Kadanoff-Baym Equations for Interacting Systems with Dissipative Lindbladian Dynamics

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The extraordinary quantum properties of nonequilibrium systems governed by dissipative dynamics have become a focal point in contemporary scientific inquiry. The nonequilibrium Green's functions (NEGF) theory provides a versatile method for addressing driven *nondissipative* systems, utilizing the powerful diagrammatic technique to incorporate correlation effects. We here present a second-quantization approach to the *dissipative* NEGF theory, reformulating Keldysh ideas to accommodate Lindbladian dynamics and extending the Kadanoff-Baym equations accordingly. Generalizing diagrammatic perturbation theory for many-body Lindblad operators, the formalism enables correlated and dissipative real-time simulations for the exploration of transient and steady-state changes in the electronic, transport, and optical properties of materials.

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Nonequilibrium systems, governed by dissipative dynamics, have broken into modern science owing to their remarkable quantum properties. Optical cavities of atoms [1,2], molecules [3,4] and solid state systems [5,6] offer an ideal platform to exploit the interplay between coherence and dissipation [7]. Special attention has thus far been dedicated to stationary states—in particular the study of nonequilibrium fixed points and critical exponents [8,9], phase transitions [10,11], entanglement [12,13], and topology [14]—as well as Floquet states [15,16].

The transient dynamics of dissipative systems subjected to ultrafast driving fields remains poorly explored. In fact, the concomitant action of external fields, correlation, and dissipation calls for innovative many-body frameworks. The Lindblad equation [17,18] serves as a solid ground to incorporate the aforementioned physics, preserving the trace and positivity of the many-body density matrix $\hat{\rho}$. However, its *brute force* numerical solution scales exponentially with the system size. Nonequilibrium Green's functions (NEGF) theory [19–21] has proven to be a versatile tool to deal with driven systems; it leverages the powerful diagrammatic technique to account for correlation effects, thus reducing from exponential to power-law the numerical scaling. The inclusion of Lindblad dissipation in NEGF has been accomplished by Sieberer *et al.* in the so-called field theory approach [22–25], which is based on the path integral technique and Schwinger-Keldysh action [26]. Alternatively, NEGF can be formulated in the second-quantization approach [19,27–29], where concepts like the Martin-Schwinger hierarchy [30], Kadanoff-Baym equations [31,32], conserving approximations [33,34], and Bethe-Salpeter equation [35,36] are employed to develop many-body schemes for the simulation of carrier [37–39] and phonon [40–42] dynamics, dephasing and thermalization [43], transient photoabsorbtion [44–47], photoemission [48,49] and Raman [50,51] spectroscopy, photoexcitations and quenches in Mott and excitonic insulators [52–55], or time-dependent quantum transport [56–62]. The question of how the second-quantization approach—and related concepts—should be extended to encompass dissipation remains to be elucidated.

In this work we offer a second-quantization perspective on the dissipative NEGF theory. We reformulate the original Keldysh idea to accommodate Lindbladian time evolutions, and extend the Kadanoff-Baym equations accordingly. We also show how to generalize the diagrammatic perturbation theory for many-body Lindblad operators. The resulting formalism paves the way for conducting real-time simulations of the correlated and dissipative dynamics of materials.

Keldysh-Lindblad formalism—For systems governed by a dissipative Lindbladian dynamics the average value of any, generally time-dependent, operator $\hat{O}(t)$ at time t is expressed as $O(t) = \mathrm{Tr}[\hat{\rho}(t)\hat{O}(t)]$, where the many-body density matrix satisfies the Lindblad equation (henceforth sum over repeated indices is implicit)

$$\frac{d\hat{\rho}}{dt} = -i[\hat{H},\hat{\rho}]_{-} + 2\hat{L}_\gamma\hat{\rho}\hat{L}_\gamma^\dagger - \hat{L}_\gamma^\dagger\hat{L}_\gamma\hat{\rho} - \hat{\rho}\hat{L}_\gamma^\dagger\hat{L}_\gamma. \quad (1)$$

Here, $\hat{H}$ is the self-adjoint Hamiltonian of the system and $\hat{L}_\gamma$ are the Lindblad operators. Equation (1) can equivalently be cast in the form of an integral equation. Let $\hat{H}_o(t) = \hat{H}(t) - i\hat{L}_\gamma^\dagger(t)\hat{L}_\gamma(t)$ be the "open system" Hamiltonian and define the nonunitary evolution operator $\hat{U}_o(t,t') = Te^{-i\int_{t'}^{t} d\bar{t}\hat{H}_o(\bar{t})}$

for $t > t'$ and $\hat{U}_o(t,t') = \bar{T} e^{-i\int_{t'}^{t} d\bar{t}\hat{H}_o^\dagger(\bar{t})}$ for $t < t'$, where T and $\bar{T}$ are the time and antitime ordering operators, respectively. Then $\hat{\rho}(t) = \hat{U}_o(t,0)\hat{\rho}(0)\hat{U}_o(0,t) + 2\int_0^t dt_1 \hat{U}_o(t,t_1)\hat{L}_{\gamma_1}(t_1)\hat{\rho}(t_1)\hat{L}^\dagger_{\gamma_1}(t_1)\hat{U}_o(t_1,t)$ solves Eq. (1), as it can easily be verified by direct differentiation. Iterating the integral equation and using the cyclic property of the trace, the time-dependent average $O(t)$ reads

$$
\begin{aligned}
O(t) = \mathrm{Tr}\Bigg[\hat{\rho}(0)\sum_{k=0}^{\infty} 2^k \int_0^t dt_1 .. \int_0^{t_{k-1}} dt_k \hat{U}_o(0,t_k) L^\dagger_{\gamma_k}(t_k)\ldots \\
\times \hat{U}_o(t_2,t_1)\hat{L}^\dagger_{\gamma_1}(t_1)\hat{U}_o(t_1,t)\hat{O}(t)\hat{U}_o(t,t_1)\hat{L}_{\gamma_1}(t_1) \\
\times \hat{U}_o(t_1,t_2)\ldots L_{\gamma_k}(t_k)\hat{U}_o(t_k,0)\Bigg]. \qquad (2)
\end{aligned}
$$

This result can be written in a more useful form if we introduce the oriented Keldysh contour $C = C_- \cup C_+ = (0,t) \cup (t,0)$. Let $z \in C$ denote a contour time; we write $z = t_\pm$ if $z \in C_\pm$. We also define the functions $\theta_\pm(z) = 1$ if $z \in C_\pm$ and zero otherwise, and $s(z) = \theta_-(z) - \theta_+(z)$. Then

$$
\hat{U}_o(t_i,t_j) = \mathcal{T}\left\{e^{-i\int_{t_{j\mp}}^{t_{i\mp}} d\bar{z}[\hat{H}(\bar{z}) - is(\bar{z})\hat{L}^\dagger_\gamma(\bar{z})\hat{L}_\gamma(\bar{z})]}\right\}, \quad t_i \gtrless t_j, \qquad (3)
$$

where $\mathcal{T}$ is the contour ordering operator. If we set the times of all operators $\hat{L}^\dagger$ on the C_+ branch and the times of all operators $\hat{L}$ on the C_- branch then the string of operators in Eq. (2) is contour ordered. Therefore, taking into account that under the $\mathcal{T}$ sign the bosonic (fermionic) operators (anti) commute, we can extend all integration limits to t and divide by $k!$. The reordering does not generate minus signs in the case of fermionic Lindblad operators since the number of interchanges is always even. In this way the series is transformed into the Taylor expansion of an exponential, and the time-dependent average simplifies to

$$
O(t) = \mathrm{Tr}\left[\hat{\rho}(0)\mathcal{T}\left\{e^{-i\int_C d\bar{z}\,\hat{H}(\bar{z},\bar{z}^*)}\hat{O}(z)\right\}\right], \qquad (4)
$$

where

$$
\hat{H}(\bar{z},\bar{z}^*) = \hat{H}(\bar{z}) - is(\bar{z})\hat{L}^\dagger_\gamma(\bar{z})\hat{L}_\gamma(\bar{z}) + 2i\theta_-(\bar{z})\hat{L}^\dagger_\gamma(\bar{z}^*)\hat{L}_\gamma(\bar{z}), \qquad (5)
$$

and $\bar{z}^* = \bar{t}_\mp$ if $\bar{z} = \bar{t}_\pm$. Notice that under integration the last term in Eq. (5) can alternatively be written as $-2i\theta_+(\bar{z})\hat{L}^\dagger_\gamma(\bar{z})\hat{L}_\gamma(\bar{z}^*)$ since $\int_C d\bar{z} F(\bar{z},\bar{z}^*) = -\int_C d\bar{z} F(\bar{z}^*,\bar{z})$ for any function F, and $\theta_\pm(\bar{z}) = \theta_\mp(\bar{z}^*)$. We also observe that in Eq. (4) the contour C can be extended to infinity, i.e., $C = (0,\infty) \cup (\infty,0)$, since $\hat{K} \equiv \mathcal{T}\{e^{-i\int_{t_-}^{t_+} d\bar{z}\,\hat{H}(\bar{z},\bar{z}^*)}\} = 1$ for all t [63]. This also implies that the contour-time z of $\hat{O}$ can be either t_+ or t_-.

In analogy with the theory of unitary evolutions we define the one-particle Keldysh-Lindblad NEGF according to

$$
G_{ij}(z,z') = \frac{1}{i}\mathrm{Tr}\left[\hat{\rho}(0)\mathcal{T}\left\{e^{-i\int_C d\bar{z}\,\hat{H}(\bar{z},\bar{z}^*)}\hat{d}_i(z)\hat{d}^\dagger_j(z')\right\}\right], \qquad (6)
$$

where the annihilation operators $\hat{d}_i$ are either bosonic or fermionic, obeying the (anti)commuation rules $[\hat{d}_i, \hat{d}^\dagger_j]_\mp = \delta_{ij}$ (upper sign for bosons and lower sign for fermions). The contour argument of $\hat{d}$ and $\hat{d}^\dagger$ in Eq. (6) fixes the position of these operators along the contour, thus rendering unambiguous the action of $\mathcal{T}$. The identity $\hat{K} = 1$ implies that the NEGF satisfies the Keldysh properties $G(t_+, t'_\pm) = G(t_-, t'_\pm)$ for $t > t'$ and $G(t_\pm, t'_+) = G(t_\pm, t'_-)$ for $t < t'$.

Using the rules for the derivative of a contour-ordered string of operators, see Ref. [19], and introducing the shorthand notation $\langle\ldots\rangle \equiv \mathrm{Tr}[\hat{\rho}(0)\mathcal{T}\{e^{-i\int_C d\bar{z}\,\hat{H}(\bar{z},\bar{z}^*)}\ldots\}]$, we find the important result

$$
\begin{aligned}
i\frac{d}{dz}G_{ij}(z,z') = &\frac{1}{i}\left\langle[\hat{d}_i(z), \hat{H}(z) - is(z)\hat{L}^\dagger_\gamma(z)\hat{L}_\gamma(z)]_-\hat{d}^\dagger_j(z')\right\rangle \\
&-2\theta_+(z)\left\langle[\hat{d}_i(z), \hat{L}^\dagger_\gamma(z)]_\mp\hat{L}_\gamma(z^*)\hat{d}^\dagger_j(z')\right\rangle \\
&\pm 2\theta_-(z)\left\langle\hat{L}^\dagger_\gamma(z^*)[\hat{d}_i(z), \hat{L}_\gamma(z)]_\mp\hat{d}^\dagger_j(z')\right\rangle \\
&+\delta(z,z'), \qquad (7)
\end{aligned}
$$

where the lower sign applies when *both* $\hat{d}_i$ and $\hat{L}_\gamma$ are fermionic operators, and the last term is the Dirac delta on the contour, i.e., $\int dz'\delta(z,z')f(z') = f(z)$ for any function f. A similar equation can be derived by differentiating with respect to z', see below and Supplemental Material [64]. The (anti)commutators in Eq. (7) generally give rise to higher-order NEGFs, the contour-time derivatives of which generate NEGFs of progressively higher order. In this manner, the Martin-Schwinger hierarchy [30] (MSH) for Lindbladian dynamics is established.

Noninteracting systems with one-body loss and gain— For quadratic self-adjoint Hamiltonians $\hat{H}(t) = \hat{H}_0(t) = h_{mn}(t)\hat{d}^\dagger_m\hat{d}_n$ and linear Lindblad operators $\hat{L}_{1\gamma}(t) = a^\gamma_n(t)\hat{d}_n$ (one-body loss) and $\hat{L}_{2\gamma}(t) = b^{\gamma *}_n(t)\hat{d}^\dagger_n$ (one-body gain) the MSH couples the n-particle NEGF exclusively to the $(n-1)$-particle NEGF, and the solution of the MSH is equivalent to Wick's theorem [64,65]. Equation (7) and its counterpart with the derivative of G with respect to z', reduce to (in matrix form)

$$
\left[i\frac{d}{dz} - \tilde{h}(z)\right]G(z,z') + 2i\ell(z^*)G(z^*,z') = \delta(z,z'), \qquad (8a)
$$

$$
G(z,z')\left[\frac{1}{i}\frac{\overleftarrow{d}}{dz'} - \tilde{h}(z')\right] - 2iG(z,z'^*)\ell(z') = \delta(z,z'), \qquad (8b)
$$

where $\tilde{h}(z=t_\pm) \equiv h(t) - is(z)[\ell^>(t) \pm \ell^<(t)]$ and $\ell(z = t_\pm) \equiv \theta_-(z)\ell^>(t) \mp \theta_+(z)\ell^<(t)$, with $\ell^>_{mn}(t) = a^{\gamma*}_m(t)a^\gamma_n(t)$ and $\ell^<_{mn}(t) = b^{\gamma*}_n(t)b^\gamma_m(t)$ positive semidefinite and self-adjoint matrices. The time dependence of $h(t)$ is generally due to external driving fields. We refer to Eqs. (8) as the noninteracting dissipative equations of motion (EOM).

Interacting systems with one-body loss and gain—In interacting systems the Hamiltonian $\hat{H}(t) = \hat{H}_0(t) + \hat{H}_{\rm int}(t)$, where $\hat{H}_{\rm int}$ is self-adjoint and at least quartic in the field operators. Expanding Eq. (6) in powers of $\hat{H}_{\rm int}$ and using Wick's theorem we obtain the Dyson equation (on the Keldysh contour) $G = G_0 + G_0\Sigma G$, where G_0 satisfies Eqs. (8) and the many-body self-energy Σ is given by the sum of all one-particle irreducible Feynman diagrams. The interacting version of the dissipative EOM follows when acting with G_0^{-1} on the Dyson equation; the outcome is Eqs. (8) with a rhs modified by the addition of $\int_C d\bar{z}\Sigma(z,\bar{z})G(\bar{z},z')$ for Eq. (8a) and $\int_C d\bar{z}G(z,\bar{z})\Sigma(\bar{z},z')$ for Eq. (8b).

To derive the Kadanoff-Baym equations (KBE) satisfied by the lesser or greater NEGF $G^{\lessgtr}(t,t') \equiv G(t_\mp, t'_\pm)$, a preliminary discussion on the Langreth rules [66] for convolutions on the Keldysh contour is essential. The many-body self-energy has the structure [19,32,67] $\Sigma_{ij}(z,z') = \delta(z,z')V_{ij}(t) + \langle \hat{\Psi}_i(z)\hat{\Psi}^\dagger_j(z')\rangle_{\rm irr}$, where $\hat{\Psi}_i \equiv [\hat{d}_i, \hat{H}_{\rm int}]_-$ and the subscript "irr" signifies the irreducible part of the average. The quantity $V_{ij}(t) \equiv \langle [\hat{d}_i(z), \hat{\Psi}^\dagger_j(z)]_\mp \rangle$ is the mean-field potential, hence the reminder is the correlation self-energy $\Sigma^{\rm corr}$. The identity $\hat{K} = 1$ [63] guarantees that also $\Sigma^{\rm corr}$ satisfies the Keldysh properties, i.e., $\Sigma^{\rm corr}(t_-, t'_\pm) = \Sigma^{\rm corr}(t_+, t'_\pm)$ for $t > t'$ and $\Sigma^{\rm corr}(t_\pm, t'_-) = \Sigma^{\rm corr}(t_\pm, t'_+)$ for $t < t'$. Therefore the Langreth rules are not affected by the Lindblad dissipators. We emphasize here the crucial role played by $L^\dagger_\gamma(\bar{z}^*)\hat{L}_\gamma(\bar{z})$ in Eq. (5). Excluding this term would leave us with two different non-Hermitian Hamiltonians, one on the forward branch and another on the backward branch, and hence $\hat{K} \neq 1$. The time-ordered and anti-time-ordered NEGF would then be independent functions, leading to significantly more intricate Langreth rules [68,69]. The KBE for $G^<$ is obtained by setting $z = t_-$ and $z' = t'_+$ in the interacting version of Eq. (8a). The second term on the lhs yields the anti-time-ordered $G^{\bar{\rm T}}(t,t') \equiv G(t_+, t'_+) = G^<(t,t') - G^{\rm A}(t,t')$, where $G^{\rm A}(t,t') = -\theta(t',t)[G^>(t,t') - G^<(t,t')]$ is the advanced NEGF. Taking into account the definition of $\tilde{h}(z)$ and $\ell(z)$ we find

$$\left[i\frac{d}{dt} - h_o(t)\right]G^<(t,t') \pm 2i\ell^<(t)G^{\rm A}(t,t') = [\Sigma^< \cdot G^{\rm A} + \Sigma^{\rm R} \cdot G^<](t,t'), \tag{9}$$

where $h_o(t) \equiv h(t) - i(\ell^>(t) \mp \ell^<(t))$ is the one-particle open-system Hamiltonian and the symbol "$\cdot$" is used for real-time convolutions between 0 and infinity [70]. As discussed in Refs. [19,55,72,73] the anti-Hermicity of $G^{\lessgtr}$ allows us to close the system of equations by solving the interacting version of Eq. (8b) for $G^>$. For $z = t_+$ and $z' = t'_-$ the second term on the lhs yields again $G^{\bar{\rm T}}$ which can also be written as $G^> - G^{\rm R}$, where $G^{\rm R}(t,t') = \theta(t,t')[G^>(t,t') - G^<(t,t')]$ is the retarded NEGF. We then find

$$G^>(t,t')\left[\frac{1}{i}\frac{\overleftarrow{d}}{dt'} - h_o^\dagger(t')\right] + 2iG^{\rm R}(t,t')\ell^>(t') = [G^> \cdot \Sigma^{\rm A} + G^{\rm R} \cdot \Sigma^>](t,t'). \tag{10}$$

Equations (9) and (10) are the *dissipative KBE* with one-body loss and gain. From these equations it is straightforward to derive the EOM for the retarded NEGF, i.e.,

$$\left[i\frac{d}{dt} - h_o(t)\right]G^{\rm R}(t,t') = \delta(t,t') + [\Sigma^{\rm R} \cdot G^{\rm R}](t,t'), \tag{11}$$

as well as to show that $G^{\rm A}(t,t') = [G^{\rm R}(t',t)]^\dagger$, see the Appendix for details on the derivation.

Lyapunov equation—The EOM for the one-particle density matrix $\rho^<(t) = \pm iG^<(t,t)$ follows by subtracting Eq. (9) from its adjoint and then setting $t = t'$:

$$\frac{d}{dt}\rho^<(t) = -ih_o(t)\rho^<(t) + i\rho^<(t)h_o^\dagger(t) + 2\ell^<(t) + I(t), \tag{12}$$

where $I(t) = \pm[\Sigma^< \cdot G^{\rm A} + \Sigma^{\rm R} \cdot G^<](t,t) + {\rm H.c.}$ is known as collision integral. Notice that for $\Sigma = 0$, and hence $I = 0$, the solution of the dissipative KBE can be written as

$$G^{\lessgtr}(t,t') = \pm G^{\rm R}(t,t')\rho^{\lessgtr}(t') \mp \rho^{\lessgtr}(t)G^{\rm A}(t,t'), \tag{13}$$

with $\rho^> = \pm iG^>(t,t) = \rho^< \pm 1$, which is identical to the nondissipative solution, see the Appendix.

In the stationary case, i.e., $(d/dt)\rho^< = 0$, and for $I = 0$ (no interaction) Eq. (12) reduces to a Lyapunov equation, whose properties, e.g., topological phases [74–76], exceptional points [24,77], and bulk-edge correspondence [78–80], are currently under intense investigation, see also Refs. [22,24,25] for an overview. A simple approach to include correlation effects is by evaluating the collision integral in the Boltzmann approximation, i.e., $I = -[(\Gamma^> + \Gamma^<), \rho^<]_+ + 2\Gamma^<$, where the rates $\Gamma^{\lessgtr}[\rho^<]$ for in or out scatterings are functionals of $\rho^<$ [81]. In this way, we revert to the noninteracting EOM with renormalized $\ell^{\lessgtr} \to \ell^{\lessgtr} + \Gamma^{\lessgtr}$. In particular the stationary solution becomes a nonlinear Lyapunov equation to be solved self-consistently.

Initial correlations—As with any set of differential equations the dissipative KBE must be solved with an initial condition. For a system in thermal equilibrium before any external driving, we have $\hat{\rho}(0) = \exp[-\beta(\hat{H} - \mu\hat{N})]/Z$, with β the inverse temperature, μ the chemical potential, $\hat{N}$ the total number of particle operator, and Z the partition function. Initial correlations can be included by extending the Keldysh contour along the imaginary time axis until the point $-i\beta$ [82,83]. This results in a generalization of the KBE since the self-energy $\Sigma(z, z')$ is nonvanishing for $z, z' \in (0, -i\beta)$. Following Refs. [19,84] we introduce the *left* $X^{\lceil}(\tau, t) \equiv X(-i\tau, t_\pm)$ and *right* $X^{\rceil}(t, \tau) \equiv X(t_\pm, -i\tau)$ correlators with one real and one imaginary time argument (in $X^{\lceil}$ and $X^{\rceil}$ we can use either t_+ or t_- since $\hat{K} = 1$). Then Eqs. (9) and (10) are modified with the inclusion of terms $[\Sigma^{\rceil} \star G^{\lceil}]$ and $[G^{\rceil} \star \Sigma^{\lceil}]$ on the rhs, respectively, where the symbol "$\star$" is used for imaginary-time convolutions between 0 and β. Taking into account that $\tilde{h}(t_\pm) - 2i\ell(t_\mp) = h_o(t)$ and $\tilde{h}(t_\pm) + 2i\ell(t_\pm) = h_o^\dagger(t)$, the interacting version of Eqs. (8) yield the following EOM for the left and right NEGF

$$\left[i\frac{d}{dt} - h_o(t)\right] G^{\rceil}(t, \tau) = [\Sigma^{\rceil} \cdot G^{\mathrm{A}} + \Sigma^{\mathrm{M}} \star G^{\rceil}](t, t'), \quad (14a)$$

$$G^{\lceil}(\tau, t')\left[\frac{1}{i}\frac{\overleftarrow{d}}{dt'} - h_o^\dagger(t')\right] = [G^{\lceil} \cdot \Sigma^{\mathrm{A}} + G^{\mathrm{M}} \cdot \Sigma^{\lceil}](t, t'). \quad (14b)$$

The Matsubara correlators $X^{\mathrm{M}}(\tau, \tau') \equiv X(-i\tau, -i\tau')$ satisfy the Dyson equation $G^{\mathrm{M}} = G_0^{\mathrm{M}} + G_0^{\mathrm{M}} \star \Sigma^{\mathrm{M}} \star G^{\mathrm{M}}$. This equation is decoupled from the left, right, lesser, and greater NEGF, and its solution provides the initial values for the dissipative KBE [19,72].

Two-particle loss—We say that the system experiences n-body losses (gains) if the Lindblad operators $\hat{L}_\gamma$ are polynomials of order n in the annihilation (creation) field operators. For $n > 1$ the analytic solution is, in general, not available. We here show how to tackle the problem by extending the many-body diagrammatic method. For the sake of definiteness we consider the set of Lindblad operators $\hat{L}_\gamma = a^\gamma_{mn}\hat{d}_m\hat{d}_n$ (two-particle loss), with $a^\gamma_{mn} = \pm a^\gamma_{nm}$ for bosons or fermions. These dissipators are relevant in the context of exciton-polariton systems [85,86]. Higher order loss and gain dissipators can be treated similarly. After some algebraic manipulation the operator in Eq. (5) can be expressed as

$$\hat{H}(\bar{z}, \bar{z}^*) = \hat{H}(\bar{z}) - \frac{1}{2}\int_C d\bar{z}' v^{2\mathrm{p}}_{ijmn}(\bar{z}, \bar{z}') \times \hat{d}_i^\dagger(\bar{z}^+)\hat{d}_j^\dagger(\bar{z}^+)\hat{d}_m(\bar{z}')\hat{d}_n(\bar{z}'), \quad (15)$$

where $v^{2\mathrm{p}}_{ijmn}(z, z') = iv^{2\mathrm{p}}_{ijmn}(t)[s(z)\delta(z', z) + 2\theta_+(z)\delta(z', z^*)]$ and $v^{2\mathrm{p}}_{ijmn}(t) = 2a^{\gamma *}_{ji}(t)a^\gamma_{mn}(t) = \pm v^{2\mathrm{p}}_{jimn}(t) = \pm v^{2\mathrm{p}}_{ijnm}(t)$.

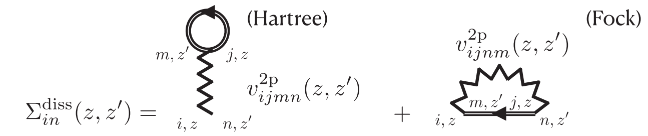

FIG. 1. Dissipation-induced self-energy diagrams—oriented double lines represent G and zigzag lines represent $v^{2\mathrm{p}}$. The $(\pm)$ prefactor of the Hartree diagram can be reabsorbed as $\pm v^{2\mathrm{p}}_{ijmn} = v^{2\mathrm{p}}_{ijnm}$, hence $\Sigma^{\mathrm{H}} = \Sigma^{\mathrm{F}}$. It is readily seen that this property holds true at any order.

The second term in Eq. (15) is quartic in the field operators and can be treated perturbatively, leading again to a Dyson equation. Unlike physical, e.g., Coulomb, interactions the contour-times z and z' are shared by two creation $(\hat{d}^\dagger\hat{d}^\dagger)$ and annihilation $(\hat{d}\,\hat{d})$ operators rather than by particle-hole-like operators $(\hat{d}^\dagger\hat{d})$. This fact gives rise to slightly different self-energy diagrams, with examples provided in Fig. 1. This difference is crucial to show that the number of topological equivalent diagrams of order k is the same as for Coulomb-like interactions, i.e., $2^k k!$, despite $v^{2\mathrm{p}}(z, z')$ being not symmetric under the exchange $z \leftrightarrow z'$, see the Appendix for the explicit proof. Thus the prefactors of the Feynman diagrams are the same as in ordinary many-body perturbation theory. Taking into account the (anti)symmetry properties of $v^{2\mathrm{p}}$, the Hartree (tadpole) and Fock (oyster) diagrams in Fig. 1 are identical, i.e., $\Sigma^{\mathrm{H}} = \Sigma^{\mathrm{F}} = \frac{1}{2}\Sigma^{\mathrm{HF}}$ with

$$\begin{aligned}\Sigma^{\mathrm{HF}}_{in}(z, z') &= \mp 2iv^{2\mathrm{p}}_{ijmn}(z, z')G_{mj}(z', z^+) \\ &= -2i[s(z)\delta(z', z) + 2\theta_+(z)\delta(z', z^*)] \\ &\quad \times v^{2\mathrm{p}}_{ijmn}(t)\rho^<_{mj}(t).\end{aligned} \quad (16)$$

At the Hartree-Fock (HF) mean-field level the rhs of the EOM Eq. (8) is modified by the addition of $\int_C d\bar{z}\,\Sigma^{\mathrm{HF}}(z, \bar{z})G(\bar{z}, z')$. Remarkably, this term renormalizes $\ell^>$ according to $\ell^>_{in}(t) \to \ell^>_{in}(t) + 2v^{2\mathrm{p}}_{ijmn}(t)\rho^<_{mj}(t)$, while it leaves $\ell^<$ unchanged, see appendix material for details on the derivation. Such asymmetry is due to the absence of two-body gain. Had we included Lindblad operators of the form $\hat{L}_\gamma = b^{\gamma *}_{mn}\hat{d}_n^\dagger\hat{d}_m^\dagger$ we would have found a similar renormalization for $\ell^<$. We infer that the mean-field treatment of two-body loss and gain is equivalent to considering one-body loss and gain.

Particle-hole loss—The treatment of mixed Lindblad operators, containing both $\hat{d}$ and $\hat{d}^\dagger$, deserves a separate discussion, but it does not pose a conceptual problem [87]. Let us consider the set $\hat{L}_\gamma = a^\gamma_{mn}\hat{d}_m^\dagger\hat{d}_n$ (particle-hole loss). As these dissipators are relevant in the context of phonon-induced relaxation of hot electrons in solids [89,90] we focus on the fermionic case. The normal-ordered form of the operator in Eq. (5) reads

$$\hat{H}(\bar{z},\bar{z}^*) = \hat{H}(\bar{z}) - is(\bar{z})V^{\mathrm{ph}}_{mn}(\bar{t})\hat{d}^\dagger_m(\bar{z})\hat{d}_n(\bar{z}) + \frac{1}{2}\int_C d\bar{z}' v^{\mathrm{ph}}_{ijmn}(\bar{z},\bar{z}')\hat{d}^\dagger_i(\bar{z}'^+)\hat{d}^\dagger_j(\bar{z}^+)\hat{d}_m(\bar{z})\hat{d}_n(\bar{z}'), \tag{17}$$

where $v^{\mathrm{ph}}_{ijmn}(z,z') = v^{\mathrm{ph}}_{ijmn}(t)[-is(z)\delta(z',z) + 2i\theta_-(z)\delta(z',z^*)]$, with $v^{\mathrm{ph}}_{ijmn}(t) = 2a^{\gamma*}_{ni}(t)a^{\gamma}_{jm}(t)$, and $V^{\mathrm{ph}}_{mn}(t) = \frac{1}{2}v^{\mathrm{ph}}_{mjnj}(t)$. The V^{ph} term renormalizes the one-particle Hamiltonian in Eqs. (8) according to $\tilde{h}(z) \to \tilde{h}(z) - is(z)V^{\mathrm{ph}}(t)$, but it does not renormalize the function $\ell(z)$. We now show that the mathematical structure of the dissipative KBE is recovered when treating v^{ph} at the HF mean-field level.

For simplicity we take $a^{\gamma*}_{mn} = a^{\gamma}_{nm}$. The diagrams with v^{ph} interaction lines are standard since the contour times z and z' are shared by particle-hole-like operators [91]. The Hartree (tadpole) diagram is easily shown to vanish whereas the Fock diagram yields

$$\Sigma^{\mathrm{F}}_{in}(z,z') = \frac{i}{2}[v^{\mathrm{ph}}_{ijnm}(z,z') + v^{\mathrm{ph}}_{ijnm}(z',z)]G_{mj}(z,z'^+) = s(z)v^{\mathrm{ph}}_{ijnm}(t)[\delta(z',z) - \delta(z',z^*)]G_{mj}(z,z'^+). \tag{18}$$

Let us discuss how this term affects the dissipative KBE, refer to appendix material for details on the calculations. The rhs of Eq. (8a) is modified by the addition of $\int_C d\bar{z}\,\Sigma^{\mathrm{F}}(z,\bar{z})G(\bar{z},z')$, the lesser component of which ($z = t_-$, $z' = t'_+$) reads $2iW^<(t)G^{\mathrm{A}}(t,t')$ where $W^<_{ij}(t) = \frac{1}{2}v^{\mathrm{ph}}_{ipjq}(t)\rho^<_{qp}(t)$. This term, together with the V^{ph}-renormalization of $\tilde{h}$, leads to a noninteracting dissipative KBE for $G^<$ with one-body loss and gain renormalized according to $\ell^{\lessgtr} \to \ell^{\lessgtr} + W^{\lessgtr}$, where $W^> = V^{\mathrm{ph}} - W^<$. Similarly, the rhs of Eq. (8b) is modified by the addition of $\int_C d\bar{z}G(z,\bar{z})\Sigma^{\mathrm{F}}(\bar{z},z')$, the greater component of which ($z = t_+$, $z' = t'_-$) reads $-2iG^{\mathrm{R}}_{in}(t,t')W^>_{nj}(t') + 2iG^>_{in}(t,t')V^{\mathrm{ph}}_{nj}(t')$. Taking into account the V^{ph} renormalization of $\tilde{h}$ we find a noninteracting dissipative KBE for $G^>$ with the *same* renormalized $\ell^{\lessgtr}$ as for $G^<$. Once again, although through a different path, the mean-field treatment reduces the problem to considering one-body loss and gain.

Beyond mean-field—The self-energy diagrams do, in general, contain both physical and dissipation-induced interaction lines. Let us inspect the structure of the total self-energy as a correlator on the Keldysh contour. In Supplemental Material [64] we show that the total self-energy can be written as $\Sigma = \Sigma^{\mathrm{HF}} + \Sigma^{\mathrm{corr}}$, where Σ^{HF} is the sum of all HF contributions and Σ^{corr} satisfies the Keldysh properties. Therefore the Langreth rules remain unchanged and the dissipative KBE are still given by Eqs. (9) and (10) with mean-field renormalized $\ell^{\lessgtr}$ and with $\Sigma \to \Sigma^{\mathrm{corr}}$.

Conclusions–The second-quantization approach of NEGF theory has been extended to dissipative Lindbladian dynamics. We have shown how to derive the MSH for the n-particle NEGF and established the dissipative KBE for $G^{\lessgtr}$. We have generalized the diagrammatic rules for approximate treatments, derived the EOM at the mean-field level, and elucidated the structure of the total self-energy as a correlator on the Keldysh contour. The dissipative KBE open the door to studies of transient phenomena and time-resolved spectra of open systems. Their applications span a wide range, from transport responses of diffusive nanoscale systems [92–94] to optical [95,96] and electronic [97] properties of materials in cavity quantum electrodynamics, as well as quantum computing dynamics in solid-state devices [98]. The dissipative KBE also offer an alternative method to solving the Lindblad equation, complementing methods such as the matrix product operator ansatz [99], quantum Monte Carlo [100], and third quantization [101]. Noteworthy, they can deal with time-dependent Hamiltonians and time-dependent Lindblad operators with no additional numerical complexity compared to their time-independent counterparts. Moreover, they can be readily implemented in available KBE codes [55,71,102,103].

We hope that our contribution inspires further developments in the theory of many-body dissipative dynamics and stimulates first-principles studies of driven correlated open systems.

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End Matter

Appendix: Dissipative KBE—The adjoint of Eqs. (9) and (10) follow from the interacting version of Eqs. (8), and read

$$\left[i\frac{d}{dt} - h_o(t)\right]G^>(t,t') + 2i\ell^>(t)G^{\rm A}(t,t') = [\Sigma^> \cdot G^{\rm A} + \Sigma^{\rm R}\cdot G^>](t,t'), \tag{A1}$$

$$G^<(t,t')\left[\frac{1}{i}\frac{\overleftarrow{d}}{dt'} - h_o^\dagger(t')\right] \pm 2iG^{\rm R}(t,t')\ell^<(t') = [G^< \cdot \Sigma^{\rm A} + G^{\rm R}\cdot\Sigma^<](t,t'). \tag{A2}$$

Acting with $[i(d/dt) - h_o(t)]$ on the retarded NEGF we then find

$$\left[i\frac{d}{dt} - h_o(t)\right]G^{\rm R}(t,t') = \delta(t,t') + \theta(t,t')\left[i\frac{d}{dt} - h_o(t)\right](G^>(t,t') - G^<(t,t')). \tag{A3}$$

To evaluate the rhs we use Eqs. (A1) and (9). Taking into account that $\theta(t,t')G^{\rm A}(t,t') = 0$ and that $\Sigma^> - \Sigma^< = \Sigma^{\rm R} - \Sigma^{\rm A}$ as well as $G^> - G^< = G^{\rm R} - G^{\rm A}$ we obtain Eq. (11). Similarly we can derive the EOM for $G^{\rm A}$:

$$\left[i\frac{d}{dt} - h_o^\dagger(t)\right]G^{\rm A}(t,t') = \delta(t,t') + [\Sigma^{\rm A}\cdot G^{\rm A}](t,t'). \tag{A4}$$

Subtracting Eq. (A2) from Eq. (9) we obtain

$$\begin{aligned}&\left(i\frac{d}{dt} + i\frac{d}{dt'}\right)G^<(t,t') - h_o(t)G^<(t,t') + G^<(t,t')h_o^\dagger(t')\\ &\pm 2i\ell^<(t)G^{\rm A}(t,t') \mp 2iG^{\rm R}(t,t')\ell^<(t')\\ &\quad= [G^<\cdot\Sigma^{\rm A} + G^{\rm R}\cdot\Sigma^< - \Sigma^<\cdot G^{\rm A} - \Sigma^{\rm R}\cdot G^<](t,t').\end{aligned} \tag{A5}$$

Taking into account that $G^{\rm R}(t^+,t) = -i$ [and hence $G^{\rm A}(t,t^+) = i$] we see that the left and right limits $t' \to t$ of Eq. (A5) are identical. In both limits the second line yields $\mp 2\ell^<(t)$, and Eq. (12) is recovered.

For $\Sigma = 0$ we can easily show that Eq. (13) is a solution of the noninteracting dissipative KBE. Using Eqs. (11) and (A4) we find (omitting the dependence on t and t')

$$i\frac{d}{dt}G^< = \pm(h_o G^{\rm R} + \delta)\rho^< \mp i(-ih_o\rho^< + i\rho^< h_o^\dagger + 2\ell^<)G^{\rm A} \mp \rho^<(h_o^\dagger G^{\rm A} + \delta).$$

The terms containing $h_o^\dagger$ and the δ function cancel and we recover Eq. (9). A similar proof holds for the greater component.

Many-body theory for two-body losses For two-particle losses we have $\hat{L}_\gamma = a^\gamma_{mn}\hat{d}_m\hat{d}_n$ and the operator in Eq. (5) reads

$$\begin{aligned}\hat{H}(z,z^*) &= \hat{H}(z) + a^{\gamma *}_{ji}(t)a^\gamma_{mn}(t)[-is(z)\hat{d}^\dagger_i(z)\hat{d}^\dagger_j(z)\hat{d}_m(z)\hat{d}_n(z) - 2i\theta_+(z)\hat{d}^\dagger_i(z)\hat{d}^\dagger_j(z)\hat{d}_m(z^*)\hat{d}_n(z^*)] \\ &= \hat{H}(z) - i\int dz' \frac{v^{\rm 2p}_{ijmn}(t)}{2}[s(z)\delta(z',z) + 2\theta_+(z)\delta(z',z^*)]\hat{d}^\dagger_i(z^+)\hat{d}^\dagger_j(z^+)\hat{d}_m(z')\hat{d}_n(z'), \qquad (A6)\end{aligned}$$

which is identical to Eq. (15). It is interesting to compare the dissipation-induced interaction with a physical, e.g., Coulomb, interaction

$$\hat{H}_{\rm int}(z) = \int dz' \frac{v^{\rm Coul}_{ijmn}(z,z')}{2}\hat{d}^\dagger_i(z^+)\hat{d}^\dagger_j(z'^+)\hat{d}_m(z')\hat{d}_n(z), \qquad (A7)$$

where $v^{\rm Coul}_{ijmn}(z,z') = \delta(z',z)v^{\rm Coul}_{ijmn}$. In Eq. (A6) the annihilation operators are evaluated in z' whereas the creation operators are evaluated in z. In Eq. (A7) we instead have a particle-hole operator in z' and another in z. Although the topology of the diagrams is identical the position of the contour times is different. For Coulomb interactions the self-energy diagrams in Fig. 1 have the orbital index n at time z and j at time z'.

Next we discuss the Feynman rules for the Green's function diagrams. To first order the expansion of $G_{ab}(z_a,z_b)$ in powers of $v^{\rm 2p}$ yields four contributions, whose diagrammatic representation is given in Fig. 2. The relabeling $i \leftrightarrow j$ and $m \leftrightarrow n$ is equivalent to a mirroring of the interaction line and maps the right diagrams onto the left diagrams since $v^{\rm 2p}_{ijmn}(t) = v^{\rm 2p}_{jinm}(t)$. For a kth order diagram we have 2^k mirrorings and $k!$ permutations of the $v^{\rm 2p}$ lines giving rise to topologically equivalent diagrams

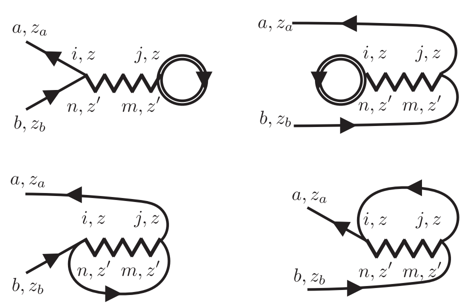

FIG. 2. First-order Green's function diagrams for a dissipation-induced interaction due to two-body losses.

with the same numerical value. Therefore we only need to consider diagrams with different topology and multiply by $2^k k!$, a procedure identical to that used for Coulomb interactions [19].

Let us show that $\Sigma^{\rm HF}$ in Eq. (16) gives rise to noninteracting dissipative EOM with $\ell^>(t)$ renormalized by the quantity $\ell^{{\rm HF},>}_{in}(t) \equiv 2v^{\rm 2p}_{ijmn}(t)\rho^<_{mj}(t)$. We have

$$\begin{aligned}&\int_C d\bar{z}\Sigma^{\rm HF}_{in}(z,\bar{z})G_{np}(\bar{z},z') \\ &= -i\ell^{{\rm HF},>}_{in}(t)\int_C d\bar{z}[s(z)\delta(\bar{z},z) + 2\theta_+(z)\delta(\bar{z},z^*)]G_{np}(\bar{z},z') \\ &= -i\ell^{{\rm HF},>}_{in}(t)[s(z)G_{np}(z,z') + 2\theta_-(z^*)G_{np}(z^*,z')],\end{aligned}$$

where in the last equality we use $\theta_+(z) = \theta_-(z^*)$. Thus, the HF approximation is equivalent to add $-is(z)\ell^{{\rm HF},>}(t)$ to $\tilde{h}(z)$, and $\theta_-(z^*)\ell^{{\rm HF},>}(t)$ to $\ell(z^*)$ in Eq. (8a). This is equivalent to renormalize $\ell^> \to \ell^> + \ell^{{\rm HF},>}$.

Many-body theory for particle-hole losses For particle-hole losses we have $\hat{L}_\gamma = a^\gamma_{mn}\hat{d}^\dagger_m\hat{d}_n$ and the operator in Eq. (5) reads

$$\begin{aligned}\hat{H}(z,z^*) = \hat{H}(z) &+ a^{\gamma *}_{ji}(t)a^\gamma_{mn}(t) \\ &\times [-is(z)\hat{d}^\dagger_i(z)\hat{d}_j(z)\hat{d}^\dagger_m(z)\hat{d}_n(z) \\ &+ 2i\theta_-(z)\hat{d}^\dagger_i(z^*)\hat{d}_j(z^*)\hat{d}^\dagger_m(z)\hat{d}_n(z)].\end{aligned}$$

In the first line all operators are evaluated at the same contour time and therefore $\hat{d}_j(z)\hat{d}^\dagger_m(z)\hat{d}_n(z) = \delta_{jm}\hat{d}_n(z) + \hat{d}^\dagger_m(z)\hat{d}_n(z)\hat{d}_j(z)$. By definition, z and z^* cannot coincide and the operators in the second line are reordered according to $\hat{d}_j(z^*)\hat{d}^\dagger_m(z)\hat{d}_n(z) = \hat{d}^\dagger_m(z)\hat{d}_n(z)\hat{d}_j(z^*)$. After the reordering $\hat{H}(z,z^*)$ becomes identical to Eq. (17). Comparing the dissipation-induced interaction with a physical, e.g., Coulomb, interaction, see Eq. (A7), we see that they have the same mathematical structure. Thus, the diagrams and the corresponding Feynman rules are the same in both cases.

Taking into account that the Hartree term vanishes the interacting version of the EOM at the HF level is given by Eqs. (8) with

$$\tilde{h}(z) \to \tilde{h}(z) - is(z)V^{\mathrm{ph}}(t) \\ = \begin{cases} h(t) - i\ell^{>}(t) + i\ell^{<}(t) - iV^{\mathrm{ph}}(t) & z = t_- \\ h(t) + i\ell^{>}(t) - i\ell^{<}(t) + iV^{\mathrm{ph}}(t) & z = t_+ \end{cases},$$

and with a rhs modified by the addition of $\int_C d\bar{z}\Sigma^{\mathrm{F}}(z,\bar{z})G(\bar{z},z')$ for Eq. (8a) and $\int_C d\bar{z}G(z,\bar{z})\Sigma^{\mathrm{F}}(\bar{z},z')$ for Eq. (8b).

Using the explicit form of Σ^{F} in Eq. (18) we find

$$\int_C d\bar{z}\Sigma^{\mathrm{F}}_{in}(z,\bar{z})G_{nj}(\bar{z},z') = is(z)\underbrace{v^{\mathrm{ph}}_{ipnq}(t)\rho^{<}_{qp}(t)}_{2W^{<}_{in}(t)} \\ \times [G_{nj}(z,z') - G_{nj}(z^*,z')]. \tag{A8}$$

Setting $z = t_-$ and $z' = t_+$ the square bracket in Eq. (A8) becomes $G^{<} - G^{\bar{\mathrm{T}}} = G^{\mathrm{A}}$. Therefore, the KBE for $G^{<}$ reads (omitting the dependence on t and t')

$$\left[i\frac{d}{dt} - (h - i\ell^{>} + i\ell^{<} - iV^{\mathrm{ph}})\right]G^{<} + 2i\ell^{<}(G^{<} - G^{\mathrm{A}}) \\ = 2iW^{<}G^{\mathrm{A}}. \tag{A9}$$

Comparing this result with Eq. (9) we infer that the HF approximation yields a noninteracting dissipative KBE with renormalized $\ell^{<} \to \ell^{<} + W^{<}$ and $\ell^{>} \to \ell^{>} + V^{\mathrm{ph}} - W^{<} = \ell^{>} + W^{>}$. We could alternatively derive this result through a direct comparison between Eqs. (A8)–(A9) and Eq. (8a).

The greater component of the adjoint EOM confirms the well-designed nature of the formalism. Using again the explicit form of Σ^{F} in Eq. (18) we find

$$\int_C d\bar{z}G_{in}(z,\bar{z})\Sigma^{\mathrm{F}}_{nj}(\bar{z},z') \\ = G_{in}(z,z')s(z')v^{\mathrm{ph}}_{npjq}(t')G_{qp}(z',z'^{+}) \\ + G_{in}(z,z'^{*})s(z'^{*})v^{\mathrm{ph}}_{npjq}(t')G_{qp}(z'^{*},z'^{+}). \tag{A10}$$

Setting $z = t_+$ and $z' = t'_-$ Eq. (A10) becomes

$$[G\Sigma^{\mathrm{F}}]^{>}_{ij}(t,t') = 2iG^{>}_{in}(t,t')W^{<}_{nj}(t') + 2iG^{\bar{\mathrm{T}}}_{in}(t,t')W^{>}_{nj}(t') \\ = 2iG^{>}_{in}(t,t')V^{\mathrm{ph}}_{nj}(t') - 2iG^{\mathrm{R}}_{in}(t,t')W^{>}_{nj}(t'),$$

where we use that $G_{qp}(t'_+,t'^{+}_-) = G^{>}_{qp}(t',t') = i(\rho^{<}_{qp} - \delta_{qp})$ and hence

$$v^{\mathrm{ph}}_{npjq}(t')G^{>}_{qp}(t',t') = 2iW^{<}_{nj}(t') - 2iV^{\mathrm{ph}}_{nj}(t') = -2iW^{>}_{nj}(t').$$

We conclude that the KBE for $G^{>}$ reads (omitting the dependence on t and t')

$$G^{>}\left[\frac{1}{i}\frac{\overleftarrow{d}}{dt'} - (h - i\ell^{>} + i\ell^{<} - iV^{\mathrm{ph}})\right] - 2i(G^{>} - G^{\mathrm{R}})\ell^{>} \\ = 2iG^{>}V^{\mathrm{ph}} - 2iG^{\mathrm{R}}W^{>}.$$

Comparing this result with Eq. (10) we again find a noninteracting dissipative KBE with the same renormalization of $\ell^{\lessgtr}$ as for $G^{<}$.