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Wigner–Lindblad Equations for Quantum Friction

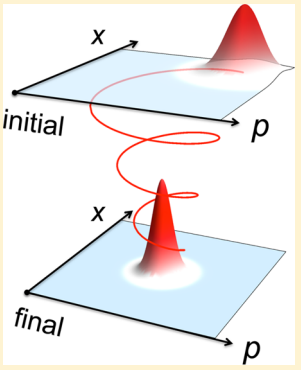
Denys I. Bondar,*[,†] Renan Cabrera,[†] Andre Campos,[†] Shaul Mukamel,[‡] and Herschel A. Rabitz[†]

[†]Princeton University, Princeton, New Jersey 08544, United States

[‡]University of California, Irvine, California 92697, United States

Supporting Information

ABSTRACT: Dissipative forces are ubiquitous and thus constitute an essential part of realistic physical theories. However, quantization of dissipation has remained an open challenge for nearly a century. We construct a quantum counterpart of classical friction, a velocity-dependent force acting against the direction of motion. In particular, a translationary invariant Lindblad equation is derived satisfying the appropriate dynamical relations for the coordinate and momentum (i.e., the Ehrenfest equations). Numerical simulations establish that the model approximately equilibrates. These findings significantly advance a long search for a universally valid Lindblad model of quantum friction and open opportunities for exploring novel dissipation phenomena.



Realistic models of quantum systems must include dissipative interactions with an environment, which may vary from a vacuum to a generic thermal bath. Nevertheless, construction of physically consistent quantum models of dissipative forces has been a long-standing problem since the birth of quantum mechanics (see, e.g., refs 1−4). A common framework for describing open quantum systems is to represent the state of the system by a density matrix, whose evolution is governed by the Lindblad equation.[5,6] In this Letter, we construct a model of quantum friction, whose classical counterpart is a velocity-dependent force acting against the particle's motion.

By employing the phase space representation of quantum mechanics,[7−9] where an observable $O = O(x,p)$ is assumed to be a real-valued function of coordinate x and momentum p and the system's state is represented by the Wigner function $W = W(x,p)$, we derive the Lindblad–Wigner equation

$$\frac{\mathrm{d}}{\mathrm{d}t}W = -\frac{\mathrm{i}}{\hbar}(H\bigstar W - W\bigstar H) + D[W] + D'[W] \tag{1}$$

$$H = p^2/(2m) + U(x) \tag{2}$$

$$D[W] = \frac{2\gamma}{\hbar}\left(A\bigstar W\bigstar A^* - \frac{1}{2}W\bigstar A^*\bigstar A - \frac{1}{2}A^*\bigstar A\bigstar W\right) \tag{3}$$

$$D'[W] = \frac{2\mathcal{D}}{\hbar^2}\left(x\bigstar W\bigstar x - \frac{1}{2}W\bigstar x\bigstar x - \frac{1}{2}x\bigstar x\bigstar W\right) = \mathcal{D}\frac{\partial^2 W}{\partial p^2} \tag{4}$$

$$\bigstar = \exp\frac{\mathrm{i}\hbar}{2}\left(\frac{\overleftarrow{\partial}}{\partial x}\frac{\overrightarrow{\partial}}{\partial p} - \frac{\overleftarrow{\partial}}{\partial p}\frac{\overrightarrow{\partial}}{\partial x}\right) \tag{5}$$

which guarantees completely positive dynamics of the density matrix underlying the Wigner function W for an arbitrary operator A. In standard derivations, one finds a family of relaxation operators A by assuming a weak coupling to a bath and expanding the dynamics perturbatively. Here we adopt a different strategy: We require that the first moments of W satisfy the Ehrenfest equations

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle x\rangle = \frac{1}{m}\langle p\rangle \tag{6}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle p\rangle = -\langle U'(x)\rangle - 2\gamma\langle \mathrm{sign}(p) f(|p|)\rangle \tag{7}$$

characterizing motion of a particle of mass m interacting with an environment-induced velocity-dependent friction. The conventional derivations of master equations (see Figure 1) do not guarantee satisfaction of these relations. Using the operational dynamical modeling (ODM) algorithm to be described below, we construct an operator A that satisfies constraints 6 and 7

$$A = \sqrt{Lf\left(|p| + \frac{\hbar}{2L}\right)}\exp(-\mathrm{i}\,\mathrm{sign}(p)x/L) \tag{8}$$

The classical limit of the Lindblad–Wigner equation (eq 1) with eq 8 recovers the appropriate Fokker–Planck equation[10]

$$D[W] = 2\gamma\frac{\partial}{\partial p}[\mathrm{sign}(p) f(|p|) W] + O(\hbar) \tag{9}$$

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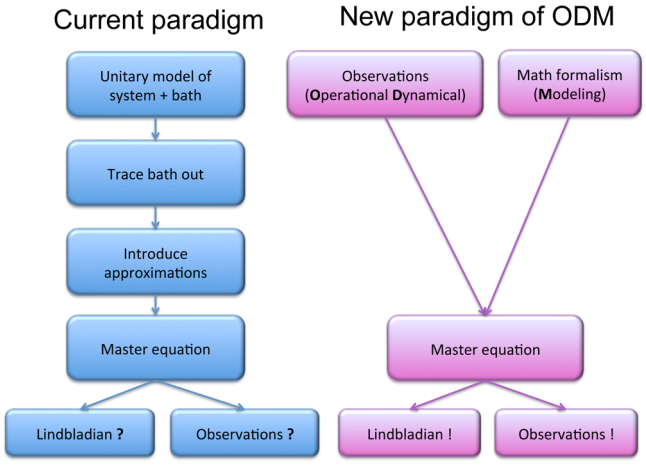

Figure 1. Current paradigm for deriving master equations governing open system dynamics versus proposed novel approach of operational dynamic modeling (ODM).

The Ehrenfest relations for the second moments may also be obtained from eq 1:

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle p^2\rangle = -2\langle pU'(x)\rangle - 2\gamma\left\langle f(|p|)\left(2|p| - \frac{\hbar}{L}\right)\right\rangle + 2\mathcal{D} \tag{10}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle xp\rangle = \frac{1}{m}\langle p^2\rangle - \langle xU'(x)\rangle - 2\gamma\langle \mathrm{sign}(p)f(|p|)x\rangle \tag{11}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle x^2\rangle = \frac{2}{m}\langle xp\rangle + \frac{\gamma\hbar L}{2}\left\langle \frac{f'(|p|)^2}{f(|p|)}\right\rangle \tag{12}$$

To employ eq 1, the following free parameters must be specified: (i) $f(p) \geq 0$, the velocity dependence of the dissipative force; (ii) $\gamma \geq 0$, a friction coefficient; (iii) $L > 0$, a length-scale constant defining the dynamics of second-order moments (eqs 10−12); and (iv) $\mathcal{D} \geq 0$, a dephasing constant chosen such that dynamics equilibrates to the Boltzmann state with some temperature.

Equation 5 defines the Moyal product,[7−9] which is a result of mapping the noncommutative matrix product in the Hilbert space into the phase space. As a result, dissipator 3 is obtained by Wigner transforming the Lindblad equation for the density matrix; thus, the Wigner function's marginals stay positive throughout the entire evolution. Dissipator 4 describes dephasing, the loss of quantum coherence,[1,11,12] whereas the dissipator 3 causes amplitude damping. The usage of sign and modulus functions in eqs 8 and 7 are necessary to ensure that the friction force acts against the particle's motion. Dissipator 3 is translationally invariant (more precisely, Galilei-covariant): a spatial displacement $W(x, p) \rightarrow W(x + c, p)$ implies $D[W](x, p) \rightarrow D[W](x + c, p)$. Numerical simulations establish that the long-time dynamics governed by eq 1 rigorously does not equilibrate; however, the dynamics can be said to approximately equilibrate. Namely, one can find a value of the dephasing constant $\mathcal{D}$ in eq 4 such that the steady state closely resembles the Boltzmann state with temperature T. In this sense, we numerically define the temperature dependence of $\mathcal{D} = \mathcal{D}(T)$.

Comparison with Other Theories. Current quantum friction models can be roughly divided into two categories: (i) Lindblad models not obeying the Ehrenfest relations have been proposed in refs 13−15. The fundamental reason for the Ehrenfest equation violation is the ubiquitous usage of A (eq 3), which is taken to be linear with respect to the coordinate and momentum (see the comment after eq 14). (ii) Non-Lindblad models obeying the Ehrenfest relations that preserve state's positivity for sufficiently high temperatures are discussed in refs 3 and 16−22. Contrary to the claims, the master equations in refs 23−25 belong to the same category. In particular, the model in ref 23 produces uncontrollable heating,[26,27] greatly spreading the wave packet. This state of the field is unsatisfactory because non-Lindblad master equations are known to lead to negative probabilities,[26,27] whereas the violation of the Ehrenfest equations lead to unphysical artifacts.[28]

A comparative review[29] of major quantum dissipation theories further revealed that no existing model is simultaneously (i) complete positive, (ii) translationally invariant, and (iii) asymptotically approaching thermal equilibrium. The present model (eq 1) exactly obeys the first two properties, whereas the latter can be satisfied approximately (this can be achieved exactly in the free particle case). Furthermore, our simulations confirm that the dynamics of our model does not cause uncontrollable spreading of the wave packet even at zero temperature and approaches thermal equilibrium at higher temperatures, thereby overcoming computational and physical inconsistencies plaguing other dissipative theories. Model 1 is obtained as a unique consequence of the Ehrenfest constrains (eqs 6 and 7) and the requirements for the dynamics to be Lindblad, translationary invariant, and state-independent [i.e., $A = A(x, p)$ in eq 3 does not depend on the Wigner function].

A difficulty of constructing physical models of quantized friction lies in fundamental limitations of the current paradigm for modeling open system dynamics (see Figure 1). First, the combined system and bath are assumed to evolve unitarily; second, the environmental degrees of freedom are traced out by making a number of approximations. This procedure neither guarantees that the resultant master equation can reproduce the observations characterizing phenomenon of interest nor that the equations have a desired mathematical structure.

It is noteworthy that the limitations of the current paradigm persist even if no approximation is necessary to trace the bath out. For example, the Hu−Paz−Zhang master equation[17−19] for a harmonic oscillator interacting with a linear passive heat bath of oscillators is exact under the assumption that the bath is initially at equilibrium and not coupled to the oscillator. The obtained non-Lindblad master equation preserves the density matrix's positivity and satisfies the Ehrenfest relations. However, the Hu−Paz−Zhang propagation of states initially uncorrelated with the environment leads to instantaneous infinite spreading of the wave packet,[30] which could be fixed by modulating the friction coefficient during the evolution.[31] Further revealed problems have led to the conclusion that the model is of very limited physical utility.[32]

To overcome these fundamental limitations, a new paradigm of ODM[33] has been recently put forth, enabling the generation of models directly from observed data (see Figure 1). To derive master equations, ODM needs two inputs: observed data recast in the form of Ehrenfest relations and a specified mathematical structure of the equation of motion. As an outcome, ODM guarantees that the resulting equations of motion have the desired physical structure to reproduce the supplied dynamical observations. This formalism has provided new interpretation of the Wigner function,[34] unveiled conceptual inconstancies in finite-dimensional quantum mechanics,[35] formulated dynamical

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models in topologically nontrivial spaces,[36] advanced the study of quantum-classical hybrids,[37] and led to development of efficient numerical techniques.[12,38]

Derivation. We begin by identifying the amplitude dumping dissipator $D[W]$ (eq 3); thus, the dephasing coefficient $\mathcal{D}$ is set to zero to ignore $D'[W]$ (eq 4). Substituting eq 1 into eqs 6 and 7 and then dropping the averaging, which is justified by A being state-independent, we obtain equations for an unknown function $A = A(x, p)$, defining the Lindblad dissipator (eq 3)

$$A^*\bigstar\frac{\partial A}{\partial p} - \frac{\partial A^*}{\partial p}\bigstar A = 0 \tag{13}$$

$$A^*\bigstar\frac{\partial A}{\partial x} - \frac{\partial A^*}{\partial x}\bigstar A = -4\mathrm{i}\,\mathrm{sign}(p) f(|p|) \tag{14}$$

The Lindblad models for Omic friction, $f(p) = |p|$, have been widely studied (see, e.g., refs 13, 14, 23, 24, 39, and 40), where A was found to be a linear combination of x and p. However, as we shall now establish, *no Lindblad dynamics with an A linear in x and p satisfies the Ehrenfest equations* (eqs 6 and 7). Indeed, substituting $A = ax + bp$ into eq 14 leads to

$$(a^*b - ab^*)x = 0, \quad (a^*b - ab^*)p = 4\mathrm{i}p \tag{15}$$

where a contradiction becomes evident. This conclusion holds in the case of Lindblad models with several such A operators. Our model (eq 8) circumvents this no-go result because of its new nonlinear dependence on x and p.

The action of the dissipative force is expected to be translationary invariant. One observes directly from the definition of the Moyal product (eq 5) that if

$$A(x, p) = g(p)\exp(\mathrm{i}Cx), \quad C^* = C \tag{16}$$

then the dissipator $D[W]$ (eq 3) is translationary invariant. Formally, the dissipator $D[W]$ with A given by eq 16 obeys

$$D[W] = F\left(p, \frac{\partial}{\partial x}, \frac{\partial}{\partial p}, \frac{\partial^2}{\partial x^2}, \frac{\partial^2}{\partial x \partial p}, \frac{\partial^2}{\partial p^2}, \cdots\right)W \tag{17}$$

where $\cdots$ denotes higher-order derivatives, and the function F explicitly does not depend on x. Additionally, eq 6 is satisfied for any real valued $g(p)$. Therefore, substituting the expansion

$$g(p) = \sum_{n=0}^{\infty} g_n(p)\hbar^n \tag{18}$$

into eqs 16 and 14, we recursively find all terms in expansion 18 (see the Supporting Information). Finally, the resultant series can be then summed up, thereby leading to the exact solution (eq 8) where L is a positive length-scale constant to balance the dimensionality. The value of L dictates the time-dynamics of second-order moments ([eqs 10−12).

A simple steady-state solution is found by additionally requiring the spatial homogeneity

$$\frac{\partial W}{\partial x} = 0, \quad \frac{\mathrm{d}W}{\mathrm{d}t} = 0, \quad U = 0, \quad \mathcal{D} = 0$$
$$\Rightarrow W = \mathrm{const}/f(|p|) \tag{19}$$

Therefore, if $f(p)$ is chosen to be inversely proportional to a thermal equilibrium state, the free particle dynamics of model 8 equilibrates without the need for the dephasing dissipator $D'[W]$ (eq 4).

Both quantum corrections in eqs 10 and 12, i.e., the terms proportional to $\hbar$, are position-independent, thereby reconfirming the translational invariance. According to eq 12, the quantum correction to Ohmic dissipation (with $f(p) = |p|$) is singular; therefore, the function $f(p)$ should be regularized. For example, we employ the following smoothing in numerical simulations (see, e.g., Figures 2−5)

$$f(p) = p^2/\sqrt{p^2 + \epsilon^2}, \quad \epsilon^2 = 0.5 \tag{20}$$

The Ehrenfest relations (eqs 6, 7, and 10−12) have been verified numerically for different values of parameters and initial conditions.

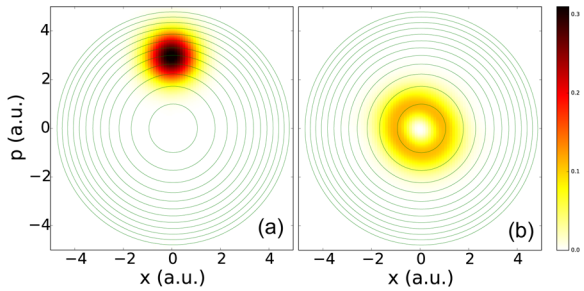

Figure 2. Initial (a) and final (b) Wigner functions for the harmonic oscillator evolving according to the model (eq 1) governing the Ohmic dissipation (with eq 20; γ = 0.07 au, L = 3 au, and $\mathcal{D} = 0$). The circular solid lines depict the level set of the Hamiltonian $H = (p^2 + x^2)/2$ au. Panel a shows the Wigner function of the ground state displaced along the momentum axis. The reached steady state (b) is not a Gaussian distribution.

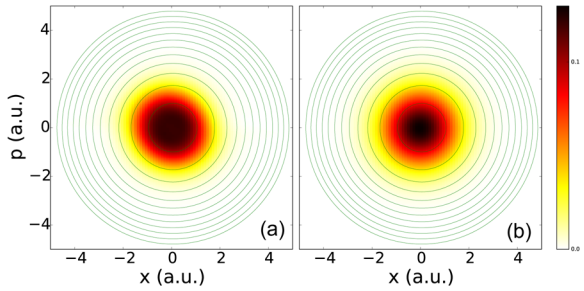

Figure 3. (a) Final Wigner function for the harmonic oscillator evolving according to the model (eq 1) governing the Ohmic dissipation (with eq 20; γ = 0.07 au, L = 3 au, and $\mathcal{D}$ = 0.0143 au). The circular solid lines depict the level set of the Hamiltonian $H = (p^2 + x^2)/2$ au. The initial Wigner function is shown in Figure 2a. Note that the steady state approaches the thermal Boltzmann state with kT = 1.166 au depicted in panel b.

Equation 12 establishes that the steady state need not coincide with thermal equilibrium. As an example, consider a harmonic oscillator. The equilibrium state is characterized by the identity $\langle xp\rangle = 0$, which contradicts the steady-state condition $\mathrm{d}\langle x^2\rangle/\mathrm{d}t = 0$ because the quantum correction in eq 12 is strictly positive. Furthermore, if the steady state is positive, then its Wigner function should be more pronounced in the second and fourth quadrants of the phase space (where $xp < 0$) to compensate for the quantum correction (this small asymmetry can be noticed in Figures 2b and 3a).

Figure 2 shows the initial state with average momentum p = 3 au (arbitrary units, $\hbar = m = 1$, are employed in the simulations) reaches the steady state with a circularly shaped

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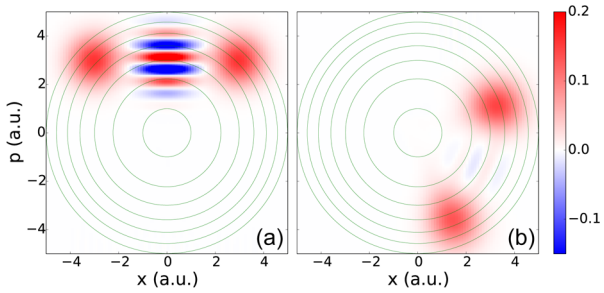

Figure 4. (a) Wigner function of the Schrödinger cat state at time t = 0. (b) Wigner function at later time t = 2 au after evolving according to the model (eq 1) governing the Ohmic dissipation (system's parameters are defined in Figure 3). As time progresses, the Wigner function's negativity vanishes and the state approaches the Boltzmann equilibrium shown in Figure 3b.

Wigner function. The latter has a characteristic asymmetry, as discussed above. The reached state does not resemble the Boltzmann thermal equilibrium.

To allow the dynamics to equilibrate approximately, we include the dephasing dissipator $D'[W]$ (eq 4) with a nonvanishing $\mathcal{D}$. In the case of a harmonic oscillator $[U(x) = m\omega^2 x^2/2]$, the fluctuation−dissipation theorem follows from the second-order Ehrenfest relations (eqs 10−12):

$$\frac{\mathcal{D}}{\gamma} = \left\langle f(|p|)\left(2|p| - \frac{\hbar}{L}\right) - \hbar L\left(\frac{m\omega}{2}\right)^2 \frac{f'(|p|)^2}{f(|p|)} \right\rangle_{\mathrm{st}} \qquad (21)$$

where $\langle\cdots\rangle_{\mathrm{st}}$ denotes averaging over a steady state.

The steady state for the model with $\mathcal{D} = 0.0143$ (au) is shown in Figure 3. For a sufficiently high value of $\mathcal{D}$, the ring in Figure 2b is washed out and the Wigner function of the steady state looks like a Gaussian (Figure 3a), which well approximates the Boltzmann equilibrium for some temperature (Figure 3b). The larger the dephasing coefficient $\mathcal{D}$, the more accurate the equilibration dynamics. Additionally, we have also verified that the approximate equilibration dynamics occurs in the case of anharmonic oscillators. Figure 4 establishes that the evolution generated by model 1 washes out the quantum interference initially present in the Schrödinger cat state, while the dynamics equilibrates.

Despite a simple look of the Wigner functions in Figures 2 and 3, full time-dependent dynamics are rich in quantum features. Figure 5 compares quantum dissipative dynamics, governed by the Lindblad−Wigner equation (eq 1), with the corresponding classical Fokker−Planck evolution (eq 9). Even though both quantum and classical master equations satisfy the same first-order Ehrenfest theorems (eqs 6 and 7), time evolution of the expectation values of the coordinate (Figure 5a) and momentum (Figure 5b) exhibit quantitative differences. Because the optical polarizability is proportional to $\langle x\rangle$, the predicted quantum corrections may be observed via nonlinear spectroscopy.[41] The correction to the second-order Ehrenfest theorems (eqs 10−12), enforcing the Heisenberg uncertainty priciple, qualitatively change open system dynamics (Figure 5c,d). As a result, the expectation value of energy in classical dissipative dynamics monotonically decreases, whereas energy revives in the quantum case at short time scales (Figure 5e).

Outlook. To describe quantum dissipative dynamics emerging in many areas of physics, there is a need for a Lindblad model satisfying the Ehrenfest relations (eqs 6 and 7, with long-time

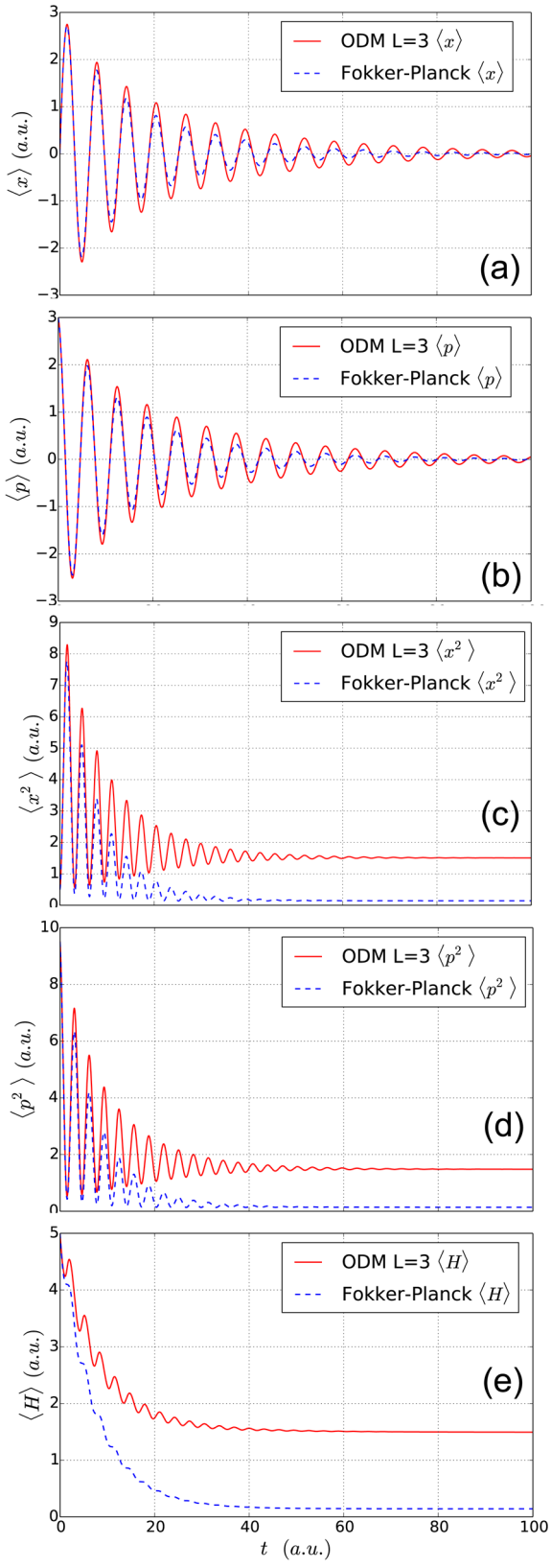

Figure 5. Quantum (solid red lines; eq 1) vs classical (dashed blue lines; eq 9) dissipative dynamic of a harmonic oscillator. Parameters for both systems are identical (parameters are specified in Figure 3). Time-evolution of the first-order (a, b) and second-order (c, d) moments; (e) total energy variation.

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dynamics converging to an equilibrium state. Currently, the lack of such a model has been substituted by a multitude of dissipative theories. Using ODM (Figure 1), we have found the translationally invariant Wigner−Lindblad model (eq 1) exactly obeying the Ehrenfest equations (eqs 6 and 7). Furthermore, according to numerical simulations, our model not only shows that a state with nonvanishing mean velocity (Figure 2a) approximately approaches the Boltzmann equilibrium (Figure 3) but also exhibits pronounced quantum corrections (Figure 5) even in the case of a harmonic oscillator.

The following Ehrenfest relation ubiquitously arises in molecular dynamics[41]

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle p\rangle(t) = -m\omega^2\langle x\rangle(t) - \int_{-\infty}^{t} \mathrm{d}\tau\, \gamma(t-\tau)\langle p\rangle(\tau) \tag{22}$$

where the time-dependent dissipation coefficient, $\gamma(t)$, is connected with the spectral density of the bath, which characterizes the nature of dissipative dynamics. Such a generalization of the developed model requires the application of ODM to non-Markovian dynamics. In this case, the Lindblad−Wigner equation (eq 1) will have to be replaced by a corresponding time-convolutionless master equation (see, e.g., ref 42), thus leading to a time-dependent extension of the relaxation operator (eq 8).

The presented derivation of the master equation directly from time evolution of expectation values embodied in Ehrenfest relations is a long-sought alternative to the current cumbersome paradigm for obtaining equations of motions (see Figure 1). A master equation is typically obtained by performing a number of approximations after the bath is traced out of a combined system−bath model. Such a derivation usually leads to either a non-Lindblad master equation or a model incapable of reproducing observations. The presented ODM-based derivation overcomes all these fundamental weaknesses by deriving Lindblad equations enforced to be compatible with the Ehrenfest equations. This formalism opens new horizons in quantum nonequilibrium statistical mechanics.

■ ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available free of charge on the ACS Publications website at DOI: 10.1021/acs.jpclett.6b00498.

Maple code for symbolic derivation of the main results of the paper (PDF)

■ AUTHOR INFORMATION

Corresponding Author

*E-mail: dbondar@princeton.edu.

Notes

The authors declare no competing financial interest.

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Supplementary material for "Wigner-Lindblad Equations for Quantum Friction"

Denys I. Bondar,[1,*] Renan Cabrera,[1] Andre Campos,[1] Shaul Mukamel,[2] and Herschel A. Rabitz[1]

[1] *Princeton University, Princeton, NJ 08544, USA*
[2] *University of California, Irvine, Irvine, CA 92697, USA*

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In deriving the main results of the paper, we have found very convenient the symbolic computational software Maple$^{\text{TM}}$ [1]. Thus, we provide below our full Maple codes used to derive and verify equations listed in the main text. The utility of the code lies beyond the discussed application and serves as a basis for symbolic derivations for quantum mechanics in phase space.

```
# Finding Lindblad friction force obeying Ehrenfest relations
restart;

# Sign of the momentum (p). Below p denotes abs(p).
# The whole code should be run twice: First time with sign_p := 1, second with sign_p := -1.
sign_p := 1;

# Number of quantum (hbar) corrections. The value of N is only limited by computer's performance
N := 5;

# Moyal product of two function A and B
MoyalStar := (A, B) -> add( (I*sign_p*hbar/2)^n /n! * add(
   binomial(n,k)*(-1)^k *diff(A,[p$k,x$(n-k)]) * diff(B,[x$k,p$(n-k)])
, k=0..n), n=0..N+1):

# Define the unknown dissipator (G must be real)
A := G*exp(-I*sign_p*x/L):
A_dagger := G*exp(+I*sign_p*x/L):

# Function generating LHS of the Ehrenfest relation for observable O
LHS := (O) -> taylor( 2*gamma/hbar*( MoyalStar(A_dagger,MoyalStar(O,A))
  - MoyalStar(MoyalStar(O,A_dagger),A)/2 - MoyalStar(A_dagger,MoyalStar(A,O))/2 ), hbar, N+2):

print("Verify the first Ehrenfest relation: ", simplify(LHS(x)));

# Find g[n] to satisfy the second Ehrenfest relation
G := add( g[n](p)*hbar^n, n=0..N):
Eq := LHS(p*sign_p) + 2*gamma*sign_p*f(p):

# Find the leading term
g[0](p) := solve(simplify(coeff(Eq, hbar, 0)), g[0](p))[1]:

# Find all quantum corrections iteratively
for n from 1 to N do
    g[n](p) := solve(simplify(coeff(Eq, hbar, n)), g[n](p)):
end do:
n := 'n':

# Compare the obtained result with the exact solution provided in the paper
A_exact := sqrt(L*f(p + hbar/(2*L)))*exp(-I*sign_p*x/L):
A_exact_dagger := sqrt(L*f(p + hbar/(2*L)))*exp(+I*sign_p*x/L):
```

*Electronic address: dbondar@princeton.edu

```
print("Verify the exact solution ",
    simplify(taylor( A_exact - A, hbar, N+1)),
    simplify(taylor( A_exact_dagger - A_dagger, hbar, N+1))
);

print("Classical limit of Linblandian");
simplify(taylor(
    2*gamma/hbar*( MoyalStar(A_exact, MoyalStar(W(x,p),A_exact_dagger))
    -MoyalStar(W(x,p), MoyalStar(A_exact_dagger, A_exact))/2
    -MoyalStar(A_exact_dagger, MoyalStar(A_exact, W(x,p)))/2 ),
hbar, 2));

print("Second order Ehrenfest relations");
print("d<p^2>/dt = ", simplify(LHS(p^2))) ;
print("d<xp>/dt = ", simplify(LHS(x*p*sign_p))) ;
print("d<x^2>/dt = ", simplify(LHS(x^2))) ;
```

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[1] http://www.maplesoft.com/products/maple/