Numerical method for integro-differential generalized Langevin and master equations

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We show that integro-differential generalized Langevin and non-Markovian master equations can be transformed into larger sets of ordinary differential equations. On the basis of this transformation we develop a numerical method for solving such integro-differential equations. Physically motivated example calculations are performed to demonstrate the accuracy and convergence of the method.

INTRODUCTION

Generalized Langevin equations (GLE) [1] and non-Markovian master equations [2, 3, 4], which arise in the treatment of systems interacting with environmental degrees of freedom, often have an integro-differential form. Unlike ordinary differential equations which can be readily solved using Runge-Kutta, Predictor-Corrector and other well known numerical schemes [5], there are no general methods for solving equations of integro-differential type. Here we show that these integro-differential equations can be converted to ordinary differential equations at the expense of introducing a new time variable which is treated as if it is of spatial type. [Similar schemes are employed to numerically solve the Schrödinger equation for time-dependent Hamiltonians [6] and as analytical tools [7]. There is also some resemblance to schemes for solving integro-differential equations of viscoelasticity [8].]

We then develop a numerical method based on this exact transformation and show that it can be used to accurately solve a variety of physically motivated examples.

Neglecting inhomogeneous terms resulting from noise, for simplicity, the generalized Langevin equations [1] for position \( q(t) \) and momentum \( p(t) \) of a damped oscillator in one dimension can be expressed in the form

\[
dq(t)/dt = \frac{p(t)}{m},
\]

\[
dp(t)/dt = -m\omega^2 q(t) - \int_{-\infty}^{t} \gamma(t, t') p(t') \ dt',
\]

where \( m \) and \( \omega \) are the mass and frequency of the oscillator and \( \gamma(t, t') \) is the memory function. Defining a space-like time variable \( u \) and a function

\[
\chi(t, u) = f(u) \int_{-\infty}^{t} \gamma(t + u, t') p(t') \ dt',
\]

it can be verified by direct substitution that \( p(t) \) and \( \chi(t, u) \) satisfy the following ordinary differential equations

\[
dp(t)/dt = -m\omega^2 q(t) - \chi(t, 0)
\]

\[
dx(t, u)/dt = f(u)\gamma(t + u, t)p(t) + \frac{\partial \chi(t, u)}{\partial u}
\]

\[
- f'(u) f(u) \chi(t, u). 
\]

Here we have introduced a differentiable damping function \( f(u) \) (with \( f(0) = 1 \)) which plays a useful role in the numerical scheme we will introduce to solve the ordinary differential equations [1, 4] and [3]. [Note that \( f'(u) = df(u)/du \)].

Neglecting inhomogeneous terms, non-Markovian master equations [2, 3, 4] can be written in the form

\[
\frac{d\rho(t)}{dt} = -i[H(t), \rho(t)] - \int_{-\infty}^{t} K(t, t') \rho(t') \ dt',
\]

where \( \rho(t) \) is the time-evolving reduced density matrix of the subsystem, \( H(t) \) is an effective Hamiltonian, and \( K(t, t') \) is a memory operator. [We employ units such that \( \hbar = 1 \).] Defining an operator

\[
\chi(t, u) = f(u) \int_{-\infty}^{t} K(t + u, t') \rho(t') \ dt',
\]

it can be verified by direct substitution that \( \rho(t) \) and \( \chi(t, u) \) satisfy ordinary differential equations

\[
\frac{d\rho(t)}{dt} = -i[H(t), \rho(t)] - \chi(t, 0)
\]

\[
\frac{d\chi(t, u)}{dt} = f(u)K(t + u, t)\rho(t) + \frac{\partial \chi(t, u)}{\partial u}
\]

\[
- f'(u) f(u) \chi(t, u). 
\]

Here \( f(u) \) is again a differentiable damping function such that \( f(0) = 1 \).

Thus, the integro-differential Langevin equations [1-4] can be expressed in the ordinary differential forms [1] and [4-6] and the integro-differential master equation [3] can be expressed as the ordinary differential equations [6-8]. To exploit these transformed equations as a practical numerical scheme we must discretize the \( u \) variable on a grid of points so that the number of ordinary differential equations is finite. Once this is achieved the ordinary differential equations can be solved using standard techniques [9]. We use an eighth order Runge-Kutta routine [10] in our calculations.

To minimize the number of grid points we choose a damping function \( f(u) \) which decreases rapidly with \( u \). In the calculations reported here we used \( f(u) = e^{-\mu u^2} \). In practice fewer grid points are needed for positive \( u \) than for negative \( u \), and we found that the points \( u_j =
which are displayed graphically in Figure 1. The solid curve is (12), the dashed is (13), the short-dashed is (14) and the dotted is (15). These memory functions were chosen to roughly represent the various functional forms which can occur physically\(^1\) and for ease in obtaining exact solutions. The constants appearing in equations (11), (14) and (15) are chosen as \(m = 1\) and \(\omega^2 = 10\). Figure 2 shows the functional form of the exact solutions \(q(t)\) (solid curve) and \(p(t)\) (dashed), which evolve from initial conditions \(q(0) = 1\) and \(p(0) = .1\), for memory function (12) over a timescale of 20 units with \(\Delta t = .04\). Solutions for the other memory functions (and the same initial conditions) are similar in appearance. These exact solutions were obtained by exploiting the fact that the above memory functions are sums of exponentials (i.e. \(W(t) = \sum_{j=1}^{\infty} a_j e^{-b_j t}\)) from which it follows that one may write

\[
dp{p}{t} = -ma_0 q(t) - \sum_{j=1}^{\infty} a_j e^{-b_j t} y_j(t) \tag{16}
\]

for \(j = 1, 2, \ldots\), and solve these ordinary differential equations using standard methods. This approach only works for memory functions of this type. Approximate solutions were obtained using \(g = 7/[(n - l)\Delta u]^2\). For negative \(u\) we set \(W(u) = W(\lvert u \rvert)\).

The negative logarithm of the absolute error in \(q(t)\),

\[
e(t) = -\log_{10} \lvert q(t) - q_{\text{approximate}}(t) \rvert, \tag{18}
\]

is shown in Figure 3 plotted against time for the values of \(n\) indicated in the inset. [The error in \(p(t)\) is similar.] As \(n\) increases \(e\) increases (on average) and hence the error decreases. The oscillations in \(e\) are caused by periodic intersections of the two solutions. In practice
it is impossible to visually distinguish the two solutions when \( \epsilon \geq 2 \). Note that after a short transient the error (on average) does not increase. This is probably a consequence of the linearity of these equations. Some decline in accuracy with time should be expected when the Langevin equations are non-linear (e.g. a particle in a double-well).

**FIG. 3: \( \epsilon(t) \) for memory function \( \sigma_z \).**

Figure 4 compares the exact solutions for \( q(t) \) (solid curve) and \( p(t) \) (short-dashed) with those obtained using our method for \( n = 150 \) (dashed and dotted, respectively) over a time of 40 units. No disagreement is visible. Convergence for memory function \( \sigma_z \) is similar.

**FIG. 4: Comparison of exact and approximate position and momentum of a damped oscillator.**

Memory functions \( \sigma_z \) and \( \sigma_x \) which take negative values and have long time tails require many grid points for convergence. Figure 5 shows the negative logarithm (base ten) of the absolute error in \( q(t) \) for this case. While many grid points are required, high accuracy solutions can clearly be obtained using our method.

For the master equation we chose an initial value problem consisting of a dissipative two-level system representing a spin interacting with environmental degrees of freedom. If the spin Hamiltonian is \( H = \frac{\omega}{2} \sigma_z + \beta \sigma_x \) and the coupling to the environment is proportional to \( \sigma_x \)

then the equation for the density matrix \( \rho(t) \) is of the form:\[\begin{align*}
\frac{d\rho(t)}{dt} &= -i\left[\frac{\omega}{2}\sigma_z + \beta \sigma_x, \rho(t)\right] \\
&\quad -C\int_0^t W(t-t')\{\sigma_x^2\rho(t') + \rho(t')\sigma_x^2 - 2\sigma_x\rho(t')\sigma_x\} \, dt'
\end{align*}\]

where the sigmas denote Pauli matrices. Parameters were set as \( \omega = 1 = \beta \) and \( C = .2 \). We chose to define \( \chi(t,u) = \int_0^t W(t-t')\rho(t') \, dt' \) which differs somewhat from the general definition employed in (7). The transformed equations are then

\[
\frac{d\rho(t)}{dt} = -i\left[\frac{\omega}{2}\sigma_z + \beta \sigma_x, \rho(t)\right] - 2C\{\chi(t,0) - \sigma_x\chi(t,0)\sigma_x\}
\]

\[
\frac{d\chi(t,u)}{dt} = e^{-gu^2}W(u)\rho(t) + \frac{\partial\chi(t,u)}{\partial u}
\]

\[+ 2gu \chi(t,u).\]

Theory predicts that the memory function \( W(t) \) for this problem is approximately gaussian in form. However, we were unable to obtain an exact solution of the master equation for this case. Instead we approximate the gaussian via the similar function \( W(t) = 14e^{-7.4t} - 13e^{-8t} \). Exact solutions for

\[
\langle \sigma_z \rangle(t) = \text{Tr}\{\sigma_z\rho(t)\} = \rho_{11}(t) - \rho_{00}(t) \quad \text{(solid curve)}
\]

\[
\langle \sigma_x \rangle(t) = \text{Tr}\{\sigma_x\rho(t)\} = \rho_{10}(t) + \rho_{01}(t) \quad \text{(dashed)}
\]

\[
\langle \sigma_y \rangle(t) = \text{Tr}\{\sigma_y\rho(t)\} = i(\rho_{10}(t) - \rho_{01}(t)) \quad \text{(short dashed)}
\]

and initial conditions \( \langle \sigma_z \rangle(0) = 1 \) and \( \langle \sigma_x \rangle(0) = 0 = \langle \sigma_y \rangle(0) \) were obtained in the same way as for the generalized Langevin equations and are plotted vs time in Figure 6. For the approximate method we used \( y = 11/[(n-l)\Delta u]^2 \) and for negative \( u \) we set \( W(u) = W(|u|) \). From Figure 7 where we plot

\[
\epsilon(t) = -\log_{10}|\langle \sigma_z \rangle(t) - \langle \sigma_z \rangle_{\text{approximate}}(t)|
\]
against time we see that convergence of the numerical method is very rapid for these equations. [Similar accuracies are achieved for $\langle \sigma_x \rangle$ and $\langle \sigma_y \rangle$.]

Thus, we have shown that accurate solutions of integro-differential equations can be obtained via transformation to a larger set of ordinary differential equations. Because this transformation is exact we expect that the method will also work for equations not considered in this manuscript. It should be possible to obtain accurate solutions for such equations via the following steps. First find an approximation of the memory function or operator which will allow exact solutions to be obtained. Optimize the numerical method by finding the best $g$ for the model equations. Finally, apply the numerical method to the original equations and look for convergence of the solutions with increasing $n$.

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[11] Laplace transforms of the exact solutions are readily obtained but inverting the transform is problematic.