QUANTUM TRANSPORT USING LIOUVILLEAN QUANTUM-FIELD DYNAMICS AND FUNCTIONAL APPROACH TO SELF-CONSISTENT MANY-BODY AND SCATTERING EFFECTS

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Abstract

Quantum dynamics in Liouville space is used for discussing quantum transport in nanoelectronics. A synergism between the two formalisms treated here, namely, the "super" Green's function technique and the generalized functional approach is expected to pave the way towards more accurate self-consistent numerical calculations of many-body and scattering effects in nanolectronics and optoelectronics.

I. INTRODUCTION

There is a need for a self-consistent treatment of the nonlinear dynamics of interacting quantized fields, e.g., interactions between electrons, ions, and electromagnetic fields. These kinds of problems arise in high frequency and/or high power nanoelectronic and optoelectronic devices. So far, highly nonequilibrium situations are treated by assuming that all the subsystems other than the one of interest are behaving classically and/or in equilibrium condition. In this paper, non-equilibrium quantum transport is formulated in terms of the Liouville space (L-space) dynamics thus treating all the fields quantum mechanically on equal footing. This description also unifies classical and quantum statistical dynamics within the L-space dynamical framework [1].

The L-space formulation is equivalent to the nonequilibrium Green's function technique [2] originated by Schwinger, and Keldysh. However the major advantage of the L-space formalism is that it allows for a straightforward application of quantized field theoretical techniques since only real-time axis is used. This is in contrast to the double-time contour of the corresponding Hilbert space (H-space) formalism which leads to awkward calculational procedure for obtaining the self-energies of interest. Another major advantage of the L-space formalism is that it provides a common starting point for a many-body functional technique, which is rooted in the powerful density functional method for calculating many-body effects [3], and the real-time Green's function technique based on the Φ-derivable method [4] for the self-energies. The synergism of these two independent techniques is expected to yield a more powerful many-body functional technique for numerically simulating *bonafide* scattering effects.

For simplicity of presentation in what follows, we focus our discussion on the electron system. The corresponding discussion of the ions and electromagnetic fields involve a parallel treatment, which will be discussed elsewhere.

II. QUANTUM DYNAMICS IN LIOUVILLE SPACE

In Liouville space quantum dynamics, the density-matrix equation formulation of the quantum statistical dynamics in H-space becomes a dynamical equation in L-space defined as follows:

$$i\hbar\frac{\partial}{\partial t}|\rho\rangle\rangle = \mathscr{L}|\rho\rangle\rangle, \tag{1}$$

where ρ is the density matrix of the system in H-space, and $|\rho\rangle\rangle$ is its corresponding supervector in L-space. Note that $\mathscr{L}|\rho\rangle\rangle$ corresponds to the commutator $[\mathscr{H},\rho]$ in H-space. Here the Liouvillean $\mathscr{L}=\hat{\mathscr{H}}-\tilde{\mathscr{H}}$, where the "hat" and "tilde" superoperators are defined below. If the set $\{|n\rangle\}$ is an orthonormal basis in H-space in the number representation of the many-body states, then the corresponding set $\{\{||m\rangle\langle n|\rangle\rangle\}\}$ is an orthonormal basis supervectors in L-space. The annihilation and the creation quantum-field operators, $\psi,\psi^\dagger$ in H-space become the "hat"("tilde") annihilation, $\hat{\psi}\,(\tilde{\psi})$ and creation, $\hat{\psi}^\dagger\,(\tilde{\psi}^\dagger)$ operators in L-space. They are defined as follows:

$$\hat{\psi}^\dagger||m\rangle\langle n|\rangle\rangle=|\psi^\dagger|m\rangle\langle n|\rangle\rangle, \tag{2}$$

$$\tilde{\psi}^\dagger||m\rangle\langle n|\rangle\rangle=(-\sigma)^{m-n+1}||m\rangle\langle n|\psi\rangle\rangle, \tag{3}$$

$$\hat{\psi}||m\rangle\langle n|\rangle\rangle=|\psi|m\rangle\langle n|\rangle\rangle, \tag{4}$$

$$\tilde{\psi}||m\rangle\langle n|\rangle\rangle=(-\sigma)^{m-n}||m\rangle\langle n|\psi^\dagger\rangle\rangle, \tag{5}$$

where σ is -1 for bosons and +1 for fermions. Due to the doubling of operators in L-space corresponding to each operator in H-space, it is more convenient to introduce a two-component annihilation and creation operators in L-space. For fermions, we have

$$\Psi=\begin{pmatrix}\hat{\psi}\\ \tilde{\psi}^\dagger\end{pmatrix}\quad and\quad \Psi^\dagger=\begin{pmatrix}\hat{\psi}^\dagger & \tilde{\psi}\end{pmatrix}. \tag{6}$$

We also define a unit supervector as $|1\rangle\rangle=\sum_m|m\rangle\langle m|$, so that the average of an arbitrary operator A can be written as $\langle A\rangle=Tr\,\rho A=\langle\langle 1|\hat{A}|\rho\rangle\rangle$.

III. NON-EQUILIBRIUM GREEN'S FUNCTION IN L- SPACE DYNAMICS

A "super" or non-equilibrium Green's function in L-space is defined as

$$\mathscr{G}=\langle T\Psi_{\overline{H}}(t)\Psi^\dagger_{\overline{H}}(t')\rangle\rangle/i\hbar, \tag{7}$$

where T is the usual time ordering operator. In the above expressions, the superoperators are written in the "super"-Heisenberg representation, e.g.,

$$\Psi_{\overline{H}}(t,t_o)=\mathscr{U}(t_o,t)\,\Psi\,\mathscr{U}(t,t_o), \tag{8}$$

where $\mathscr{U}(t,t_o)=T\exp\left\{-\frac{i}{\hbar}\int_{t_o}^{t}\mathscr{L}\,dt'\right\}$. Thus, in the "super"-interaction representation in L-space, we can also write Eq. (7) as

$$\mathscr{G}=\langle\langle 1|\bar{S}(\infty,t)\Psi_I(t)\bar{S}(t,t')\Psi_I^\dagger(t')\bar{S}(t',-\infty)|\rho_{eq}\rangle\rangle/\langle\langle 1|\bar{S}(\infty,-\infty)|\rho_{eq}\rangle\rangle, \tag{9}$$

where $\bar{S}(t,t_o)$ is the "super"-S-matrix, obtained by substituting $\mathscr{L}$ in $\mathscr{U}(t,t_o)$ by $\mathscr{L}_I^{(1)}=\hat{\mathscr{H}}_I^{(1)}-\tilde{\mathscr{H}}_I^{(1)}$ in the "super"-interaction picture. In Eq. (9), the time axis is from $-\infty$ *to* $+\infty$ and therefore the theory is formally the same as for the "zero-temperature" Green's function. Similar equations for the respective Green's functions can be constructed for the ion and electromagnetic fields. The full dynamics of ion motion including phonons is described by the correlation function of the ion positions.

We will now develop the transport equations in L-space from the above Green's functions. Following the Keldysh approach in H-space, the transport equations for nonequilibrium plasmas and radiation has been given by DuBois [5]. A similar transport equation for a system of ions may be found in Kwok [6], which is based on the Green function associated with ion positions. In a

separate paper [7], we will derive the appropriate transport equations for the coupled system of electrons, ions, and electromagnetic fields.

IV. TRANSPORT EQUATIONS AND SELF-ENERGIES

In terms of the familiar correlation functions, $G^{>}$,and $G^{<}$, the matrix equation for the "super"-Green's function, $\mathscr{G}$, is exactly the same as the following expression

$$\mathscr{G} = \begin{pmatrix} G^{c} & -G^{<} \\ G^{>} & -G^{ac} \end{pmatrix}, \tag{10}$$

where G^{c} and G^{ac}, which can be expressed in terms of $G^{>}$ and $G^{<}$, are the chronological and antichronological Green's functions respectively. Equation (10) is exactly the same as the nonequilibrium matrix Green's function expression obtained by other authors [2], using the time contour formulation of Schwinger and Keldysh. Integro-differential transport equations for the matrix elements of $\mathscr{G}$, can be readily obtained from $\mathscr{G}^{-1}\mathscr{G} = \delta$ and its adjoint. We make use of the relations: $F^{<,>\dagger} = -F^{<,>}$, $F^{c\dagger} = -F^{ac}$, to obtain the transport equations for all the matrix elements of $\mathscr{G}$:

$$\begin{aligned} i\hbar(\partial/\partial t + \partial/\partial t')G^{>,<} = &\left[-\hbar^2\nabla^2/2m + \varphi_{eff} + \mathrm{Re}\,\Sigma^{r}, G^{>,<}\right] \\ &+\left[\Sigma^{>,<}, \mathrm{Re}\,G^{r}\right] + i\left\{A, \Sigma^{>,<}\right\}/2 - i\left\{\Gamma, G^{>,<}\right\}/2, \end{aligned} \tag{11}$$

$$i\hbar(\partial/\partial t + \partial/\partial t')G^{c} = \left[-\hbar^2\nabla^2/2m + \varphi_{eff} + \Sigma^{c}, G^{c}\right] + G^{<}\Sigma^{>} - \Sigma^{<}G^{>}, \tag{12}$$

$$i\hbar(\partial/\partial t + \partial/\partial t')G^{ac} = \left[-\hbar^2\nabla^2/2m + \varphi_{eff} - \Sigma^{ac}, G^{ac}\right] + \Sigma^{>}G^{<} - G^{>}\Sigma^{<}, \tag{13}$$

where G^{r} *and* Σ^{r} represent the retarded Green's function and its associated self-energy, and φ_{eff} is the effective potential. It is clear from the last two equations that the term $G^{<}\Sigma^{>} - \Sigma^{<}G^{>}$ and its counterpart describe effects beyond the finite-lifetime quasi-particle concept, and represent *bonafide* nonequilibrium scattering effects. These are similar to those occurring in the last two terms of Eq. (11) for $G^{>,<}$. The equation for $G^{>,<}$ is exactly identical to the Keldysh results [2], while the equations for G^{c} and G^{ac} also contain collision terms.

The "super" self-energy has formally the same functional form as that of the "zero-temperature" self-energy. In the L-space approach, each of the self-energy matrix elements is calculated using the equation of motion of the "hat" and "tilde" superoperators, which is a straightforward application of quantum field theoretical techniques. Similar transport equations are deduced [7] for the ion and electromagnetic fields from their respective Green functions and self-energies. The self-energies depend on all the field variables exhibiting the mutual interactions among the fields. Thus all the Green's functions become mutually coupled, requiring thereby a self-consistent analysis.

V. FUNCTIONAL TECHNIQUE IN L-SPACE DYNAMICS

The stationary action principle is the foundation of the time-dependent density functional theory of pure-state quantum mechanical systems. The "Schrodinger" Eq. (1), also provides a stationary action principle for nonequilibrium statistical mechanics.

We write the functional of the action in the form

$$W(t,t_o) = \frac{1}{2}\int_{t_o}^{t}\left\langle\left\langle \Phi(t')\middle|\left(i\hbar\frac{\partial}{\partial t} - \mathscr{L}\right)\middle|\rho(t')\right\rangle\right\rangle dt', \tag{14}$$

subject to the thermal equilibrium initial condition for the ρ. Thus by varying the left supervector and setting the result equal to zero, we obtain the superket Eq. (1). The factor 1/2 is chosen to account for the presence of "twins" (doubling) in L-space.

It is shown elsewhere [8], that $W(t,t_o)$ is a functional of averaged fields and they completely characterize the supervector $|\rho\rangle\rangle$. We use the "physical" functional given by $\langle\langle\Phi(t)| = \langle\langle 1|$ in Eq.(14) which is now stationary with respect to the variations of the average currents $J_\mu(\vec{r}t)$, average electromagnetic potentials $A_\mu(\vec{r}t)$, and average ion positions $\vec{R}(l\kappa t)$, where l represents the lattice point and κ labels the ion species, for a system of electrons, ions, and electromagnetic fields. Thus the stationarity of W leads to the equations:

$$\delta W/\delta J_\mu = 0, \quad \delta W/\delta A_\mu = 0, \quad and \quad \delta W/\delta \vec{R} = 0. \tag{15}$$

The first of the equations in Eq.(15) leads to an effective one-particle Schrodinger equation, the second leads to an effective Maxwell's equation, and the third leads to an effective Newton's equation for the ions. In general, these equations involve "effective potentials", equal to the average potentials in addition to terms describing the mutual interactions with other fields.

By re-expressing these equations in terms of the Green function language, we can identify the terms corresponding to self-energies of the respective fields, given by the "super" Green function approach. Thus, we can incorporate the functional form of the appropriate diagrammatic expressions into a self-consistent scheme within the functional approach for calculating many-body effects which now includes the effects of scatterings. These are discussed in more detail by the authors in a separate paper [8].

VI. SUMMARY AND CONCLUDING REMARKS

The functional theory discussed here provides a self-consistent method for incorporating many-body and scattering effects in the self-energy to be used in the transport equations. By inserting the diagrammatic approximation to the self-energy in a self-consistent loop of the coupled equations in functional theory, a more accurate self-consistent self-energy can be generated. This algorithm may be considered as a generalization in device physics of the well-known self-consistent method of solving the Poisson equation along with the quantum transport equation [2]. For numerical simulation, it is desirable to take the Weyl transform [2] of Eqs.(11-13, 15). It is hoped that this work would lead to the numerical implementation of the algorithm proposed here in self-consistent analyses of nanoelectronics and optoelectronics problems.

ACKNOWLEDGMENT: This work is supported in part by the Office of Naval Research.

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