RESPONSE FUNCTIONS OF OSCILLATORY SYSTEMS

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1. The response function

The purpose of this short note is to clarify some conceptual issues around the linear response of non-dissipative systems (mathematically: the Fourier transform of causal functions). This is an elementary problem, but with a remarkably deep structure. In the literature on response functions in quantum mechanics, these technical issues are often glossed over, or treated in an ad-hoc way. We will consider very general models, in order to separate general statements from details of specific physical systems.

Consider a nonlinear time-invariant (autonomous) system

$$\dot{x} = F(x)$$

near an equilibrium x_*. We perturb this system with an external time-dependent source with intensity $I(t)$, resulting in the non-autonomous system

$$\dot{x} = F(x, I(t)).$$

In a neighborhood of x_* we can linearize[1] in the displacement with respect to equilibrium $\delta x = x - x_*$:

$$\dot{\delta x} = \partial_x F \delta x + \partial_I F I(t) + O(|\delta x|^2 + |I(t)|^2)$$

where the derivatives of F are evaluated at $(x_*, 0)$.

Assume that the system is at rest ($\delta x = 0$) at $t = -\infty$, and that I is switched on at a finite time ($I(t) = 0$ for $t < t_0$). Ignoring the remainder terms, we get

$$\delta x = \int_{-\infty}^{t} e^{(t-t')\partial_x F} \partial_I F I(t') dt'$$

which is a convolution between I and the *impulse response function*. If $O(x)$ is an output quantity of interest, then its displacement with respect to equilibrium $\delta O = O(x(t)) - O(x_*)$ is (again to first order)

$$\begin{aligned} \delta O(t) &= \int_{-\infty}^{t} \langle \nabla O, e^{(t-t')\partial_x F} \partial_I F \rangle I(t') dt' \\ &= (R * I)(t) \end{aligned}$$

where R is the response function

$$\boxed{R(t) = \theta(t) \langle \nabla O, e^{t\partial_x F} \partial_I F \rangle} \tag{1}$$

with θ the Heaviside function ($\theta(t) = 1$ for $t \geq 0$, $\theta(t) = 0$ for $t < 0$). This is also called the impulse response, because when I is a Dirac impulse at time 0, $\delta O = R$. Characteristically of linear time-invariant systems, knowing the response to a single impulse allows us to reconstruct the full response to any signal by convolution. This response function is *causal* ($R(t) = 0$ for $t < 0$). In the rest of this document, we will consider response functions of the form (1).

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[1]Note that we assume here that the problem is real, or, if complex, that F is holomorphic, so that $\partial_I F$ is a complex-linear map. If this is not the case, one needs to split real and imaginary parts.

2. Stable responses

It is clear that the properties of the operator $L = \partial_x F$ are crucial. If L has spectrum with purely negative real part, then the system is stable: $R(t)$ goes to zero exponentially fast. It is then possible to take the Fourier transform of R

$$\widehat{R}(\omega) = \int_0^{+\infty} R(t) e^{i\omega t} dt \tag{2}$$

as a well-defined integral. The unusual convention of taking $e^{i\omega t}$ instead of $e^{-i\omega t}$ (and, therefore, $e^{-i\omega t}$ as the elementary oscillation instead of $e^{i\omega t}$) is done for consistency with quantum mechanics (where the elementary solution of the Schrödinger equation is e^{-iEt}). The Fourier transform represents the oscillatory (AC) response to an applied periodic perturbation. To see this, it is convenient to rewrite $\widehat{R}(\omega)$ as

$$\begin{aligned} \widehat{R}(\omega) &= \lim_{T\to\infty} e^{i\omega T} \int_0^T R(t) e^{i\omega(t-T)} dt = \lim_{T\to\infty} e^{i\omega T} \int_0^T R(T-t) e^{i\omega t} dt \\ &= \lim_{T\to\infty} e^{i\omega T} (R * \theta(t) e^{i\omega t})(T) \end{aligned} \tag{3}$$

which means that when the input is a pure oscillation $I(t) = \theta(t) e^{i\omega t}$, the output is asymptotic for large times to $\widehat{R}(\omega) e^{-i\omega T}$.

Assume that the system is finite-dimensional and that L is diagonalizable: $L = PDP^{-1}$. Denoting by u_i and $\overline{v_i}$ the columns of P and P^{-1} respectively, we can write

$$L = \sum_{i=1}^N \lambda_i |u_i\rangle\langle v_i|$$

with $\langle u_i, v_j\rangle = \delta_{ij}$. It follows that

$$\begin{aligned} R(t) &= \theta(t) \sum_{i=1}^N e^{t\lambda_i} \langle \nabla O, u_i\rangle \langle v_i, \partial_I F\rangle \\ \widehat{R}(\omega) &= -\sum_{i=1}^N \frac{1}{\lambda_i + i\omega} \langle \nabla O, u_i\rangle \langle v_i, \partial_I F\rangle \end{aligned} \tag{4}$$

This function is naturally defined in the upper complex plane and the real axis (as this is where the integral (2) makes sense). In this case it even extends to a meromorphic function on the whole complex plane (with poles at $\omega = i\lambda_i$ in the lower complex plane), but this is not necessarily the case for response functions of infinite-dimensional systems, which can have a more complicated analytic structure.

Example 1 (Damped harmonic oscillator)**.** *Consider the equation*

$$\ddot{x} + \eta \dot{x} + \omega_0^2 x = I(t) \tag{5}$$

with $\eta > 0$, equilibrium $x = 0$ and observable $O = x$. The response function has two components with exponents λ solutions of $\lambda^2 + \eta\lambda + \omega_0^2 \lambda = 0$, which are located in the left-hand complex plane, and converge towards $\pm i\omega_0$ as $\eta \to 0^+$. The Fourier transform, defined on the real axis and above, has two poles in the lower complex plane which approach the real axis as $\eta \to 0^+$.

3. Oscillatory responses

The expression of $\widehat{R}(\omega)$ is informative as to the frequency content of the response. It can however not be defined as such for for systems that are not stable: in these situations, R is not decaying, and therefore neither (2) nor (3) are defined. For truly unstable systems (with eigenvalues with positive real part) the Fourier transform for real ω is not really meaningful, and one has to be content with the Laplace transform (Fourier transform for ω in the upper complex plane). An intermediate case of particular interest in quantum mechanics (and more generally Hamiltonian systems) is when all the eigenvalues of L have zero real part (purely oscillatory dynamics). This is in particular the case of Hamiltonian systems at energy minima. In this case, (2) does not make sense, as the integral is not convergent (the various oscillation modes do not decay). It is however possible to give a meaning to the Fourier transform in various ways.

Throughout, we will illustrate using the following example:

Example 2 (Linearized Schrödinger equation, 1 degree of freedom)**.** Consider the equation with source term

$$i\dot{x} = Ex + I(t). \tag{6}$$

with equilibrium $x = 0$ and $O(x) = x$. The response function in time is easily calculated as

$$f(t) = -i\theta(t)e^{-iEt}. \tag{7}$$

This example is an extremely simplified version of the Schrödinger equation, with major differences with respect to actual quantum mechanics: it is 1D, has a dissipation, and the perturbation acts as a source term, not multiplicatively on the state as in quantum mechanics. It is best seen as a slightly simpler variant of the forced harmonic oscillator, with one (complex) degree of freedom instead of two (real). It serves as a useful intermediate stepping stone towards the linearized Schrödinger equation.

3.1. **Method 0: steady state.** If $\widehat{R}(\omega)$ it to be interpreted as the steady-state response of the system to an oscillatory input $e^{-i\omega t}$ (recall the unusual sign of the Fourier transform), we can just set I to that value and look for a steady state in δx. This is appealing, but not precise enough. For instance, on the example above, by setting $I(t) = e^{i\omega t}$ and $x(t) = \widehat{R}(\omega)e^{i\omega t}$, we find

$$\widehat{f}(\omega) = \frac{1}{\omega - E}?$$

This result is *almost* correct, but is insufficiently precise in describing what is going on at $\omega = E$. For instance, it appears to lead to the (incorrect) conclusion that the imaginary part of $\widehat{f}$ is identically zero (which contradicts various general statements, for instance sum rules or Kramers-Kronig relations). It also gives a divergent result for systems with infinitely many degrees of freedom, as we will see later.

3.2. **Method 1: physical dissipation.** Often Hamiltonian systems are idealizations of dissipative systems where dissipative effects are neglected. In the case of mechanical systems this is usually easy to see: for instance the harmonic oscillator $\ddot{x}+\omega_0^2 x = 0$ is the limit case of the damped oscillator $\ddot{x} + \eta\dot{x} + \omega_0^2 x = 0$. It is also easy in linearized dynamics, by simply adding a dissipative term: in the example above, we can modify it to $i\dot{x} = Ex - i\eta x + I(t)$.

In (not linearized) quantum systems this is harder as dissipation is more complicated to build in the framework of quantum theory (this can be ultimately justified using the theory of open quantum systems, which we will not go into here). Using this, one can compute the Fourier transform of the dissipative system, then take the dissipationless limit $\eta \to 0^+$ (η goes to 0 through positive values). This is perhaps the most insightful and physically relevant method, but we will not discuss it further because it modifies R in a system-dependent way, and is not "black-box", in contrast to the next methods.

3.3. **Method 2: artificial dissipation.** This method just adds dissipation artificially to R:

$$\widehat{R}_2(\omega) := \lim_{\eta\to 0^+} \int_0^{+\infty} R(t)e^{i\omega t}e^{-\eta t}dt = \lim_{\eta\to 0^+} \widehat{R}(\omega + i\eta) \tag{8}$$

In the example above, we obtain

$$\widehat{f}(\omega) = \lim_{\eta\to 0^+} \frac{1}{\omega + i\eta - E}. \tag{9}$$

We will discuss this limit later. Note that $\widehat{R}_1(\omega + i\eta)$ is a Laplace transform: this method defines the Fourier transform as the limit of the Laplace transform as the frequency parameter approaches the real axis.

3.4. **Method 3: Cesaro regularization.** The problem in defining $R(\omega) = \lim_{t\to+\infty} \int_0^t R(t')e^{i\omega t'}dt'$ is that this integral typically oscillates with t. We can regularize these oscillations by looking at the average behavior of this function of t:

$$\widehat{R}_3(\omega) := \lim_{T\to+\infty} \frac{1}{T} \int_0^T \int_0^t R(t')e^{i\omega t'}dt'dt$$

3.5. **Method 4: adiabatic switching.** The oscillations come from the fact that we perturbed our system brutally (with an impulse). This triggers oscillations that would not have occured had the system been disturbed more gently (think of a water surface set in motion brutally). To compute the Fourier transform of R at frequency ω (which we think of as the steady-state response of the system to an input $e^{-i\omega t}$), we ramp up the input gradually:

$$I(t) = \begin{cases} e^{-i\omega t}e^{\eta t} & \text{for } t < 0 \\ e^{-i\omega t} & \text{for } t \geq 0 \end{cases}$$

This results in

$$\delta O_\eta(t) = \int_{-\infty}^{t} e^{(-i\omega+\eta)t'} R(t-t')dt'.$$

We then hope that the output looks like $\widehat{R}(\omega)e^{-i\omega t}$ for $t \geq 0$, and so set

$$\begin{aligned} \widehat{R}_4(\omega) &= \lim_{\eta\to 0^+} \delta O_\eta(0) = \lim_{\eta\to 0^+} e^{i\omega t}\int_{-\infty}^{t} e^{(-i\omega+\eta)t'} R(t-t')dt' \\ &= \lim_{\eta\to 0^+} e^{\eta t}\int_{-\infty}^{0} e^{(-i\omega+\eta)t''} R(-t'')dt'' = \lim_{\eta\to 0^+} e^{\eta t}\int_{0}^{+\infty} e^{(i\omega-\eta)t''} R(t'')dt''. \end{aligned} \tag{10}$$

In the limit $\eta \to 0$ this is independent on t and directly equivalent to method 2.

3.6. **Method 5: distributional Fourier transform.** It is possible to give a weak sense to the Fourier transform of a continuous non-decaying function, as long as that function does not grow faster than polynomially at infinity. To do so, we give up the idea of defining $\widehat{R}(\omega)$ pointwise, but rather only measure averages. This makes sense as measurements never observe an exact frequency (which would correspond to measuring a system for an infinite time), but rather *near* a frequency ω with accuracy $\delta\omega$ (related to the observation time by $T \approx \frac{1}{\delta\omega}$). Therefore we have to give a meaning to $\int_{\mathbb{R}} \widehat{R}(\omega)\widehat{\phi}(\omega)d\omega$ for test functions $\widehat{\phi}(\omega)$. We require the test functions to form a set rich enough that such integrals can identify $\widehat{R}$ uniquely, but restricted to smooth and decaying functions (so that their Fourier transforms are decaying and smooth); technically we use the Schwartz class, see any textbook covering distribution theory. Using the formula

$$\int_{\mathbb{R}} \overline{\widehat{f}(\omega)}\widehat{g}(\omega)d\omega = 2\pi\int \overline{f(t)}g(t)dt,$$

which is valid for functions f and g that decay, one can *define*

$$\text{“}\int_{\mathbb{R}} \overline{\widehat{R}_4(\omega)}\widehat{\phi}(\omega)d\omega\text{”} := 2\pi\int \overline{R(t)}\phi(t)dt, \tag{11}$$

this last integral converging because ϕ is local in time. This definition of distributional Fourier transform allows many formal statements (such as the Fourier transform of $e^{-i\omega t}$ being $2\pi\delta_\omega$) to have a rigorous mathematical meaning, and it is the one in which singular limits make sense.

4. General equivalences

We have seen that method 0 (steady state) is incorrect. Method 1 (physical dissipation) is system-dependent (but is equivalent to method 2, artificial dissipation). Method 4 (adiabatic switching) is equivalent to method 2. We then have to clarify the relationship between methods 2 (artificial dissipation), 3 (Cesaro regularization) and 5 (distributional transform).

4.1. **Distributional sense.** In the distributional sense, all methods work and give the same result

Theorem. *If R is causal, continuous and of polynomial growth (there are $C, p > 0$ such that $|R(t)| \leq C(1+|t|^p)$), then method 5 (distributional transform) is well-defined. The limits in methods 2 (artificial dissipation) and 3 (Cesaro regularization) are well-defined in the distributional sense, and all the methods agree in the distributional sense.*

Proof. If the function is of polynomial growth, it defines a tempered distribution and its distributional transform is well-defined (see any textbook on distribution theory).

The sequence $R(t)e^{-\eta t}$ converges in the sense of distributions to $R(t)$ as $\eta \to 0^+$ (recall that R is causal), and so the distributional Fourier transform of $R(t)e^{-\eta t}$ converges to that of $R(t)$. It follows that methods 2 and 5 agree.

Let $\phi \in S(\mathbb{R})$. We have

$$\int_{\mathbb{R}} d\omega \widehat{\phi}(\omega) \frac{1}{T} \int_0^T dt \int_0^t dt' \overline{R(t')} e^{-i\omega t'} = \frac{2\pi}{T} \int_0^T dt \int_0^t dt' \overline{R(t')} \phi(t') \to \int_0^{+\infty} \overline{R(t)} \phi(t) dt$$

which is the definition of the convergence of the Cesaro regularization of $\widehat{R}$ towards $\widehat{R}$ in the sense of distributions, and therefore methods 3 and 5 agree. □

4.2. **Pointwise sense.** Recall that convergence in the sense of distributions does not imply pointwise convergence (for instance, in the sense of distributions, e^{inx} converges to zero as $n \to \infty$). When pointwise values are of interest, the theory of distribution is not of much use, but the Cesaro and dissipation methods still give the same result, with the dissipation method being "stronger" (applies in more cases).

Theorem. *Let R be continuous and causal. For a given $\omega \in \mathbb{R}$, if method 3 converges, then method 2 converges, and both give the same result.*

Proof. We use the following lemma, establishing the link between the Cesaro and Abel methods of regularizing $\lim_{t\to\infty} F(t)$ (this type of results are called "Abelian-Tauberian theorems").

Lemma. *Let F be continuous. If the Cesaro limit*

$$\lim_{T\to+\infty} \frac{1}{T} \int_0^T F(t) dt$$

converges, then so does the Abel limit

$$\lim_{\eta\to 0^+} \eta \int_0^{+\infty} e^{-\eta t} F(t) dt$$

and both results are equal.

Assuming the lemma and defining $F(t) = \int_0^t R(t')dt'$, we have

$$\eta \int_0^{+\infty} e^{-\eta t} F(t) dt = \int_0^{+\infty} e^{-\eta t} R(t) dt$$

which proves the theorem.

The lemma is classical (see for instance Widder '71, An Introduction to Transform Theory, Chap. 8, Theorem 2.3); we reproduce the sketch of the proof here. Let C be the Cesaro sum. We write

$$\eta \int_0^{+\infty} e^{-\eta t} F(t) dt = \eta^2 \int_0^{+\infty} e^{-\eta t} \left(\int_0^t F(t') dt' \right) dt$$

Now we have $\int_0^t F(t')dt' = Ct + r(t)$ where $\frac{r(t)}{t} \to 0$. From the formula $\int_0^{+\infty} te^{-\eta t} dt = \eta^{-2}$ it follows that we only have to prove that

$$\eta^2 \int_0^{+\infty} e^{-\eta t} r(t) dt \to 0.$$

For all $\varepsilon > 0$, there is a $C_\varepsilon > 0$ such that $r(t) \leq C_\varepsilon + \varepsilon t$. Then, using $\int_0^{+\infty} e^{-\eta t} dt = \eta^{-1}$ and $\int_0^{+\infty} te^{-\eta t} dt = \eta^{-2}$, we get

$$\left| \eta^2 \int_0^{+\infty} e^{-\eta t} r(t) dt \right| \leq C_\varepsilon \eta + \varepsilon$$

and the result follows. □

5. The Plemelj-Sokhotski formula

We have seen above that the limit $\lim_{\eta\to 0^+} \widehat{R}(\omega + i\eta)$ makes sense in the sense of distributions (when integrated against test functions). It is instructive to make the limit more explicit in the example $f(t) = -i\theta(t)e^{-iEt}$, where

$$\widehat{f}(\omega) = \lim_{\eta\to 0^+} \frac{1}{\omega - E + i\eta}.$$

At finite η, we have

$$\frac{1}{\omega - E + i\eta} = \frac{\omega - E}{(\omega - E)^2 + \eta^2} - \frac{\eta i}{(\omega - E)^2 + \eta^2}$$

The real part is a regularized $1/(\omega - E)$ function, and the imaginary part is a regularized Dirac delta (see Figure 1). It is an easy exercise in the theory of distributions to show that, in the sense

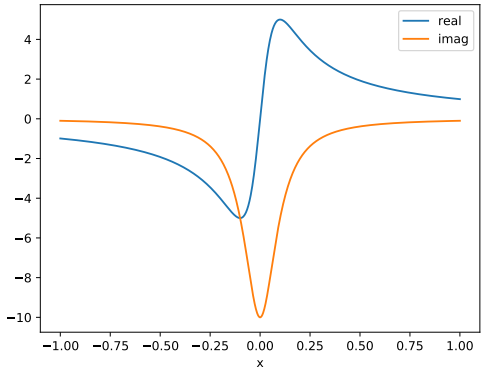

FIGURE 1. The Plemelj-Sokhotski formula: real and imaginary parts of $\frac{1}{x+i\eta}$ (here for $\eta = 0.1$).

of distributions,

$$\lim_{\eta \to 0^+} \frac{1}{\omega - E + i\eta} = P\frac{1}{\omega - E} - i\pi\delta(\omega - E) \tag{12}$$

where P denotes the Cauchy principal value (note that taking the limit $\eta \to 0^-$ reverses the sign of the imaginary part). This equation is sometimes known as the Plemelj-Sokhotski formula.

6. Towards more complex systems

We will consider progressively more complicated refinements of the very simple example 2 above.

6.1. N degrees of freedom.

Consider first the equation

$$i\dot{x} = Lx + I(t)c \tag{13}$$

with equilibrium $x = 0$, observable $O(x) = \langle b, x\rangle$, where b and c are N-dimensional vectors and L a N-dimensional Hermitian matrix. The response function is

$$R(t) = \langle b, e^{-iLx}c\rangle$$

By decomposing on an orthonormal set of eigenvectors v_n and eigenvalues E_n of L, we see that

$$\begin{aligned}\widehat{R}(\omega) &= \lim_{\eta \to 0^+} \sum_{n=1}^{N} \frac{\langle b, v_n\rangle\langle v_n, c\rangle}{\omega - E_n + i\eta} \\ &= \sum_{n=1}^{N} \langle b, v_n\rangle\langle v_n, c\rangle \left(P\frac{1}{\omega - E_n} - i\pi\delta(\omega - E_n)\right)\end{aligned} \tag{14}$$

in the sense of distributions. This has singularities at each of the energies E_n.

6.2. Identity multiplication operator.

Now consider an infinite-dimensional model. To start with, consider L to be a simple multiplication operator:

$$\begin{aligned} i\dot{x}(E,t) &= Ex(E,t) + I(t)c(E) \\ O(t) &= \int_{\mathbb{R}} b(E)x(E)dE\end{aligned} \tag{15}$$

for $x(E,t)$. This leads directly to

$$\begin{aligned} R(t) &= -i\int_{\mathbb{R}} b(E)c(E)e^{-iEt}dE \\ \widehat{R}(\omega) &= \lim_{\eta \to 0^+} \int_{\mathbb{R}} \frac{b(E)c(E)}{\omega - E + i\eta}dE \\ &= P\int_{\mathbb{R}} \frac{b(E)c(E)}{\omega - E + i\eta}dE - i\pi b(\omega)c(\omega).\end{aligned} \tag{16}$$

Remarkably, the imaginary part is not singular anymore! Seeing this model as the limit case of a discrete problem, the eigenvalues have densified to a continuum, and the poles have merged to a continuous function. This is not unusual in complex analysis; consider for instance

$$\int_{-1}^{1} \frac{1}{\omega - E} dE = \log\left(\frac{\omega - 1}{\omega + 1}\right).$$

Characteristically, such functions are multivalued, with branch points at the "spectrum edges" (here ± 1). This makes it important to specify the branch by an appropriate limit process (for instance, taking the limit $\eta \to 0^-$ above would have flipped the sign of the imaginary part of $\widehat{R}(\omega)$). An imperfect physical analogy is the electrostatic potential produced by a surface of uniform charge, which has a finite but discontinuous value across the surface; this is by contrast to a discrete array of charges, which produces a continuous potential.

6.3. **General multiplication operator.** As an additional step in complexity, consider a non-trivial multiplication operator

$$i\dot{x}(k,t) = E(k)x(k,t) + I(t)c(k) \tag{17}$$
$$O(t) = \int_{\mathbb{R}} b(k)x(k)dk$$

modeling a field of excitations with dispersion relation $E(k)$. We have

$$\widehat{R}(\omega) = \lim_{\eta \to 0^+} \int_{\mathbb{R}} \frac{b(k)c(k)}{\omega - E(k) + i\eta} dk$$

It is instructive to compute more explicitly the imaginary part with the help of the co-area formula:

$$-\frac{1}{\pi}\mathrm{Im}(\widehat{R}(\omega)) = \int_{E(k)=\omega} \frac{b(k)c(k)}{|\nabla E(k)|} dk$$

The physical picture is that the disturbance at frequency ω excites all the excitations k matching the frequency $E(k) = \omega$. The quantity $\int_{E(k)=\omega} \frac{1}{|\nabla E(k)|}$ is the density of states at energy ω, which are here weighted by the "matrix element" $b(k)c(k)$ (with $c(k)$ quantifying how much k couples to the disturbance, and $b(k)$ the output k produces).

6.4. **General case.** Finally, the model

$$i\dot{x}(t) = Lx(t) + I(t)c$$

where L is a general self-adjoint operator can have a mixed behavior (displaying both a discrete and a continuous part). The generalization of the previous formulas is

$$-\frac{1}{\pi}\mathrm{Im}(\widehat{R}(\omega)) = \langle b, \pi_L(\omega)c\rangle$$

where π_L is the projector-valued spectral measure associated with L.

7. Application to quantum mechanics

The main difficulty in applying the above formalism to Schrödinger equations of the form

$$i\partial_t \psi = (H + I(t)V)\psi(t)$$

is that the stationary solutions are not naturally solutions of $H\psi = 0$ but rather of $H\psi = E\psi$. This is easily remedied in the *interaction picture* (also called Duhamel or Dyson formula): changing variables to $\psi(t) = e^{-iHt}\phi(t)$, we get

$$i\partial_t \phi = e^{iHt} I(t) V e^{-iHt} \phi(t)$$

from where the first-order expansion near an eigenstate can proceed, resulting in a response function of the form above.

Another solution is to use density matrix (projectors). Setting $P = |\psi\rangle\langle\psi|$, we obtain

$$i\partial_t P = [(H + I(t)V), P]$$

which has an equilibrium when ψ is an eigenfunction of H. In this formalism, the operator L is the Liouvillian.

Both these methods generalize to nonlinear equations (such as time-dependent density functional theory). In applying the above theory, we have to take care that these equations are not necessarily compatible with the complex structure (because the density involves conjugates of the orbitals, or because the space of Hermitian matrices (and therefore density matrix variations) is not a complex

vector space): we then have to separate real and imaginary part (or couple frequencies $+\omega$ and $-\omega$), resulting in a 2×2 block matrix structure.