IC/83/172

INTERNATIONAL CENTRE FOR
THEORETICAL PHYSICS

PROJECTED INTERACTION PICTURE OF FIELD OPERATORS AND MEMORY SUPEROPERATORS. A MASTER EQUATION FOR THE SINGLE-PARTICLE GREEN'S FUNCTION IN A LIOUVILLE SPACE

Horacio Grinberg

INTERNATIONAL
ATOMIC ENERGY
AGENCY

UNITED NATIONS
EDUCATIONAL,
SCIENTIFIC
AND CULTURAL
ORGANIZATION

1983 MIRAMARE-TRIESTE

International Atomic Energy Agency
and
United Nations Educational Scientific and Cultural Organization

INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS

PROJECTED INTERACTION PICTURE OF FIELD OPERATORS AND MEMORY SUPEROPERATORS. A MASTER EQUATION FOR THE SINGLE-PARTICLE GREEN'S FUNCTION IN A LIOUVILLE SPACE *

Horacio Grinberg **
International Centre for Theoretical Physics, Trieste, Italy.

ABSTRACT

The projection operator method of Zwanzig and Feshbach is used to construct the time dependent field operators in the interaction picture. The formula developed to describe the time dependence involves time-ordered cosine and sine projected evolution (memory) superoperators, from which a master equation for the interaction-picture single-particle Green's function in a Liouville space is derived.

MIRAMARE - TRIESTE
November 1983

* To be submitted for publication.

** MCIC, Consejo Nacional de Investigaciones Cientificas y Tecnicas (CONICET), Argentina.
Permanent address: Laboratorio de Fisica Teorica, Departamento de Fisica, Facultad de Ciencias Exactas, Universidad Nacional de La Plata, C.C. No. 67 (1900) La Plata, Argentina.

I INTRODUCTION

A fundamental challenge pervading theoretical physics is the problem of understanding the properties of systems possessing large or infinite numbers of degrees of freedom in terms of the underlying interactions between constituents. In particular, in recent years much progress has been made in our understanding the role of many-electron effects in non-linear optical phenomena such as two-photon absorption, Raman and fluorescence spectra, multiphoton absorption, and ionization of atoms and molecules.[1] Indeed, the considerable interest addressed to understand the influence of such effects in the formation of electron[2-8] and X-ray emission[9-12] molecular (and, naturally, atomic) spectra is due, to a considerable extent, to the introduction of various many-particle theories to molecular physics.

The present report constitutes a preliminary study aimed to investigate some of the many-electron effects of such events (in molecular systems with completely closed orbitals) by using the Green's function formalism.[2,13,14]

As it is well known, the equation of motion of the double-time Green's functions leads to an infinite set of equations which couple the original Green's functions to the higher-order ones. Approximate solutions are obtained by the decoupling of the higher-order Green's functions, at a certain stage, to set up a closed system of equations for the original Green's functions.

It has also been realized that it is possible to develop a systematic approach called the self-consistent many-body theory to the double-time Green's function with an exact Dyson-type equation.[15,16] The idea to derive a Dyson equation is a straightforward extension of the Zwanzig-Mori projection operator technique.[17,18] In this work this concept is taken up in order to derive a master equation (in interaction-picture) for the single-particle Green's function. Specifically, it consists of a direct application of the Zwanzig[19]-Feshbach[20] projection operator scheme to the time dependence of the field operators (expanded in an arbitrary complete set of one-particle wave functions).

In Sec.II, some simple considerations on the evolution superoperator associated with the interaction-picture Hamiltonian operator of a many-fermion system are made. In Sec.III, formally exact solutions for the projected parts of the time dependent field operators are given. These are generalizations of Turner and Dahler's[21] earlier studies for time dependent wave functions which incorporate arbitrary initial conditions. The analysis of Sec.IV shows that this transcription reveals a much simpler interpretation of the (memory) superoperators, namely as the self-adjoint (and anti-self-adjoint) parts of a Lie group element generated by the coupling between the two projected subspaces (in interaction representation). As a part of a Lie group element, the memory superoperator does not preserve norm, which reflects the leakage of probability density from one subspace to the other. However, an appropriate sum of the self-adjoint and anti-self-adjoint parts does form a group element so that the norm of the total field operator is conserved. This property is used to derive a master equation (in a Liouville space) for the interaction-picture single-particle Green's function in terms of the projection representation of the interaction-picture motion group element.

II TIME DEPENDENCE OF THE FIELD OPERATORS AND MEMORY SUPEROPERATORS

H, the second-quantized Hamiltonian of an interacting many-fermion system, can be decomposed into the sum of two parts

$$H_0 = \int d\xi_1 \int d\xi_1' \, \psi^+(\xi_1,t)\, \mathcal{H}_0(\xi_1|\xi_1')\, \psi(\xi_1',t) \tag{1a}$$

and

$$H' = \frac{1}{2}\int d\xi_1 \int d\xi_2 \int d\xi_1' \int d\xi_2' \, \psi^+(\xi_1,t)\,\psi^+(\xi_2,t) \times \mathcal{H}'(\xi_1\xi_2|\xi_1'\xi_2')\,\psi(\xi_2',t)\,\psi(\xi_1',t) \tag{1b}$$

where terms involving interaction of more than two bodies have been neglected. $\mathcal{H}_0(\xi_1|\xi_1')$ and $\mathcal{H}'(\xi_1\xi_2|\xi_1'\xi_2')$ are the kernels of the one- and two-particle Schrodinger operators H_0 and H' respectively and $\psi^+(\xi,t)$, $\psi(\xi,t)$ are the time-dependent field operators in the Heisenberg picture ($\hbar$ = 1 is used throughout this paper)

$$\psi^+(\xi,t) = \exp(iHt)\,\psi^+(\xi)\,\exp(-iHt) \tag{2a}$$

$$\psi(\xi,t) = \exp(iHt)\,\psi(\xi)\,\exp(-iHt) \tag{2b}$$

where $\psi^+(\xi)$ and $\psi(\xi)$ are the field operators at $t = 0$,

$$\psi^+(\xi) \equiv \psi^+(\xi,0) \tag{3a}$$

$$\psi(\xi) \equiv \psi(\xi,0) \tag{3b}$$

and ξ denotes the full set of coordinates of a particle (i.e., the position vector q and the z component of spin, ζ). These operators can be generated by an arbitrary single-particle wave functions system $\{\phi_m(\xi)\}$

$$\psi^+(\xi,t) = \sum_{m=0}^{\infty} a_m^+(t)\,\phi_m^*(\xi) \tag{4a}$$

$$\psi(\xi,t) = \sum_{m=0}^{\infty} a_m(t)\,\phi_m(\xi) \tag{4b}$$

where $a_n^+(t)$ and $a_n(t)$, the time dependent creation and annihilation fermionic operators respectively, are the generators of a Grassman algebra. Consequently, the field operators (2a,2b) satisfy the canonical anticommutation relations

$$[\psi(\xi,t),\psi(\xi',t)]_+ = [\psi^+(\xi,t),\psi^+(\xi',t)]_+$$

$$= [\psi(\xi,t),\psi^+(\xi',t)]_+ - \delta(\xi-\xi') = 0 \qquad (5)$$

where $\delta(\xi-\xi')$ is the generalized Dirac-Kronecker symbol

$$\delta(\xi-\xi') = \delta(q-q')\,\delta_{\zeta\zeta'} \qquad (6)$$

Associated with these operators are the corresponding commutation superoperators

$$\mathcal{O}_o \equiv [H_o,\ ]_- \qquad (7a)$$

$$\mathcal{O}' \equiv [H',\ ]_- \qquad (7b)$$

whose sum

$$\mathcal{O} = (\mathcal{O}_o + \mathcal{O}') \equiv [H,\ ]_- \qquad (8)$$

is the generator of motion for the field operators $\psi^+(\xi,t)$, $\psi(\xi,t)$. As seen, $\mathcal{O}_o$, $\mathcal{O}'$, and $\mathcal{O}$ are Liouville type superoperators, i.e., (linear hermitian) operators that work in the Hilbert space of operators rather than the space of states. Consequently (with similar expressions, from now on, involving $\psi^+(\xi,t)$), $\psi(\xi,t)$ evolves according to the Heisenberg equation of motion

$$i\frac{\partial}{\partial t}\psi(\xi,t) = -\mathcal{O}\psi(\xi,t)$$

$$= \int d\xi_1'\,\mathcal{H}_o(\xi|\xi_1')\,\psi(\xi_1')$$

$$+\int d\xi_1\int d\xi_2\int d\xi_1'\,\psi^+(\xi_1,t)\,\mathcal{H}'(\xi\xi_1|\xi_1'\xi_2)\,\psi(\xi_2,t)\,\psi(\xi_1',t) \qquad (9)$$

Using Eq.(9) and its adjoint, the time derivative of an operator containing products of n creation and n annihilation operators will yield an expression involving at most products of n+1 creation and annihilation operators, so that the evolution of expectation values of n-body operators will necessarily be coupled with expectation values of n+1 particle operators.

The formal solution of Eq.(9)

$$\psi(\xi,t) = \exp\{i\mathcal{O}(t-t')\}\,\psi(\xi,t') \qquad (10)$$

gives the Schrodinger picture description of the time evolution of the field operator $\psi(\xi,t)$. Although the specific situation envisioned here is the physical event representing any of the above mentioned optical phenomena, the formal results obtained in this section will be applicable to any system with a Liouville superoperator analogous to $\mathcal{O} = \mathcal{O}_o + \mathcal{O}'$ of (9).

It is convenient to replace $\psi(\xi,t)$ with the interaction picture field operator

$$\psi_I(\xi,t) = \exp(-i\mathcal{O}_o t)\,\psi(\xi,t) \qquad (11)$$

The equation of motion of this operator is

$$i\frac{\partial}{\partial t}\psi_I(\xi,t) = -\mathcal{U}(t)\,\psi_I(\xi,t) \tag{12}$$

where $\mathcal{U}(t) = [U(t), \,]_-$ denotes the evolution superoperator associated with the interaction-picture Hamiltonian operator

$$U(t) = \exp(-i\mathcal{L}_0 t)\,H' \tag{13}$$

The superoperator $\mathcal{U}(t)$ is the generator of the motion group $\mathcal{G}$ whose elements

$$\mathcal{G}(t,t') = \mathcal{T}\exp\left\{ i\int_{t'}^{t} ds\,\mathcal{U}(s)\right\} \tag{14}$$

(defined in terms of the Dyson[22] time-ordering or chronological superoperator $\mathcal{T}$) exhibit the group properties

$$\mathcal{G}(t,t')^{+} = \mathcal{G}(t',t)$$

$$\mathcal{G}(t,t')\,\mathcal{G}(t',s) = \mathcal{G}(t,s) \tag{15}$$

$$\mathcal{G}(t,t) = 1$$

and propagate the field operator $\psi(\xi,t)$ according to the prescription

$$\psi_I(\xi,t) = \mathcal{G}(t,t')\,\psi_I(\xi,t') \tag{16}$$

III PROJECTED INTERACTION PICTURE OF THE FIELD OPERATORS

The decomposition of the density operator into relevant and irrelevant parts accomplished by the Zwanzig[19]-Feshbach[20] projection operator technique will be applied to the interaction-picture field operator $\psi_I(\xi,t)$. The expectation at t can be calculated in two ways: by following the evolution of either the ensemble density or the dynamical variable. It is a matter of convenience which is preferred. Therefore, earlier formulation of projected evolution superoperators as applied to inelastic scattering[23] will be followed here to investigate the connection of the (projected) interaction-picture field operators with evolution (memory) superoperators. Thus, the results of successively operating on Eq.(12) with the projection superoperators $\mathcal{P}$ and $\mathcal{Q} \equiv 1-\mathcal{P}$ are the coupled differential equations

$$\frac{\partial}{\partial t}\psi_{\mathcal{P}}(\xi,t) - i\mathcal{U}_{\mathcal{P}\mathcal{P}}(t)\,\psi_{\mathcal{P}}(\xi,t) = i\mathcal{U}_{\mathcal{P}\mathcal{Q}}(t)\,\psi_{\mathcal{Q}}(\xi,t) \tag{17}$$

and

$$\frac{\partial}{\partial t}\psi_{\mathcal{Q}}(\xi,t) - i\mathcal{U}_{\mathcal{Q}\mathcal{Q}}\,\psi_{\mathcal{Q}}(\xi,t) = i\mathcal{U}_{\mathcal{Q}\mathcal{P}}(t)\,\psi_{\mathcal{P}}(\xi,t) \tag{18}$$

for the two orthogonal complements of the field operator, $\psi_{\mathcal{P}}(\xi,t) \equiv \mathcal{P}\psi_I(\xi,t)$ and $\psi_{\mathcal{Q}}(\xi,t) \equiv \mathcal{Q}\psi_I(\xi,t) \equiv (1-\mathcal{P})\,\psi_I(\xi,t)$ respectively. The superoperators $\mathcal{U}_{\mathcal{Q}\mathcal{J}}(t)$ appearing in Eqs.(17) and (18) are defined in the manner

$$\mathcal{U}_{\mathcal{R}\mathcal{S}}(t) = \mathcal{R}\,\mathcal{U}(t)\mathcal{S};\quad \mathcal{R},\mathcal{S} = \mathcal{P},\mathcal{Q} \tag{19}$$

Associated with each projection $\mathcal{S}\,(=\mathcal{P},\mathcal{Q})$ is the group of time-dependent superoperators

$$\mathcal{G}_{\mathcal{S}}(t,s) = \mathcal{S}\,\mathcal{T}\exp\left\{i\int_s^t ds_1\,\mathcal{U}_{\mathcal{S}\mathcal{S}}(s_1)\right\}\mathcal{S} \tag{20}$$

generated by the corresponding $\mathcal{S}$-space, interaction-picture Liouville superoperator $\mathcal{U}_{\mathcal{S}\mathcal{S}}(t)$. These groups can be used to convert the differential equations (17) and (18) and their associated initial conditions at time t' into the pair of coupled integral equations

$$\psi_{\mathcal{P}}(\xi,t) = \mathcal{G}_{\mathcal{P}}(t,t')\psi_{\mathcal{P}}(\xi,t') + i\int_{t'}^{t} ds\,\mathcal{G}_{\mathcal{P}}(t,s)\,\mathcal{U}_{\mathcal{P}\mathcal{Q}}(s)\,\psi_{\mathcal{Q}}(\xi,s) \tag{21}$$

and

$$\psi_{\mathcal{Q}}(\xi,t) = \mathcal{G}_{\mathcal{Q}}(t,t')\psi_{\mathcal{Q}}(\xi,t') + i\int_{t'}^{t} ds\,\mathcal{G}_{\mathcal{Q}}(t,s)\,\mathcal{U}_{\mathcal{Q}\mathcal{P}}(s)\,\psi_{\mathcal{P}}(\xi,s) \tag{22}$$

The result of substituting Eq.(22) into Eq.(21) is the linear, inhomogeneous integral equation

$$\begin{aligned}\psi_{\mathcal{P}}(\xi,t) = {} & \mathcal{G}_{\mathcal{P}}(t,t')\psi_{\mathcal{P}}(\xi,t') - \int_{t'}^{t} ds \int_{t'}^{s} ds'\,\mathcal{G}_{\mathcal{P}}(t,s)\,\mathcal{U}_{\mathcal{P}\mathcal{Q}}(s) \\ & \times \mathcal{G}_{\mathcal{Q}}(s,s')\,\mathcal{U}_{\mathcal{Q}\mathcal{P}}(s')\,\psi_{\mathcal{P}}(\xi,s') \\ & + i\int_{t'}^{t} ds\,\mathcal{G}_{\mathcal{P}}(t,s)\,\mathcal{U}_{\mathcal{P}\mathcal{Q}}(s)\,\mathcal{G}_{\mathcal{Q}}(s,t')\,\psi_{\mathcal{Q}}(\xi,t')\end{aligned} \tag{23}$$

for $\psi_{\mathcal{P}}(\xi,t)$. This particular form of Zwanzig's generalized master equation, involving time dependent Hamiltonians and Liouville superoperators, is the consequence of applying projection superoperators to the interaction-picture Heisenberg equation of motion

Because $\psi(\xi,t)$ is a linear functional of $\psi_{\mathcal{P}}(\xi,t')$ and $\psi_{\mathcal{Q}}(\xi,t')$, the solution of Eq.(23) can be expressed in the form

$$\psi_{\mathcal{P}}(\xi,t) = \mathcal{G}_{\mathcal{P}}(t,t')\left[\mathcal{M}_{\mathcal{P}\mathcal{Q}\mathcal{P}}(t,t')\psi_{\mathcal{P}}(\xi,t') + \mathcal{N}_{\mathcal{P}\mathcal{Q}}(t,t')\psi_{\mathcal{Q}}(\xi,t')\right] \tag{24}$$

By substituting this expression for $\psi_{\mathcal{P}}(\xi,t)$ and $\psi_{\mathcal{Q}}(\xi,s)$ into Eq.(23) and then invoking the independence of $\psi_{\mathcal{P}}(\xi,t')$ and $\psi_{\mathcal{Q}}(\xi,t')$ it can be verified that the memory superoperator $\mathcal{M}_{\mathcal{P}\mathcal{Q}\mathcal{P}}(t,t')$ must satisfy the Volterra integral equation (here written for an arbitrary pair of complementary projectors $\mathcal{R}$ and $\mathcal{S}$)

$$\mathcal{M}_{\mathcal{S}\mathcal{R}\mathcal{S}}(t,t') = \mathcal{S} - \int_{t'}^{t} ds\,\mathcal{W}_{\mathcal{S}\mathcal{R}\mathcal{S}}(t,s;t')\,\mathcal{M}_{\mathcal{S}\mathcal{R}\mathcal{S}}(s,t') \tag{25}$$

whose kernels

$$\mathcal{W}_{\mathcal{S}\mathcal{R}\mathcal{S}}(t,s;t') \equiv \left\{\int_s^t ds'\,\mathcal{B}_{\mathcal{S}\mathcal{R}}(t',s')\right\}\mathcal{B}_{\mathcal{R}\mathcal{S}}(t',s) \tag{26}$$

involve superoperators

$$\mathcal{B}_{\mathcal{S}\mathcal{R}}(t,s) \equiv -\,\mathcal{G}_{\mathcal{S}}(t,s)\,\mathcal{U}_{\mathcal{S}\mathcal{R}}(s)\,\mathcal{G}_{\mathcal{R}}(s,t) \tag{27}$$

which couple the $\mathcal{R}$- and $\mathcal{S}$-subspaces at the common instant of time t. This coupling proceeds by propagation through $\mathcal{R}$-space backward in time from t to s, a subsequent direct coupling between the two subspaces mediated by $\mathcal{U}_{\mathcal{S}\mathcal{R}}(s)$, and a final forward propagation through $\mathcal{S}$-space from s to t. The kernel $\mathcal{W}_{\mathcal{S}\mathcal{R}\mathcal{S}}(t,s;t')$ defined by Eq.(26) couples the $\mathcal{S}$- and $\mathcal{R}$-spaces at time t' through motions forward to s and back again to t'. The integral of $\mathcal{B}_{\mathcal{S}\mathcal{R}}(t',s')$ from s'=s to s'=t then recouples to $\mathcal{S}$-space the dynamic information which has been accumulated in $\mathcal{R}$-space during this interval.

The same procedure which has just been used to generate the integral equation (25) for $\mathcal{M}_{\mathcal{S}\mathcal{R}\mathcal{S}}$ leads to the formula

$$\mathcal{N}_{\mathcal{P}\mathcal{Q}}(t,t') = i\int_{t'}^{t} ds\, \mathcal{B}_{\mathcal{P}\mathcal{Q}}(t',s)\,\mathcal{M}_{\mathcal{Q}\mathcal{Q}\mathcal{P}}(s,t') \tag{28}$$

for the coefficient superoperator $\mathcal{N}_{\mathcal{P}\mathcal{Q}}(t,t')$ of $\psi_{\mathcal{Q}}(\xi,t')$ appearing in Eq.(24). It then follows that $\psi_{\mathcal{P}}(\xi,t')$ and $\psi_{\mathcal{Q}}(\xi,t')$ determine $\psi_{\mathcal{P}}(\xi,t)$ and, by analogy $\psi_{\mathcal{Q}}(\xi,t)$, according to the formulas

$$\psi_{\mathcal{P}}(\xi,t) = \mathcal{G}_{\mathcal{P}}(t,t')\,\mathcal{M}_{\mathcal{P}\mathcal{Q}\mathcal{P}}(t,t')\,\psi_{\mathcal{P}}(\xi,t') + i\,\mathcal{G}_{\mathcal{P}}(t,t')\int_{t'}^{t} ds\, \mathcal{B}_{\mathcal{P}\mathcal{Q}}(t',s)\,\mathcal{M}_{\mathcal{Q}\mathcal{Q}\mathcal{P}}(s,t')\,\psi_{\mathcal{Q}}(\xi,t') \tag{29}$$

and

$$\psi_{\mathcal{Q}}(\xi,t) = \mathcal{G}_{\mathcal{Q}}(t,t')\,\mathcal{M}_{\mathcal{Q}\mathcal{P}\mathcal{Q}}(t,t')\,\psi_{\mathcal{Q}}(\xi,t') + i\,\mathcal{G}_{\mathcal{Q}}(t,t')\int_{t'}^{t} ds\, \mathcal{B}_{\mathcal{Q}\mathcal{P}}(t',s)\,\mathcal{M}_{\mathcal{P}\mathcal{Q}\mathcal{P}}(s,t')\,\psi_{\mathcal{P}}(\xi,t') \tag{30}$$

respectively.

The integral equation (25) is equivalent to the integrodifferential equation,

$$\frac{\partial}{\partial t}\mathcal{M}_{\mathcal{S}\mathcal{R}\mathcal{S}}(t,t') = -\mathcal{B}_{\mathcal{S}\mathcal{R}}(t',t)\int_{t'}^{t} ds'\, \mathcal{B}_{\mathcal{R}\mathcal{S}}(t',s')\,\mathcal{M}_{\mathcal{S}\mathcal{R}\mathcal{S}}(s',t') \tag{31}$$

accompanied by the initial condition

$$\mathcal{M}_{\mathcal{S}\mathcal{R}\mathcal{S}}(t',t') = \mathcal{S} \tag{32}$$

These equations for the memory superoperators can be solved formally by iteration. Thus, it is an immediate consequence of Eq.(25) that

$$\begin{aligned}\mathcal{M}_{\mathcal{S}\mathcal{R}\mathcal{S}}(t,t') &= \mathcal{S} + \sum_{n\geq 1}(-)^n \int_{t'}^{t} ds_1 \int_{t'}^{s_1} ds_2 \cdots \int_{t'}^{s_n} ds_n\, \mathcal{W}_{\mathcal{S}\mathcal{R}\mathcal{S}}(t,s_1;t') \\ &\quad \times \mathcal{W}_{\mathcal{S}\mathcal{R}\mathcal{S}}(s_1,s_2;t')\cdots \mathcal{W}_{\mathcal{S}\mathcal{R}\mathcal{S}}(s_{n-1},s_n;t') \\ &\equiv \mathcal{S}\,\mathcal{T}'\exp\left\{-\int_{t'}^{t} ds\, \mathcal{W}_{\mathcal{S}\mathcal{R}\mathcal{S}}(t,s;t')\right\}\mathcal{S}\end{aligned} \tag{33}$$

with

$$\int_{t'}^{t} ds\, \mathcal{W}_{\mathcal{S}\mathcal{R}\mathcal{S}}(t,s;t') = \int_{t'}^{t} ds' \int_{t'}^{s'} ds\, \mathcal{B}_{\mathcal{S}\mathcal{R}}(t',s')\,\mathcal{B}_{\mathcal{R}\mathcal{S}}(t',s) \tag{34}$$

and where $\mathcal{T}'$ denotes a Dyson-like superoperator which orders both the limits of integration and the pairs of arguments of the integrand factors $\mathcal{W}_{\mathcal{S}\mathcal{R}\mathcal{S}}$.

For the evaluation of the memory superoperators $\mathcal{M}_{\mathcal{S}\mathcal{R}\mathcal{S}}$, the superoperators $\mathcal{B}_{\mathcal{S}\mathcal{R}}$ and $\mathcal{B}_{\mathcal{R}\mathcal{S}}$ act in analogy to raising and lowering operators, that is, the superoperator $\mathcal{B}_{\mathcal{S}\mathcal{R}}$ "raises" the system from the $\mathcal{S}$ space to the $\mathcal{R}$ space (at the same time t through an intermediate time s) while $\mathcal{B}_{\mathcal{R}\mathcal{S}}$ "lowers" the system from the $\mathcal{S}$ space to the $\mathcal{R}$ space. Again in analogy to the fact that a raising operator is the adjoint of a lowering operator, so here is $\mathcal{B}_{\mathcal{S}\mathcal{R}}(t,s)$ the superoperator adjoint of $\mathcal{B}_{\mathcal{R}\mathcal{S}}(t,s)$. It is thus profitable to define the self-adjoint superoperator

$$\mathcal{B}(t,s) \equiv \mathcal{B}_{\mathcal{P}\mathcal{Q}}(t,s) + \mathcal{B}_{\mathcal{Q}\mathcal{P}}(t,s) = \mathcal{B}(t,s)^{+} \qquad (35)$$

Then, because the two projection superoperators $\mathcal{S}$ and $\mathcal{R}$ ($\mathcal{P}$ and $\mathcal{Q}$) are orthogonal complements of one another, the first and second terms of the series (33) can be written as

$$\int_{t'}^{t} ds_1\, W_{\mathcal{S}\mathcal{R}\mathcal{S}}(t,s_1;t') = \mathcal{S}\int_{t'}^{t} ds_1 \int_{s_1}^{t} ds_1'\, \mathcal{B}(t',s_1')\,\mathcal{B}(t',s_1)\,\mathcal{S}$$

$$= \mathcal{S}\int_{t'}^{t} ds_1' \int_{t'}^{s_1'} ds_1\, \mathcal{B}(t',s_1')\,\mathcal{B}(t',s_1)\,\mathcal{S} \qquad (36)$$

and

$$\int_{t'}^{t} ds_1 \int_{t'}^{s_1} ds_2\, W_{\mathcal{S}\mathcal{R}\mathcal{S}}(t,s_1;t')\, W_{\mathcal{S}\mathcal{R}\mathcal{S}}(s_1,s_2;t')$$

$$= \mathcal{S}\int_{t'}^{t} ds_1' \int_{t'}^{s_1'} ds_1 \int_{t'}^{s_1} ds_2' \int_{t'}^{s_2'} ds_2\, \mathcal{B}(t',s_1')\,\mathcal{B}(t',s_1)\,\mathcal{B}(t',s_2')\,\mathcal{B}(t',s_2)\,\mathcal{S} \qquad (37)$$

respectively. These and the higher order terms as well, can readily be identified as successive, even-powered terms in an ordinary, time-ordered exponential superoperator. Consequently, it is apparent that

$$\mathcal{M}_{\mathcal{S}\mathcal{R}\mathcal{S}}(t,t') = \mathcal{S}\mathcal{M}^{C}(t,t')\,\mathcal{S} \qquad (38)$$

and

$$\int_{t'}^{t} ds\, \mathcal{B}_{\mathcal{R}\mathcal{S}}(t',s)\,\mathcal{M}_{\mathcal{S}\mathcal{R}\mathcal{S}}(s,t') = \mathcal{R}\mathcal{M}^{S}(t,t')\,\mathcal{S} \qquad (39)$$

wherein

$$\mathcal{M}^{C}(t,t') = \sum_{n\geq 0}(-)^{n}\int_{t'}^{t} ds_1 \int_{t'}^{s_1} ds_2 \cdots\cdots \int_{t'}^{s_{2n-1}} ds_{2n}\, \mathcal{B}(t',s_1)\,\mathcal{B}(t',s_2)$$

$$\cdots\cdots \mathcal{B}(t',s_{2n}) = \mathcal{T}\cos\left\{\int_{t'}^{t} ds\, \mathcal{B}(t',s)\right\} \qquad (40)$$

and

$$\mathcal{M}^{S}(t,t') = \sum_{n\geq 0}(-)^{n}\int_{t'}^{t} ds_1 \int_{t'}^{s_1} ds_2 \cdots\cdots \int_{t'}^{s_{2n}} ds_{2n+1}\, \mathcal{B}(t',s_1)\,\mathcal{B}(t',s_2)$$

$$\cdots\cdots \mathcal{B}(t',s_{2n+1}) = \mathcal{T}\sin\left\{\int_{t'}^{t} ds\, \mathcal{B}(t',s)\right\} \qquad (41)$$

From Eqs.(38) and (39) it then follows that the formulas (29) and (30) can be written as

$$\Psi_{\mathcal{P}}(\xi,t) = \mathcal{G}_{\mathcal{P}}(t,t')\left[\mathcal{M}^{C}(t,t')\,\Psi_{\mathcal{P}}(\xi,t') + i\,\mathcal{M}^{S}(t,t')\,\Psi_{\mathcal{Q}}(\xi,t')\right]$$

$$= \left[\Psi_{\mathcal{P}}(\xi,t')\,\mathcal{M}^{C}(t,t')^{+} - i\,\Psi_{\mathcal{Q}}(\xi,t')\,\mathcal{M}^{S}(t,t')^{+}\right]\mathcal{G}_{\mathcal{P}}(t,t')^{+} \qquad (42)$$

and

$$\psi_{\mathcal{Q}}(\xi,t) = \mathcal{G}_{\mathcal{Q}}(t,t')[\mathcal{M}^{c}(t,t')\psi_{\mathcal{Q}}(\xi,t') + i\mathcal{M}^{s}(t,t')\psi_{\mathcal{P}}(\xi,t')]$$

$$= [\psi_{\mathcal{Q}}(\xi,t')\mathcal{M}^{c}(t,t')^{+} - i\psi_{\mathcal{P}}(\xi,t')\mathcal{M}^{s}(t,t')^{+}]\mathcal{G}_{\mathcal{Q}}(t,t')^{+} \quad (43)$$

Because $\mathcal{B}(t,s)$ generally will be complex valued, the superoperators $\mathcal{M}^{C}$ and $\mathcal{M}^{S}$ are not necessarily real. The memoryless approximation obtained by setting $\mathcal{B}(t,s)$ equal to zero replaces $\mathcal{M}^{C}$ with 1 and $\mathcal{M}^{S}$ with 0, with the consequence that $\psi_{\mathcal{S}}(\xi,t) \longrightarrow \mathcal{G}_{\mathcal{S}}(t,t')\psi_{\mathcal{S}}(\xi,t')$ for $\mathcal{S} = \mathcal{P}$ and $\mathcal{Q}$. In this approximation there is no coupling between the $\mathcal{P}$- and $\mathcal{Q}$-space motions, regardless of how the two are defined.

IV MASTER EQUATION FOR THE INTERACTION PICTURE SINGLE-PARTICLE GREEN'S FUNCTION

Eqs.(42) and (43) provide formally exact expressions for the $\mathcal{P}$- and $\mathcal{Q}$-space components of the interaction-picture field operators, from which the conventional single-particle Green's function can be constructed

$$G(\xi t,\xi' t') \equiv -i\langle T\{\psi(\xi,t)\psi^{+}(\xi',t')\}\rangle \quad (44)$$

where T is the Wick time-ordering operator and the bracket indicates the ground-state expectation value is to be taken over the full Hamiltonian $H = H_0 + H'$ of Eqs.(1) (though the results are generalizable to ensemble averages). Expanding T in terms of the Heaviside unit-step function, the master equation for the projected single-particle Green's function (diagonal parts) in the two orthogonal complementary spaces $\mathcal{P}$ and $\mathcal{Q} = 1 - \mathcal{P}$ becomes, using Eqs. (42) and (43) together with their Hermitian conjugates $\psi_{\mathcal{P}}^{+}(\xi,t)$ and $\psi_{\mathcal{Q}}^{+}(\xi,t)$,

$$G_{\mathcal{P}\mathcal{P}}(\xi t,\xi' t') = -i\theta(t-t')\langle[\psi_{\mathcal{P}}(\xi)\mathcal{M}^{c}(t,0)^{+} - i\psi_{\mathcal{Q}}(\xi)\mathcal{M}^{s}(t,0)]$$

$$\times\mathcal{G}_{\mathcal{P}}(t,t')^{+}[\mathcal{M}^{c}(t',0)\psi_{\mathcal{P}}^{+}(\xi') + i\mathcal{M}^{s}(t',0)\psi_{\mathcal{Q}}^{+}(\xi')]\rangle$$

$$+ i\theta(t'-t)\langle[\psi_{\mathcal{P}}^{+}(\xi')\mathcal{M}^{c}(t',0)^{+} - i\psi_{\mathcal{Q}}^{+}(\xi')\mathcal{M}^{s}(t',0)^{+}]$$

$$\times\mathcal{G}_{\mathcal{Q}}(t,t')[\mathcal{M}^{c}(t,0)\psi_{\mathcal{P}}(\xi) + i\mathcal{M}^{s}(t,0)\psi_{\mathcal{Q}}(\xi)]\rangle \quad (45)$$

and

$$G_{\mathcal{Q}\mathcal{Q}}(\xi t,\xi' t') = \Pi_{\mathcal{P}\mathcal{Q}}\, G_{\mathcal{P}\mathcal{P}}(\xi t,\xi' t') \quad (46)$$

where $\Pi_{\mathcal{P}\mathcal{Q}}$ means interchanging the indices $\mathcal{P}$ and $\mathcal{Q}$ in Eq.(45).

On the other hand, it can easily be verified, by using $\mathcal{P}\mathcal{Q} \equiv 0$, that

$$G_{\mathcal{P}\mathcal{Q}}(\xi t,\xi' t') = -i\theta(t-t')\langle\psi_{\mathcal{P}}(\xi,t)\psi_{\mathcal{Q}}^{+}(\xi',t')\rangle$$

$$+ i\theta(t'-t)\langle\psi_{\mathcal{Q}}^{+}(\xi',t')\psi_{\mathcal{P}}(\xi,t)\rangle = 0 \quad (47)$$

and

$$G_{\mathcal{Q}\mathcal{P}}(\xi t,\xi' t') = 0 \quad (48)$$

For the two orthogonal space components (non-diagonal parts) of the projected single-particle Green's function.

The present analysis has to be pursued a little further in order to get a master equation for the Green's function in a Liouville space. Thus, because $\mathcal{M}^c = \mathcal{P}\mathcal{M}^c\mathcal{P} + \mathcal{Q}\mathcal{M}^c\mathcal{Q}$ and $\mathcal{M}^s = \mathcal{P}\mathcal{M}^s\mathcal{Q} + \mathcal{Q}\mathcal{M}^s\mathcal{P}$, the sum of (42) and (43) can be written as

$$\psi_I(\xi,t) = \psi_{\mathcal{P}}(\xi,t) + \psi_{\mathcal{Q}}(\xi,t) = \mathcal{G}_{\mathcal{D}}(t,t')\,\mathcal{G}_{\mathcal{C}}(t,t')\,\psi_I(\xi,t') \qquad (49)$$

which enables the master equation for the interaction-picture single-particle Green's function to be cast in the form

$$\begin{aligned} G_I(\xi t,\xi' t') &= G_{\mathcal{P}\mathcal{P}}(\xi t,\xi' t') + G_{\mathcal{Q}\mathcal{Q}}(\xi t,\xi' t') \\ &= -i\,\theta(t-t')\langle \psi(\xi)\,\mathcal{G}_{\mathcal{C}}(t,t')^{+}\,\mathcal{G}_{\mathcal{D}}(t,t')^{+}\,\psi^{+}(\xi')\rangle \\ &\quad + i\,\theta(t'-t)\langle \psi^{+}(\xi')\,\mathcal{G}_{\mathcal{C}}(t,t')\,\mathcal{G}_{\mathcal{D}}(t,t')\,\psi(\xi)\rangle \end{aligned} \qquad (50)$$

with

$$\begin{aligned} \mathcal{G}_{\mathcal{D}}(t,t') &\equiv \mathcal{G}_{\mathcal{P}}(t,t') + \mathcal{G}_{\mathcal{Q}}(t,t') \\ &= \mathcal{T}\exp\left\{i\int_{t'}^{t} ds\,\mathcal{U}_{\mathcal{P}\mathcal{P}}(s)\right\} + \mathcal{T}\exp\left\{i\int_{t'}^{t} ds\,\mathcal{U}_{\mathcal{Q}\mathcal{Q}}(s)\right\} \end{aligned} \qquad (51)$$

an element of the motion group descriptive of decoupled ($\mathcal{D}$) $\mathcal{P}$- and $\mathcal{Q}$-space dynamics, whereas

$$\mathcal{G}_{\mathcal{C}}(t,t') \equiv \mathcal{M}^c(t,t') + i\,\mathcal{M}^s(t,t') = \mathcal{T}\exp\left\{i\int_{t'}^{t} ds\,\mathcal{B}(t',s)\right\} \qquad (52)$$

belongs to a group of propagators pertaining only to the motion coupling ($\mathcal{C}$) the two subspaces. The elements of this second group are sums of the $\mathcal{M}^C$ and $\mathcal{M}^S$ superoperators, neither set of which separately forms a group. A comparison of Eqs.(15) and (49) establishes that $\mathcal{G}_{\mathcal{D}}(t,t')\mathcal{G}_{\mathcal{C}}(t,t')$ is the projection representation of the interaction picture group element $\mathcal{G}(t,t')$.

By expanding the Schrodinger operators $\psi(\xi)$, $\psi^{+}(\xi)$ according to Eqs.(4), one gets, from Eq.(50)

$$G_I(\xi t,\xi' t') = \sum_{n,n'=0}^{\infty} G_I(nt,n't')\,\phi_n(\xi)\,\phi^{*}_{n'}(\xi') \qquad (53)$$

where $G_I(nt,n't')$, the transform of $G_I(\xi t,\xi' t')$ with respect to the functions $\phi_n(\xi)$, is given by

$$G_I(nt,n't') = -i\langle T\left\{a_n\,\mathcal{G}_{\mathcal{C}}(t,t')\,\mathcal{G}_{\mathcal{D}}(t,t')\,a^{+}_{n'}\right\}\rangle \qquad (54)$$

where a_n and a^{+}_n are the annihilation and creation fermionic operators at t=0.

This memory superoperator formulation can, of course, be adapted to the Schrodinger picture, in which case $\mathcal{U}(t)$ is replaced wherever it occurs by the full quantum Liouville operator $\mathcal{O}$ and the quantities $\psi_{\mathcal{P}}(\xi,t) \equiv \mathcal{P}\psi_I(\xi,t)$ by the corresponding projections $\tilde{\psi}_{\mathcal{P}} = \mathcal{P}\psi(\xi,t)$ of the Schrodinger picture field operator $\psi(\xi,t)$. It should also be pointed out that a general procedure for determination of Liouvillian Green's functions and their associated proper transition self-energies has recently been developed [24] and applied to the theory of spectral line shape. In this connection, the above description of the Schrodinger picture can be used to demonstrate that the formally exact time dependent solution of the Heisenberg equation (9) is identical to the usual Laplace transform solution,[23] thus leading to a Lehmann-type representation[25] in terms of memory superoperators. Work along these lines is underway and will be given at a later time.

ACKNOWLEDGMENTS

The author would like to thank Professors Abdus Salam and Luciano Bertocchi, the International Atomic Energy Agency and UNESCO for hospitality at the International Centre for Theoretical Physics, Trieste, as well as Professor Erico Tosatti for a critical reading of the manuscript. The stay of the author at the Centre has been made possible through a Federation Agreement between the International Centre for Theoretical Physics and the Subsecretaryat of Science and Technology (SUBCYT), Argentina. The grant of study leave by the CONICET, Argentina, is also gratefully acknowledged.

REFERENCES

1 S. Mukamel, Phys. Rep., 93, 1 (1982).

2 L. S. Cederbaum and W. Domcke, Adv. Chem. Phys., 36, 205 (1977).

3 J. Schirmer, J. Cederbaum L. S. Domcke, and W. von Niessen, Chem. Phys., 26, 149 (1977).

4 P. S. Bagus and E. K. Vinnikka, Phys. Rev., A15, 1486 (1977).

5 M. Ohno and G. Wendin, J. Phys., B12, 1305 (1979).

6 G. Howat, T. Aberg, and O. Goscinski, J. Phys., B11, 1575 (1978).

7 G. Wending, Daresbury Laboratory Report, DL/SC1/R11 (1978).

8 A. V. Kondratenko, Chem. Phys. Lett., 86, 156 (1982).

9 T. Aberg, Phys. Rev., 4, 1735 (1971).

10 A. V. Kondratenko, L. N. Mazalov, and K. M. Neyman, Opt. Spektrosk., 48, 1072 (1980).

11 L. A. Demekhina and V. V. Timoshevskaja, Opt. Spektrosk., 51, 685 (1981).

12 A. V. Kondratenko and L. N. Mazalov, Theor. Chim. Acta (Berl.), 62, 537 (1983).

13 A. A. Abrikosov, L. P. Gor'kov, and I. E. Dzyaloshinsky, Quantum Field Theoretical Methods in Statistical Physics (Oxford, Pergamon Press, 1965).

14 A. B. Migdal, Theory of Finite Fermi Systems and Applications to Atomic Nuclei (John Wiley, London, 1967).

15 A. J. Fedro and R. S. Wilson, Phys. Rev., B11, 2148 (1975).

16 R. Kishore, Phys. Rev., B19, 3822 (1979).

17 R. Zwanzig, in Lectures in Theoretical Physics, Boulder 1969, Colorado, Vol.III, W. E. Brittin, B. W. Downs and Downs, Eds. (New York, 1961).

18 H. Mori, Progr. Theor. Phys., 33, 423 (1965).

19 a) R. Zwanzig, J. Chem. Phys., 33, 1338 (1960); b) R. Zwanzig, Physica, 30, 1109 (1964).

20 H. Feshbach, Ann. Phys. N. Y., 19, 287 (1962).

21 R. E. Turner and J. S. Dahler, J. Phys., B13, 161 (1980).

22 F. J. Dyson, Phys. Rev., 75, 486 (1949).

23 R. E. Turner, J. S. Dahler, and R. F. Snidder, Can. J. Phys., 60, 1371 (1982).

24 a) M. D. Girardeau, Phys. Rev., A28, 1056 (1983); b) M. D. Girardeau and C. F. Hart, ibid., A28, 1072 (1983).

25 H. Lehmann, Nuovo Cimento, 11, 342 (1954). See also A. L. Fetter and J. D. Walecka, Quantum Theory of Many-Particle Systems (McGraw-Hill, New York, 1971).