{cases} +\delta(t_1-t_1') & t_1, t_1' \in C_1 \\ -\delta(t_1-t_1') & t_1, t_1' \in C_2. \end{cases} \tag{28}$$

The matrix forms of equations (26) (27) are

$$\left(\mathrm{i}\frac{\partial}{\partial t_1}-\epsilon_1\right)\mathscr{G}(11') = \Delta(1-1')+\frac{\mathrm{i}\kappa}{2\Omega\hbar}\sum_{2\bar{2}}(V(12\bar{1}\bar{2})+\kappa V(12\bar{2}\bar{1}))v\mathscr{G}^{(2)}(\bar{1}\bar{2}21'),$$

$$t_1 = t_2 = \bar{t}_2 = \bar{t}_1 \tag{29}$$

$$\mathscr{G}^{(2)}_{a_1a_2a_3a_4}(1234) := G^{(2)}(1234)\sigma_{a_3}\sigma_{a_4}, \qquad t_i \in C_{a_i}. \tag{30}$$

When a perturbation expansion is made of the two-particle Green function the second term on the right-hand side is generated by terms represented by the diagram of figure 4(*a*). Therefore

$$\left(\mathrm{i}\frac{\partial}{\partial t_1}-\epsilon_1\right)\mathscr{G}(11') = \mathscr{C}(11')+\int_{t_0}^{t_p}\mathrm{d}t_2\,\mathrm{d}t_3\sum_{23}\mathscr{C}(12)\mathscr{M}(23)\mathscr{G}(31')$$

$$\left(-\mathrm{i}\frac{\partial}{\partial t_1'}-\epsilon_1'\right)\mathscr{G}(11') = \mathscr{E}(11')+\int_{t_0}^{t_p}\mathrm{d}t_2\,\mathrm{d}t_3\sum_{23}\mathscr{G}(12)\mathscr{M}(23)\mathscr{E}(37'). \tag{31}$$

The derivation of the second of these equations is similar to that of the first. These are the generalized Kadanoff and Baym equations. The perturbation expansion of M can be divided into two parts: the sum M^c of terms which contain clusters; and the sum

M^{u} of terms which do not. Then using the $\Delta(1-1')$ contained in $\mathscr{C}$ and $\mathscr{E}$

$$\left(\mathrm{i}\frac{\partial}{\partial t_1}-\epsilon_1\right)\mathscr{G}(11')=\Delta(1-1')+\int_{t_0}^{t_{\mathrm{P}}}\mathrm{d}t_2\sum_2\mathscr{M}^{\mathrm{u}}(12)\mathscr{G}(21')+\mathscr{I}(11')$$

$$\left(-\mathrm{i}\frac{\partial}{\partial t_1'}-\epsilon_1'\right)\mathscr{G}(11')=\Delta(1-1')+\int_{t_0}^{t_{\mathrm{P}}}\mathrm{d}t_2\sum_2\mathscr{G}(12)\mathscr{M}^{\mathrm{u}}(21')+\mathscr{J}(11'). \tag{32}$$

Initial correlation effects are contained in $\mathscr{I}$ and $\mathscr{J}$ hence on neglect of initial correlations equations of the usual Kadanoff and Baym kind result (I, § 2). $\mathscr{I}$ and $\mathscr{J}$ can easily be expressed in terms of $\mathscr{M}^{\mathrm{c}}$, $\mathscr{M}$, $\mathscr{E}$, $\mathscr{C}$ and $\mathscr{G}$.

4. Conclusions

By generalizing the statistical Wick's theorem to include a cluster decomposition of initial correlations a complete non-equilibrium many-body theory has been derived based on a diagrammatic perturbation method. This diagrammatic perturbation method is a simple extension of the usual one for statistical Green functions. The non-equilibrium statistical Green function and its time derivatives can in principle be expressed in terms of a few functions including a self-energy function as in the equilibrium case. However, three other functions are also needed because of the initial correlations.

Non-equilibrium Green functions have already been used to study a variety of problems, and it is to be expected that the formalism developed in this paper can be used to extend the range greatly.

Appendix 1. Diagrammar

A diagram contributing to the nth order term in the perturbation series for the single particle Green function has:

(*a*) n potential bonds
(*b*) $2n+1$ directed lines such that:

each line begins and ends on a vertex except for one ingoing and one outgoing line; there are two ingoing and two outgoing lines to each potential bond;

(*c*) a single correlation bond may be joined once to any line to link any number of the lines;
(*d*) all lines carry a different time–momentum label at each end.

All topologically different diagrams contribute. The topology includes the effect of line direction but care must be taken in this because of dummy labels. Topology also includes whether a line is joined to the correlation bond, but not the manner in which it is joined. Diagrams having an unlinked part or a CDS give zero contribution.

When constructing diagrams with clusters rule (*c*) is replaced by:

(*c'*) any line may be joined once by one cluster bond to any number of other lines. Subject to this and the availability of lines there may be any number of clusters.

Diagrams with different clusterings have different topology.

Using *time-path functions* the corresponding expression in the perturbation expansion is obtained by writing

(1*a*) for every potential bond with ingoing labels $r's'$ and outgoing labels rs

$$\int_c \mathrm{d}t_r \sum_{\substack{rs \\ r's'}} \frac{\mathrm{i}}{\Omega\hbar} V(rsr's'), \qquad t_r = t_s = t'_r = t'_s$$

(1*b*) for every line not joined to a correlation or cluster bond and starting with label s and ending with label r $G_0(rs)$;

(1*c*) for the correlation bond if any $(-\mathrm{i}\kappa)^m \gamma^0_m(1 \ldots s \ldots m, m' \ldots s' \ldots 1')$, or for cluster bonds $(-\mathrm{i}\kappa)^m \chi^0_m(1 \ldots s \ldots m, m' \ldots s' \ldots 1')$ where $11'$, ss' and mm' are ending and beginning labels of lines joined to the bond. The precise ordering of the pairs is unimportant.

(1*d*) An overall factor κ^L where L is the number of closed particle loops.

Using *real-time matrix functions* the expression is obtained by writing

(2*a*) for the potential bond

$$\int_{t_0}^{t_\mathrm{P}} \mathrm{d}t_r \sum_{\substack{rs \\ r's'}} \sum_{\substack{a_r a_s \\ a'_r a'_s}} \left(\frac{\mathrm{i}}{\Omega\hbar}\right) V(rsr's') v_{a_r a_s a'_r a'_s}, \qquad t_r = t_s = t'_r = t'_s$$

a_r etc $= 1$ or 2, $v_{1111} = -v_{2222} = 1$ other elements zero

(2*b*) for the line $\mathscr{G}^0_{a_r a_s}(rs)$;

(2*c*) for a line running from a correlation or cluster bond to label r $\exp[-\mathrm{i}\epsilon_r(t_r - t_0)]\mu_{a_r}$

for a line running to a correlation or cluster bond from label r' $\exp[\mathrm{i}\epsilon'_r(t'_r - t_0)]\bar{\mu}_{a'_r}$

for the bond $(-\mathrm{i}\kappa)^m \gamma_m(\boldsymbol{p}_1 \ldots \boldsymbol{p}_r \ldots \boldsymbol{p}_m, \boldsymbol{p}'_m \ldots \boldsymbol{p}'_r \ldots \boldsymbol{p}'_1 t_0)$ or $(-\mathrm{i}\kappa)^m \chi_m$;

(2*d*) as (1*d*).

It is also possible to use *time-ordered matrix functions*. Diagrams are given an explicit time direction; a convenient choice has physical time running from right to left as in the Prigogine (1962) and Fujita (1966) diagrams. Potential bonds are drawn so that their ends have the same time (vertically). The correlation and cluster bonds are drawn at the earliest time (extreme right). (In practice this is not entirely essential as long as the bond is understood to be in this place.) Diagrams are now different if the time ordering of the potential vertices is different. The interpretation is now

(3*a*) as (2*a*) but the time integral runs from t_0 to the time associated with the next later vertex;

(3*b*) as (2*b*) but a line running with time is interpreted as $\mathscr{G}^+$ and against time as $\mathscr{G}^-$ (see I equations (11))

(3*c*, *d*) as (2*c*, *d*).

The matrix rules simplify when there are parallel elements (I appendix A).

Appendix 2. Dentate structure theorems

The graph of figure 5 has a part containing a potential bond not joined to the rest of the diagram except by lines first joined to the correlation bond. Such a graph has a correla-

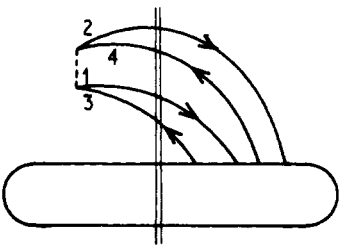

Figure 5.

tion dentate structure (CDS) and contributes nothing to the perturbation series. From the rules (A.2) the matrix parts of the contributions from this diagram are

$$\sum_{a_1a_2a_3a_4} \bar{\mu}_{a_1}\bar{\mu}_{a_2}v_{a_1a_2a_3a_4}\mu_{a_4}\mu_{a_3} = 0. \tag{A.3}$$

'Left dentate structure' (LDS) (Fujita 1966) refers to a part of a time-ordered graph as in figure 6 containing a potential bond at a later time than any bond to which it is immediately connected. Any number of the lines can be connected to a correlation bond. A diagram containing an LDS contributes nothing.

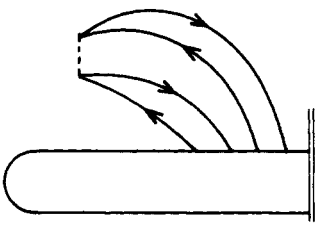

Figure 6.

Again only the matrix parts are required and the possible contributions are shown in expressions (A.4) with a summation over the index $e = 1, 2$. The μ and σ can be combined to give the first simplification. The elements of $\mathcal{G}^+_{e1}$ and $\mathcal{G}^+_{e2}$ are equal (I, equations (11)) for any e and $\mathcal{G}^+$ can be ignored. The elements of $\mathcal{G}^-_{1e}$ and of $\mathcal{G}^-_{2e}$ change sign only under e. The sign of the $e = 2$ contribution relative to the $e = 1$ contribution is given in the final column; in every case it is negative. Summing over e gives zero contribution.

$$\begin{aligned}
&\mathcal{G}^-_{ae}\mathcal{G}^-_{be}\sigma_e\mathcal{G}^+_{ec}\mathcal{G}^+_{ed} \to \mathcal{G}^-\mathcal{G}^-\sigma \to (-)(-)(-)\\
&\mathcal{G}^-_{ae}\bar{\mu}_e\sigma_e\mathcal{G}^+_{ec}\mathcal{G}^+_{ed} \to \mathcal{G}^- \to (-)\\
&\bar{\mu}_e\bar{\mu}_e\sigma_e\mathcal{G}^+_{ec}\mathcal{G}^+_{ed} \to \sigma \to (-)\\
&\mathcal{G}^-_{ae}\mathcal{G}^-_{be}\sigma_e\mu_e\mathcal{G}^+_{ed} \to \mathcal{G}^-\mathcal{G}^-\sigma \to (-)(-)(-)\\
&\mathcal{G}^-_{ae}\mathcal{G}^-_{be}\sigma_e\mu_e\mu_e \to \mathcal{G}^-\mathcal{G}^-\sigma \to (-)(-)(-)\\
&\mathcal{G}^-_{ae}\bar{\mu}_e\sigma_e\mu_e\mathcal{G}^+_{ed} \to \mathcal{G}^- \to (-)\\
&\bar{\mu}_e\bar{\mu}_e\sigma_e\mu_e\mathcal{G}^+_{ed} \to \sigma \to (-)\\
&\mathcal{G}^-_{ae}\bar{\mu}_e\sigma_e\mu_e\mu_e \to \mathcal{G}^- \to (-).
\end{aligned} \tag{A.4}$$

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