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Exact functional differential variant of the generalized Kadanoff-Baym ansatz

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We derive an exact functional differential relation for the physical Green's function $g_{\gtrless}(1;2)$ in terms of its retarded and advanced counterparts and the equal-time function $g_{\gtrless}(1;\mathbf{x}_2,t_1)$. This exact, formal, functional differential relation is a variant of the generalized Kadanoff-Baym GKB ansatz, and we examine the approximations involved in reducing it to the GKB ansatz.

I. INTRODUCTION: REVIEW OF GAUGE PROPERTIES

The microscopic quantum dynamical formulation of a Boltzmann-type transport equation involves the appearance of the physical Green's function $g_{\gtrless}$ (1;2) in the scattering term (upon an approximate Green's function factorization[1–3]) resulting in a closed integro-differential equation. Kadanoff and Baym[2] (KB) proposed an ansatz which expresses the physical Green's function in terms of a spectral function related to the retarded and advanced Green's functions and the physical Green's function at equal time $g_{\gtrless}(1;\mathbf{x}_2,t_1)$ expressed as a nonequilibrium distribution function. However, this ansatz violates the group property of the time evolution operator for finite external field. Recently, Lipavský, Spička, and Velický[4] proposed a generalized Kadanoff-Baym (GKB) ansatz which maintains a semigroup property of the time evolution operator, in that its validity is limited to zero scattering time. In this paper, we derive an exact functional differential relation for the physical Green's function $g_{\gtrless}(1;2)$ in terms of its retarded and advanced counterparts and the equal time function $g_{\gtrless}(1;\mathbf{x}_2,t_1)$, which constitutes an exact result, albeit formal. This exact functional differential relation is a variant of the GKB ansatz.

In the presence of current producing external electromagnetic fields $\mathbf{A}(1)$ and $\phi(1)$ turned on at time t_0 [$A_\mu(1)$ in four-vector notation], one must address the gauge properties of the Green's function. The potentials appear explicitly in the one-electron part of the Hamiltonian H^0 as

$$H^0(t_1)=\int d\mathbf{x}_1\hat{\Psi}^\dagger(1^+)h(1)\hat{\Psi}(1) ,$$

where

$$h(\mathbf{p},\mathbf{x};t)=\frac{[\mathbf{p}-e\,\mathbf{A}(\mathbf{x},t)]^2}{2m}+e\phi(\mathbf{x},t) , \quad (1)$$

and $\hat{\Psi}^\dagger,\hat{\Psi}$ are the field operators (spin is ignored here). Scattering interactions (phonons, impurities, etc.) are devoid of any explicit appearance of the potentials, and are in fact gauge invariant. In consequence of this, one should immediately expect that the gauge-dependent part of the Green's function (with scattering) should be the same as the gauge-dependent part of the one-electron Green's function, as it arises from the gauge transformation properties of $\hat{\Psi}$ and $\hat{\Psi}^\dagger$. The latter have the same form with and without scattering. Schwinger[5] extracted the gauge-dependent part of the Green's function in constant uniform electric and magnetic fields and also for plane-wave fields, but in the absence of scattering interactions. Ashby[6] and Serimaa *et al.*[7] obtained corresponding results for arbitrary electromagnetic fields, expressed in terms of the Wigner function. In all cases, the gauge-dependent factor of the Green's function has the form $\exp[ie\int_L dx_\mu A_\mu(x_\mu)]$ where L is a straight trajectory joining $(\mathbf{x}_1,t_1)$ and $(\mathbf{x}_2,t_2)$. In the absence of scattering, we may express this result in terms of the spectral weight $A^0(1;2)$ of the retarded and advanced Green's function $G^0_\pm(1;2)$: $A^0(1;2)$ is defined by

$$A^0(1;2)=i[G^0_+(1;2)-G^0_-(1;2)] , \quad (2)$$

where

$$G^0_\pm(1;2)=\pm\eta_\pm(t_1-t_2)[G^0_>(1;2)-G^0_<(1;2)] , \quad (3)$$

with $\eta_+(t)$ as the Heaviside step function and $\eta_-(t)=1-\eta_+(t)$. Here, $G^0_\gtrless$ is the null-scattering, null-source limit of the generating Green's function $G_\gtrless$ which is defined quite generally by

$$G(1;2;t_c)=-i\varepsilon(1;2)\frac{\mathrm{Tr}[S(t_c+\tau;t_c)(\hat{\Psi}(1)\hat{\Psi}^\dagger(2))_+]}{\mathrm{Tr}[S(t_c+\tau;t_c)]} , \quad (4)$$

where

$$\varepsilon(1;2)=\pm 1$$

for fermions accordingly as $t_1 \gtrless t_2$ and the weighting factor $S(t_c+\tau;t_c)$ is given in terms of time development generated by the complete Hamiltonian H_c which includes all scatterings, self-interactions, and sources as well as external fields $[H_c(t)=H(t)+H'(t)$ where $H(t)$ and $H'(t)$ are given in Eqs. (12) and (14) below]

$$S(t_c+\tau;t_c)=\left[\exp\left[-i\int_{t_c}^{t_c+\tau} d\bar{t}\, H_c(\bar{t})\right]\right]_- , \tag{5}$$

with $\tau=-i/kT$, kT is thermal energy. ($[\cdots]_-$ refers to the negative time ordering.) In this $G_>, G_<$ (as well as $g_>, g_<$ below) are defined in the usual way in accordance with the two time orderings of $(\hat{\Psi}(1)\hat{\Psi}^\dagger(2))_+$ under the trace. The generating Green's function G differs from the physical Green's function g defined as

$$g(1;2)=-i\varepsilon(1;2)\frac{\mathrm{Tr}[\rho_0(\hat{\Psi}(1)\hat{\Psi}^\dagger(2))_+]}{\mathrm{Tr}[\rho_0]} \tag{6}$$

in that the weighting factor of the trace for G is $S(t_c+\tau;t_c)$ instead of the initial equilibrium density matrix ρ_0 for g in the absence of sources and external fields (but including scatterings and self-interactions). It should be noted[3] that when the real time parameter t_c is less than the time t_0 at which the external fields are turned on, then $G(1;2)\to g(1;2)$ for null sources.

Since the absence of scattering processes makes possible a purely one-electron description, $A^0(1;2)$ may be written alternatively as

$$A^0(1;2)=\langle \mathbf{x}_1,t_1|\mathbf{x}_2,t_2\rangle , \tag{7}$$

where $|\mathbf{x},t\rangle$ is the eigenvector of the density operator for a single electron. In these terms, the extraction of the gauge dependence is given by (no scattering and no sources)

$$A^0(1;2)=\exp\left[ie\int_L dx_\mu A_\mu(x_\mu)\right]A^{0\prime}(1;2) . \tag{8}$$

Here $A^{0\prime}(1;2)$ is the gauge-independent part of the spectral weight function. As we have purely one-electron dynamics in the absence of scattering, the field operators evolve in time according to

$$\hat{\Psi}(1)=\int d\mathbf{x}' G^0_+(1;\mathbf{x}',t_0)\hat{\Psi}(\mathbf{x}',t_0) \tag{9}$$

and

$$\hat{\Psi}^\dagger(2)=\int d\mathbf{x}'\hat{\Psi}^\dagger(\mathbf{x}',t_0)G^0_-(\mathbf{x}',t_0;2), \tag{10}$$

for t_1 and t_2 later than the turn-on time of $A_\mu(x_\mu)$, t_0. Clearly, the physical Green's function has the same gauge-dependent factor as above,

$$g^0_{\gtrless}(1;2)=\exp\left[ie\int_L dx_\mu A_\mu(x_\mu)\right]g^{0\prime}_{\gtrless}(1;2) \tag{11}$$

with $g^{0\prime}_{\gtrless}(1;2)$ gauge independent (no scattering, no sources).

II. SCATTERING CONSIDERATIONS AND GROUP PROPERTIES: DEVELOPMENT OF AN EXACT FUNCTIONAL DIFFERENTIAL VARIANT OF THE GKB ANSATZ

In the presence of scatterers (phonons, impurities, etc.), the time evolution of $\hat{\Psi}$ and $\hat{\Psi}^\dagger$ can no longer be described by the retarded and advanced electron Green's functions [Eqs. (9) and (10)] alone, because of coupling to other dynamical fields. In this case, we consider the total Hamiltonian $H_c(t)$ to be comprised of a part including electron kinematics, fields, self- and scattering interactions $H(t)$ and a source part $H'(t)$, where

$$H(t_1)=\int d\mathbf{x}_1\hat{\Psi}^\dagger(1^+)h(1)\hat{\Psi}(1)+\sum_\alpha H_s[Q_\alpha(t_1)] + \tfrac{1}{2}\int d\mathbf{x}_1\int d\mathbf{x}_2\hat{\Psi}^\dagger(1^+)\hat{\Psi}^\dagger(\mathbf{x}_2,t_1^+)v(\mathbf{x}_1-\mathbf{x}_2)\hat{\Psi}(\mathbf{x}_2,t_1)\hat{\Psi}(1)+\int d\mathbf{x}_1\sum_\alpha \hat{\Psi}^\dagger(1^+)\hat{\Psi}(1)H_I[Q_\alpha(t_1),\mathbf{x}_1] . \tag{12}$$

In this, $\{Q_\alpha(t)\}$ are state variables of the scatterers, $H_I[Q_\alpha(t),\mathbf{x}]$ describes the interaction between electrons and scatterers, and $\sum_\alpha H_s[Q_\alpha(t)]$ is the kinematic Hamiltonian of the scatterers. We assume

$$[\hat{\Psi}(t),Q_\alpha(t)]=[\hat{\Psi}^\dagger(t),Q_\alpha(t)]=0 . \tag{13}$$

For the source Hamiltonian, we employ the non-gauge-invariant form

$$H'(t_1)=\int d\mathbf{x}_1[\hat{\Psi}^\dagger(1)\xi(1)+\xi^*(1)\hat{\Psi}(1)]+\sum_\alpha\{Q_\alpha(t_1)\}\eta_\alpha(t_1) , \tag{14}$$

with electron particle sources ξ,ξ^* and scatterer sources η_α. The associated electron field equation of motion may be written in the form

$$\left[i\frac{\partial}{\partial t_1}-h(1)-\xi^*(1)-\int d(3)V(1;3)i\frac{\delta}{\delta\xi(3^+)}i\frac{\delta}{\delta\xi^*(3)}-\sum_\alpha H_I\left[\left\{i\frac{\delta}{\delta\eta_\alpha(t_1)}\right\},\mathbf{x}_1\right]\right]\mathrm{Tr}[S(t_c+\tau;t_c)\hat{\Psi}(1)\hat{\Psi}^\dagger(2)]=0 , \tag{15}$$

and its adjoint counterpart is

$$\mathrm{Tr}[S(t_c+\tau;t_c)\hat{\Psi}(1)\hat{\Psi}^{\dagger}(2)]\left[-i\frac{\partial^T}{\partial t_2}-h^{\dagger}(2)-\xi(2)-\int d(3)i\frac{\delta^T}{\delta\xi^*(3)}i\frac{\delta^T}{\delta\xi(3^+)}V(3;2)-\sum_{\alpha}H_I\left[\left\{i\frac{\delta^T}{\delta\eta_\alpha(t_2)}\right\},\mathbf{x}_2\right]\right]=0\,, \tag{16}$$

with $V(1;2)=v(\mathbf{x}_1-\mathbf{x}_2)\delta(t_1-t_2)$. Following Schwinger,[8] we employ an asymmetric point of view which involves an auxiliary variational operator which generates interaction dynamics involving the electron-electron and electron-scatterer Hamiltonian couplings. In this, we define $\hat{A}(1;2)$ and $\hat{A}^{T}(1;2)$ as variational differential operator counterparts of spectral weight, as given by

$$\hat{A}(1;2)=\exp\left[-i\int_{t_2}^{t_1}d(3)\int_{t_2}^{t_1}d(4)\left[i\frac{\delta}{\delta\xi(3^+)}i\frac{\delta}{\delta\xi^*(3)}V(3;4)+\sum_{\alpha}H_I\left[\left\{i\frac{\delta}{\delta\eta_\alpha(t_4)}\right\},\mathbf{x}_4\right]\delta(3;4)\right]\times i\frac{\delta}{\delta\xi(4^+)}i\frac{\delta}{\delta\xi^*(4)}\right]A^0(1;2) \tag{17}$$

and

$$\hat{A}^{T}(1;2)=A^0(1;2)\exp\left[-i\int_{t_2}^{t_1}d(3)\int_{t_2}^{t_1}d(4)i\frac{\delta^T}{\delta\xi(3^+)}i\frac{\delta^T}{\delta\xi^*(3)}\times\left[V(3;4)i\frac{\delta^T}{\delta\xi(4^+)}i\frac{\delta^T}{\delta\xi^*(4)}+\sum_{\alpha}H_I\left[\left\{i\frac{\delta^T}{\delta\eta_\alpha(t_3)}\right\},\mathbf{x}_3\right]\delta(3;4)\right]\right]\,. \tag{18}$$

In Eqs. (17) and (18), $A^0(1;2)=\langle\mathbf{x}_1,t_1|\mathbf{x}_2,t_2\rangle$ differs from the corresponding one-electron quantity of Eq. (7) (without all scattering and self-interactions) in that the effects of sources are present here. The variational derivatives with a superscript T in the above equations act to the left, whereas those without a superscript T act to the right. These variational differential actions apply to $A^0(1;2)$ and any other functionals multiplied into $A^0(1;2)$ (unless interrupted by the symbol ‡ which indicates termination of the action of variational derivatives). In accordance with Schwinger's interpretation, we may think of a single electron as moving under the influence of the other electrons of the medium and of the scatterers. The variational derivatives are regarded as the state variables of the medium electrons and the scatterers. For convenience, we define associated retarded and advanced auxiliary variational Green's function operators as

$$\hat{G}_+(1;2)=-i\eta_+(t_1-t_2)\hat{A}(1;2) \tag{19}$$

and

$$\hat{G}_-(1;2)=i\eta_-(t_1-t_2)\hat{A}^{T}(1;2)\,. \tag{20}$$

Using the fact that the variational derivatives

$$i\frac{\delta}{\delta\xi(\mathbf{x}_3,t_3^+)}i\frac{\delta}{\delta\xi^*(\mathbf{x}_3,t_3)}\,,$$

acting on $A^0(1;2)=\langle\mathbf{x}_1,t_1|\mathbf{x}_2,t_2\rangle$ yields

$$\langle\mathbf{x}_1,t_1|\hat{\Psi}^{\dagger}(\mathbf{x}_3,t_3^+)\hat{\Psi}(\mathbf{x}_3,t_3)|\mathbf{x}_2,t_2\rangle$$

if t_3 is between t_1 and t_2, and noting that $\hat{\Psi}^{\dagger}(\mathbf{x}_3,t_1^+)\hat{\Psi}(\mathbf{x}_3,t_1)$ just measures the electron density at t_1 with eigenvalue $\delta(\mathbf{x}_1-\mathbf{x}_3)$ in its operation on the density eigenstate $|\mathbf{x}_1,t_1\rangle$, we obtain

$$i\frac{\delta}{\delta\xi(\mathbf{x}_3,t_1^+)}i\frac{\delta}{\delta\xi^*(\mathbf{x}_3,t_1)}\hat{G}_+(1;2)=\delta(\mathbf{x}_1-\mathbf{x}_3)\hat{G}_+(1;2) \tag{21}$$

and

$$\hat{G}_-(1;2)i\frac{\delta^T}{\delta\xi(\mathbf{x}_3,t_2^+)}i\frac{\delta^T}{\delta\xi^*(\mathbf{x}_3,t_2)}=\delta(\mathbf{x}_2-\mathbf{x}_3)\hat{G}_-(1;2)\,. \tag{22}$$

With Eqs. (17)–(22) in view, one may readily verify that

$$\left[i\frac{\partial}{\partial t_1}-h(1)-\xi^*(1)-\int d(3)V(1;3)i\frac{\delta}{\delta\xi(3^+)}i\frac{\delta}{\delta\xi^*(3)}-\sum_{\alpha}H_I\left[\left\{i\frac{\delta}{\delta\eta_\alpha(t_1)}\right\},\mathbf{x}_1\right]\right]\hat{G}_+(1;2)=\delta(1;2) \tag{23}$$

and

$$\hat{G}_-(1;2)\left[-i\frac{\partial^T}{\partial t_2}-h^{\dagger}(2)-\xi(2)-\sum_{\alpha}H_I\left[\left\{i\frac{\delta^T}{\delta\eta_\alpha(t_2)}\right\},\mathbf{x}_2\right]-\int d(3)i\frac{\delta^T}{\delta\xi^*(3)}i\frac{\delta^T}{\delta\xi(3^+)}V(3;2)\right]=\delta(1;2). \tag{24}$$

In Eqs. (17) and (18) we may verify the extraction of the gauge dependence in the presence of scattering and self-interactions by noting that such interaction effects are generated by the action of the combination $[i\delta/\delta\xi(3^+)][i\delta/\delta\xi^*(3)]$ which induces field operators in the density formation $\hat{\Psi}^\dagger(3^+)\hat{\Psi}(3)$, which is gauge invariant: subsequent to such action, we take the zero-source limit, and then we may employ Eq. (8) to extract the gauge dependence of the associated retarded and advanced auxiliary variational Green's-function operators, whence

$$\hat{G}_\pm(1;2)=\exp\left[ie\int_L dx_\mu A_\mu(x_\mu)\right]\hat{G}'_\pm(1;2)\ , \tag{25}$$

for t_1 and t_2 later than the turn-on time of A_μ, t_0. $\hat{G}'_\pm(1;2)$ is of course gauge independent in the null-source limit. We note that the initial values[9] of $\hat{G}_\pm$ are given by

$$\hat{G}_\pm(\mathbf{x}_1,t_0^\pm;\mathbf{x}_2,t_0)=\mp i\delta(\mathbf{x}_1-\mathbf{x}_2) \tag{26}$$

and furthermore, for $t_1,t_2>t_0$, $\hat{G}_\pm$ obeys the homogeneous counterpart of Eqs. (23) and (24). With this in view, one may readily verify that the forward time development of $\mathrm{Tr}[S(t_c+\tau;t_c)\hat{\Psi}(1)\hat{\Psi}^\dagger(2)]$, starting from its initial value at t_0, is given by

$$\begin{aligned}\mathrm{Tr}[S(t_c+\tau;t_c)\hat{\Psi}(1)\hat{\Psi}^\dagger(2)]&=\int d\mathbf{x}_3\int d\mathbf{x}_4\hat{G}_+(1;\mathbf{x}_3,t_0)\mathrm{Tr}[S(t_c+\tau;t_c)\hat{\Psi}(\mathbf{x}_3,t_0)\hat{\Psi}^\dagger(\mathbf{x}_4,t_0)]\hat{G}_-(\mathbf{x}_4,t_0;2)\\&=\exp\left[ie\int_L dx_\mu A_\mu(x_\mu)\right]\\&\quad\times\int d\mathbf{x}_3\int d\mathbf{x}_4\hat{G}'_4(1;\mathbf{x}_3,t_0)\mathrm{Tr}[S(t_c+\tau;t_c)\hat{\Psi}(\mathbf{x}_3,t_0)\hat{\Psi}^\dagger(\mathbf{x}_4,t_0)]\hat{G}'_-(\mathbf{x}_4,t_0;2)\end{aligned} \tag{27}$$

(with the limit of null sources understood after the action of the variational derivatives is carried out) since for $t_1,t_2>t_0$, Eqs. (23) and (24) assure the vanishing required by Eqs. (15) and (16) and at the initial time $t_1=t_2=t_0$, the spatial δ function of Eq. (26) assures the initial value of $\mathrm{Tr}[S(t_c+\tau;t_c)\hat{\Psi}(1)\hat{\Psi}^\dagger(2)]$. The physical Green's function, $g_>(1;2)$, may then be expressed[3,9,10] as

$$\begin{aligned}g_>(1;2)=&\lim_{t_c\to t_0^-}\exp\left[ie\int_L dx_\mu A_\mu(x_\mu)\right]\\&\times\frac{\int d\mathbf{x}_3\int d\mathbf{x}_4\hat{G}'_+(1;\mathbf{x}_3,t_0)\mathrm{Tr}[S(t_c+\tau;t_c)\hat{\Psi}(\mathbf{x}_3,t_0)\hat{\Psi}^\dagger(\mathbf{x}_4,t_0)]\hat{G}'_-(\mathbf{x}_4,t_0;2)}{\mathrm{Tr}[S(t_c+\tau;t_c)]}\ ,\end{aligned} \tag{28}$$

after the null-source limits $\xi\to 0$ and $\eta_\alpha\to 0$ are taken. In this, we have noted that the gauge-dependent exponent is given by

$$\begin{aligned}\exp\left[ie\int_L dx_\mu A_\mu(x_\mu)\right]&=\exp\left[ie\int_2^1 dx_\mu A_\mu(x_\mu)\right]\\&=\exp\left[ie\int_{(\mathbf{x}_3,t_0)}^1 dx_\mu A_\mu(x_\mu)\right]\exp\left[ie\int_2^{(\mathbf{x}_4,t_0)} dx_\mu A_\mu(x_\mu)\right]\ .\end{aligned}$$

It should be remarked that

$$\mathrm{Tr}[S(t_c+\tau;t_c)\hat{\Psi}(\mathbf{x}_3,t_0)\hat{\Psi}^\dagger(\mathbf{x}_4,t_0)]$$

is certainly gauge invariant since there is no external field before t_0. Similarly, we obtain

$$g_<(1;2)=\lim_{t_c\to t_0}\exp\left[ie\int_L dx_\mu A_\mu(x_\mu)\right]\frac{\int d\mathbf{x}_3\int d\mathbf{x}_4\hat{G}'_+(1;\mathbf{x}_3,t_0)\mathrm{Tr}[S(t_c+\tau;t_c)\hat{\Psi}^\dagger(\mathbf{x}_3,t_0)\hat{\Psi}(\mathbf{x}_4,t_0)]\hat{G}'_-(\mathbf{x}_4,t_0;2)}{\mathrm{Tr}[S(t_c+\tau;t_c)]} \tag{29}$$

in the null-source limit. In regard to gauge, it is clear that the extraction of gauge dependence for the physical Green's function is given by

$$g_{\gtrless}(1;2)=\exp\left[ie\int_L dx_\mu A_\mu(x_\mu)\right]g'_{\gtrless}(1;2)\ , \tag{30}$$

in the presence of scatterers, as in their absence, in the null-source limit $\xi\to 0$ and $\eta_\alpha\to 0$.

It is worthwhile to observe that $\hat{G}_\pm$ obeys group properties in accordance with Eqs. (17)–(22) as

$$\int d\mathbf{x}_3 \hat{G}_+(1;3)\hat{G}_+(3;2) = -\int d\mathbf{x}_3 \exp\left[\int_{t_3}^{t_1} dt\, F\left[i\frac{\delta}{\delta\xi(t)}, i\frac{\delta}{\delta\xi^*(t)}; i\frac{\delta}{\delta\eta(t)}; t\right]\right]$$
$$\times A^0(1;3)\exp\left[\int_{t_2}^{t_3} dt\, F\left[i\frac{\delta}{\delta\xi(t)}, i\frac{\delta}{\delta\xi^*(t)}; i\frac{\delta}{\delta\eta(t)}; t\right]\right] A^0(3;2)$$
$$= -\int d\mathbf{x}_3 \exp\left[\int_{t_3}^{t_1} dt\, F\left[i\frac{\delta}{\delta\xi(t)}, i\frac{\delta}{\delta\xi^*(t)}; i\frac{\delta}{\delta\eta(t)}; t\right]\right]$$
$$\times \exp\left[\int_{t_2}^{t_3} dt\, F\left[i\frac{\delta}{\delta\xi(t)}, i\frac{\delta}{\delta\xi^*(t)}; i\frac{\delta}{\delta\eta(t)}; t\right]\right] A^0(1;3) A^0(3;2)$$
$$= -\exp\left[\int_{t_2}^{t_1} dt\, F\left[i\frac{\delta}{\delta\xi(t)}, i\frac{\delta}{\delta\xi^*(t)}; i\frac{\delta}{\delta\eta(t)}; t\right]\right] A^0(1;2)$$
$$= -i\hat{G}_+(1;2) \tag{31}$$

for $t_1 > t_3 > t_2$ with

$$F\left[i\frac{\delta}{\delta\xi(t_3)}, i\frac{\delta}{\delta\xi^*(t_3)}; i\frac{\delta}{\delta\eta(t_3)}; t_3\right] = -i\int d\mathbf{x}_3 \int d\mathbf{x}_4 \left\{\left[i\frac{\delta}{\delta\xi(3^+)} i\frac{\delta}{\delta\xi^*(3)} v_c(\mathbf{x}_3;\mathbf{x}_4)\right.\right.$$
$$\left.\left. + \sum_\alpha H_I\left[\left\{i\frac{\delta}{\delta\eta_\alpha(t_3)}\right\}, \mathbf{x}_4\right]\delta(\mathbf{x}_3-\mathbf{x}_4)\right] i\frac{\delta}{\delta\xi(\mathbf{x}_4, t_3^+)} i\frac{\delta}{\delta\xi^*(\mathbf{x}_4, t_3)}\right\} .$$

In this we have employed the corresponding group property of $G^0_\pm$. Similarly,

$$\int d\mathbf{x}_3 \hat{G}_-(1;3)\hat{G}_-(3;2) = i\hat{G}_-(1;2) . \tag{32}$$

Employing Eq. (31), we rewrite Eq. (27) for $t_1 > t_2$ as

$$\mathrm{Tr}[S(t_c+\tau;t_c)\hat{\Psi}(1)\hat{\Psi}^\dagger(2)] = \int d\mathbf{x}_3 \int d\mathbf{x}_4 \int d\mathbf{x}_5 \hat{G}_+(1;\mathbf{x}_5,t_2)\hat{G}_+(\mathbf{x}_5,t_2;\mathbf{x}_3,t_0)$$
$$\times \mathrm{Tr}[S(t_c+\tau;t_c)\hat{\Psi}(\mathbf{x}_3,t_0)\hat{\Psi}^\dagger(\mathbf{x}_4,t_0)]\hat{G}_-(\mathbf{x}_4,t_0;2) ,$$

so that

$$g_<(1;2) = \lim_{t_c \to t_0^-} i\frac{\int d\mathbf{x}_3 \hat{G}_+(1;\mathbf{x}_3,t_2)\mathrm{Tr}[S(t_c+\tau;t_c)\hat{\Psi}^\dagger(\mathbf{x}_3,t_2)\hat{\Psi}(\mathbf{x}_2,t_2)]}{\mathrm{Tr}[S(t_c+\tau;t_c)]} . \tag{33}$$

Similarly, for $t_1 < t_2$, we obtain

$$g_<(1;2) = \lim_{t_c \to t_0^-} i\frac{\int d\mathbf{x}_3 \mathrm{Tr}[S(t_c+\tau;t_c)\hat{\Psi}^\dagger(\mathbf{x}_1,t_1)\hat{\Psi}(\mathbf{x}_3,t_1)]\hat{G}_-(\mathbf{x}_3,t_1;2)}{\mathrm{Tr}[S(t_c+\tau;t_c)]} . \tag{34}$$

It is useful to define a differently normalized Green's function

$$G^c_>(1;2) = -i\frac{\mathrm{Tr}[S(t_c+\tau;t_c)\hat{\Psi}(1)\hat{\Psi}^\dagger(2)]}{\mathrm{Tr}[\rho_0]} \tag{35}$$

and

$$G^c_<(1;2) = i\frac{\mathrm{Tr}[S(t_c+\tau;t_c)\hat{\Psi}^\dagger(2)\hat{\Psi}(1)]}{\mathrm{Tr}[\rho_0]} , \tag{36}$$

where we choose ρ_0 as the initial equilibrium density matrix in the absence of sources and external fields [as defined in connection with Eq. (6), including scattering and self-interactions]. Then we may rewrite Eqs. (33) and (34) in a compact form as

$$g_{\gtrless}(1;2) = \lim_{t_c \to t_0^-} i\int d\mathbf{x}_3 [\hat{G}_+(1;\mathbf{x}_3,t_2)G^c_{\lessgtr}(\mathbf{x}_3,t_2;2)$$
$$- G^c_{\lessgtr}(1;\mathbf{x}_3,t_1)\hat{G}_-(\mathbf{x}_3,t_1;2)] , \tag{37}$$

where we have noted that $\mathrm{Tr}[S(t_c+\tau;t_c)]$ is just ρ_0 for $t_c < t_0$, and one should observe that the Heaviside functions in $\hat{G}_\pm$ mandate that only one of the two terms on the right-hand side of Eq. (37) contributes at a given time. These relations are exact and constitute a functional differential variant of the GKB ansatz.

III. RELATION TO THE GKB ANSATZ

In order to gain insight into the exact functional differential relation of Eq. (37) as it bears on the approximate GKB ansatz, we now neglect all initial electron-scatterer interactions in the initial state at t_0, just as the external field is switched on, so that the initial state trace may be decoupled as

$$\mathrm{Tr}[S(t_c+\tau;t_c)\hat{\Psi}(1)\hat{\Psi}^\dagger(2)]_{t_1=t_2=t_0^-}$$
$$=\mathrm{Tr}[S_s(t_c+\tau;t_c)]\times\mathrm{Tr}[S_0(t_c+\tau;t_c)\hat{\Psi}(1)\hat{\Psi}^\dagger(2)]_{t_1=t_2=t_0^-} . \tag{38}$$

In this, $S_s(t_c+\tau;t_c)$ is the kinematic time evolution operator of the scatterers including their sources, and $S_0(t_c+\tau;t_c)$ is the time evolution operator of the carriers including their sources, with the decoupling due to cutting the carrier-scatterer interaction in the initial state. To simplify our considerations, we further neglect the carrier-carrier interactions so that the variational derivatives with respect to phonon sources in $\hat{G}_\pm$ of Eq. (37) act only on the scatterer trace $\mathrm{Tr}[S_s(t_c+\tau;t_c)]$. Recalling Eqs. (28) and (29) (reabsorbing the gauge dependence with $\hat{G}'_\pm\to\hat{G}_\pm$), we form the retarded and advanced Green's function $G_\pm(1;2)$ defined in analogy to Eq. (3) and note that for $t_c\to t_0^-$, the generating Green's function $G_\gtrless$ is identical to the physical Green's function $g_\gtrless$ in the absence of sources, so that

$$G_\pm(1;2)=\pm\eta_\pm(t_1-t_2)[g_>(1;2)-g_<(1;2)] . \tag{39}$$

Since the difference $(g_>-g_<)$ involves field operators referred to the same initial time t_0, their commutator is readily evaluated by the canonical commutation relations, yielding the retarded Green's function as (henceforth we always understand that the null-source limit is to be taken after carrying out indicated variational differentiations)

$$\begin{aligned}G_+(1;\mathbf{x}_2,t_0)&=\lim_{t_c\to t_0^-}\frac{\int d\mathbf{x}_3\hat{G}_+(1;\mathbf{x}_3,t_0)\mathrm{Tr}[S_s(t_c+\tau;t_c)]\mathrm{Tr}[S_0(t_c+\tau;t_c)]\delta(\mathbf{x}_3-\mathbf{x}_2)}{\mathrm{Tr}[S_s(t_c+\tau;t_c)]\mathrm{Tr}[S_0(t_c+\tau;t_c)]}\\&=\lim_{t_c\to t_0^-}\frac{\hat{G}_+(1;\mathbf{x}_2,t_0)\mathrm{Tr}[S_s(t_c+\tau;t_c)]}{\mathrm{Tr}[S_s(t_c+\tau;t_c)]} .\end{aligned} \tag{40}$$

Similarly, for the advanced Green's function G_-, we have

$$G_-(\mathbf{x}_1,t_0;2)=\lim_{t_c\to t_0^-}\frac{\mathrm{Tr}[S_s(t_c+\tau;t_c)]\hat{G}_-(\mathbf{x}_1,t_0;2)}{\mathrm{Tr}[S_s(t_c+\tau;t_c)]} . \tag{41}$$

Generally speaking, these retarded and advanced Green's functions do not satisfy the group property

$$\int d\mathbf{x}_3G_+(1;3)G_+(3;2)\neq-iG_+(1;2) \tag{42}$$

and

$$\int d\mathbf{x}_3G_-(1;3)G_-(3;2)\neq iG_-(1;2) , \tag{43}$$

because the variational derivative acts on $\mathrm{Tr}[S_s]$, which has no reference corresponding to the real time domain, such as exists for $A^0(1;2)$ in Eq. (31). However, following Lipavsky, Špička, and Velický[4] in the assertion of equality in Eqs. (42) and (43) for both t_1 and t_2 later than t_0, corresponding to the "semigroup" property for $G_\pm$ under the model assumption of zero collision time, we can proceed to make contact with the generalized Kadanoff-Baym ansatz. Rewriting Eq. (42) for G_+ with substitution of Eq. (40) into the integrand, we have (recall the symbol ‡ for stopping variational differentiation)

$$-iG_+(1;\mathbf{x}_2,t_0)=\lim_{t_c\to t_0^-}\int d\mathbf{x}_3\frac{\hat{G}_+(1;3)\mathrm{Tr}[S_s(t_c+\tau;t_c)]\ddagger\hat{G}_+(3;\mathbf{x}_2,t_0)\mathrm{Tr}[S_s(t_c+\tau;t_c)]}{\mathrm{Tr}[S_s(t_c+\tau;t_c)]\mathrm{Tr}[S_s(t_c+\tau;t_c)]} \tag{44}$$

for $t_1,t_3>t_0$. Reabsorbing gauge dependence, Eq. (29) becomes

$$g_<(1;2)=\lim_{t_c\to t_0^-}\frac{\int d\mathbf{x}_3\int d\mathbf{x}_4\hat{G}_+(1;\mathbf{x}_3,t_0)\mathrm{Tr}[S_s(t_c+\tau;t_c)]}{\mathrm{Tr}[S_s(t_c+\tau;t_c)]}\frac{\mathrm{Tr}[S_0(t_c+\tau;t_c)\hat{\Psi}^\dagger(\mathbf{x}_3,t_0)\hat{\Psi}(\mathbf{x}_4,t_0)]\hat{G}_-(\mathbf{x}_4,t_0;2)}{\mathrm{Tr}[S_0(t_c+\tau;t_c)]} . \tag{45}$$

Noting that the part of the integrand of the above equation given by $\hat{G}_+\mathrm{Tr}[S_s]\ddagger/\mathrm{Tr}[S_s]$ is in fact G_+, which may be reexpressed in terms of Eq. (44), we find that $g_<(1;2)$ takes the form $(t_1>t_2)$

$$g_<(1;2)\simeq i\frac{\int d\mathbf{x}_5\hat{G}_+(1;\mathbf{x}_5,t_2)\mathrm{Tr}[S_s]}{\mathrm{Tr}[S_s]}\ddagger\frac{\int d\mathbf{x}_3\int d\mathbf{x}_4\hat{G}_+(\mathbf{x}_5,t_2;\mathbf{x}_3,t_0)\mathrm{Tr}[S_s]\mathrm{Tr}[S_0\hat{\Psi}^\dagger(\mathbf{x}_3,t_0)\hat{\Psi}(\mathbf{x}_4,t_0)]\hat{G}_-(\mathbf{x}_4,t_0;2)}{\mathrm{Tr}[S_s]\mathrm{Tr}[S_0]}$$

$$\simeq i\int d\mathbf{x}_5\int d\mathbf{x}_3\int d\mathbf{x}_4 G_+(1;\mathbf{x}_5,t_2)\frac{\hat{G}_+(\mathbf{x}_5,t_2;\mathbf{x}_3,t_0)\mathrm{Tr}[S_s]\mathrm{Tr}[S_0\hat{\Psi}^\dagger(\mathbf{x}_3,t_0)\hat{\Psi}(\mathbf{x}_4,t_0)]\hat{G}_-(\mathbf{x}_4,t_0;2)}{\mathrm{Tr}[S_s]\mathrm{Tr}[S_0]}$$

$$\simeq i\int d\mathbf{x}_5 G_+(1;\mathbf{x}_5,t_2)g_<(\mathbf{x}_5,t_2;\mathbf{x}_2,t_2)\ . \tag{46}$$

Similarly for $t_1<t_2$, we obtain

$$g_<(1;2)\simeq -i\int d\mathbf{x}_5 g_<(1;\mathbf{x}_5,t_1)G_-(\mathbf{x}_5,t_1;2)\ . \tag{47}$$

Moreover, we obtain the GKB ansatz[4] from these considerations,

$$g_\gtrless(1;2)\simeq i\int d\mathbf{x}_3[G_+(1;\mathbf{x}_3,t_2)g_\gtrless(\mathbf{x}_3,t_2;2)-g_\gtrless(1;\mathbf{x}_3,t_1)G_-(x_3,t_1;2)]\ . \tag{48}$$

It should be noted that, apart from the neglect of initial scattering interactions (as well as dropping electron-electron interactions completely), the only approximation involves the assertion of the semigroup properties[4] of $G_\pm$, with no approximation pertaining to the equal-time Green's function $g_\gtrless(1;\mathbf{x}_2,t_1)$.

Finally, we make contact with the ordinary Kadanoff-Baym ansatz[2] with definitions analogous to Eqs. (40) and (41) to introduce the spectral weight function $A(1;2)$ as

$$A(1;\mathbf{x}_2,t_0)=\lim_{t_c\to t_0^-}\frac{\hat{A}(1;\mathbf{x}_2,t_0)\mathrm{Tr}[S_s(t_c+\tau;t_c)]}{\mathrm{Tr}[S_s(t_c+\tau;t_c)]}$$

$$=\lim_{t_c\to t_0^-}\frac{\mathrm{Tr}[S_s(t_c+\tau;t_c)]\hat{A}(\mathbf{x}_1,t_0;2)}{\mathrm{Tr}[S_s(t_c+\tau;t_c)]}\ . \tag{49}$$

We further assume that the equal-time Green's functions $g_\gtrless(1;\mathbf{x}_2,t_1)$ and $g_\gtrless(\mathbf{x}_1,t_2;2)$ vary slowly within the time interval $t_1\to t_2$ and in this spirit they are represented by their midpoint values $g_\gtrless(\mathbf{x}_1,(t_1+t_2)/2;\mathbf{x}_2,(t_1+t_2)/2)$. Notwithstanding the violation of group properties which this entails, it leads to

$$g_\gtrless(1;2)\simeq i\int d\mathbf{x}_3[G_+(1;\mathbf{x}_3,t_2)g_\gtrless(\mathbf{x}_3,(t_1+t_2)/2;\mathbf{x}_2,(t_1+t_2)/2)-g_\gtrless(\mathbf{x}_1,(t_1+t_2)/2;\mathbf{x}_3,(t_1+t_2)/2)G_-(\mathbf{x}_3,t_1;2)]\ . \tag{50}$$

Since $g_\gtrless$ is evaluated at equal times here, it may be referred to the Wigner function $f(\mathbf{k};\mathbf{R},(t_1+t_2)/2)$. Considered jointly with Eqs. (19), (20), and (49), we obtain the KB ansatz

$$g_\gtrless(\mathbf{k};t_1,t_2)\simeq \mp iA(\mathbf{k};t_1,t_2)\times\begin{cases}1-f(\mathbf{k};\mathbf{R},(t_1+t_2)/2)\\ f(\mathbf{k};\mathbf{R},(t_1+t_2)/2)\ .\end{cases} \tag{51}$$

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[1]P. C. Martin and J. Schwinger, Phys. Rev. **115**, 1342 (1959).
[2]L. P. Kadanoff and G. Baym, *Quantum Statistical Mechanics* (Benjamin, New York, 1962), p. 153.
[3]H. C. Tso, Ph.D. thesis, Stevens Institute of Technology, Hoboken, New Jersey, 1990.
[4]P. Lipavský, V. Špička, and B. Velický, Phys. Rev. B **34**, 6933 (1986).
[5]J. Schwinger, Phys. Rev. **82**, 664 (1951).
[6]N. Ashby, Ph.D. thesis, Harvard University, Cambridge, Massachusetts, 1961.
[7]O. Serimaa *et al.*, Phys. Rev. A **33**, 2913 (1986).
[8]J. Schwinger, *Quantum Kinematics and Dynamics* (Benjamin, New York, 1970), p. 285.
[9]N. J. M. Horing and H. L. Cui, Phys. Rev. B **38**, 10 907 (1988).
[10]N. J. M. Horing (unpublished).