Approximate Dynamical Systems

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Abstract

Working notes on setting up approximate dynamical systems and nonlinear eigenvalue problems, here embedded within the theory of complex nonlinear dynamics. Computations parallel those of linear quantum theory except that we use functional methods rather than Hilbert space.

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I. INTRODUCTION

This covers basic concepts behind the theory of *approximate dynamical systems* [1], the theory of generalized quantum dynamics, functional methods, theory of propagators, and the basics of nonlinear spectral theory and nonlinear functional analysis.

It begins with the key idea of the subject, namely the use of *action principles* to define, and obtain *approximate dynamical systems*. Subsequently we see some examples of useful systems of this kind that generate nonlinear equations.

II. ACTION PRINCIPLES AND APPROXIMATION THEORY

What we really need, to make the business of practical computations efficient, is a *larger mathematics* which contains both exact and approximate equations of motion — treated in a unified manner. This is best done working from the principle of least action.

At the deepest level, physical theories when considered as dynamical systems, derive from action principles. It easy to state these in complete generality, as a shell into which we plug a Lagrangian and turn the crank. Here we concentrate upon *equations of motion* as “solutions” of the variational problem

\[
\frac{\delta}{\delta x(t)} \int_{t=t_0}^{t=t_f} L[x, \dot{x}, t] \, dt = 0.
\]

The lovely thing about an action principle, when we look at it this way, is that it provides a recipe for constructing new equations of motion that are the result of replacing \( L[x, \dot{x}, t] \) by some conveniently chosen approximation \( L_{\text{app}}[x, \dot{x}, t] \approx L[x, \dot{x}, t] \).

If we make sure that our system of mathematics is *large enough* to capably handle all useful kinds of approximation, then — once we have formalized these in the abstract — we will obtain an entire new system of generalized quantum dynamics.

So, the goal is to replace *exact* action principles by *approximate* action principles and so obtain entire *approximate dynamical systems*. Then we look at these, study and classify them, the better to understand their particular merits and deficiencies.
III. DECORRELATION AS A STANDARD APPROXIMATION

Practical approximations are designed to leave some effect out to make things simple. In quantum theory the one generic effect which makes the theory hard to calculate with, and visualize, is quantum correlation and quantum entanglement. In the theory of approximate dynamical systems we use some simple tricks to suppress this effect and simplify things.

Here is one simple semi–classical example

$$\langle \frac{\hat{p}^2}{2m} + k\hat{x}^2 \rangle \approx \langle \hat{p} \rangle^2 \frac{2m}{2m} + k\langle \hat{x} \rangle^2,$$

(2)

where the quantum expectation is replaced by its semi–classical counterpart. A familiar many–body example is the Hartree approximation

$$\int \psi^*(x_1, x_2)V(|x_1 - x_2|)\psi(x_1, x_2) d^3x_1 d^3x_2 \approx \int \psi_1^*(x_1)\psi_2^*(x_2)V(|x_1 - x_2|)\psi_1(x_1)\psi_2(x_2) d^3x_1 d^3x_2,$$

(3)

where $\psi(x_1, x_2)$ has been replaced by a factorized pair of wave–functions.

In both cases we neglect correlations, or enforce disentanglement, and so modify the degree of the original expression in $\psi$ and $\psi^*$. It is this modification of degree which is the cause of induced nonlinearity, as we now see with a simple example.

IV. CLASSICAL SCHRÖDINGER EQUATION

The easiest way to express the correspondence between classical and quantum physics is via the Ehrenfest theorem. Starting with the quantum equations:

$$\frac{d\langle \hat{p} \rangle}{dt} = -\langle H_x(\hat{x}, \hat{p}) \rangle, \text{ and } \frac{d\langle \hat{x} \rangle}{dt} = +\langle H_p(\hat{x}, \hat{p}) \rangle;$$

(4)

we introduce the obvious semi–classical approximation:

$$\langle H_x(\hat{x}, \hat{p}) \rangle \approx H_x(\langle \hat{x} \rangle, \langle \hat{p} \rangle), \text{ and } \langle H_p(\hat{x}, \hat{p}) \rangle \approx H_p(\langle \hat{x} \rangle, \langle \hat{p} \rangle);$$

(5)

and thus obtain the approximate equations:

$$\frac{d\langle \hat{p} \rangle}{dt} \approx -H_q(\langle \hat{x} \rangle, \langle \hat{p} \rangle), \text{ and } \frac{d\langle \hat{x} \rangle}{dt} \approx +H_p(\langle \hat{x} \rangle, \langle \hat{p} \rangle).$$
If we now take these as defining a new dynamical system (i.e. we replace $\approx$ by $=$) then our equations reduce to those of Hamilton,

$$\frac{dP}{dt} = -H_x(X, P), \quad \text{and} \quad \frac{dX}{dt} = +H_p(X, P);$$

(7)

where we make the obvious identification:

$$X(t) = \langle \hat{x}(t) \rangle \quad \text{and} \quad P(t) = \langle \hat{p}(t) \rangle.$$  

(8)

In taking these steps one reduces the quantum problem to a classical problem, in a manner that ignores certain features of the full quantum treatment.

Now let us apply this analysis of the Ehrenfest theorem, as a decorrelation approximation, at the general level of the exact quantum action principle

$$\frac{\delta}{\delta \psi^*} \int i\hbar \langle \psi | \frac{d}{dt} |\psi \rangle - \langle \psi | H(\langle \hat{x} \rangle, \langle \hat{p} \rangle) |\psi \rangle dt = 0.$$  

(9)

Taking variations with this we obtain

$$i\hbar \frac{d}{dt} |\psi \rangle = \hat{H}(\hat{x}, \hat{p}) |\psi \rangle,$$

(10)

as the general equation of motion. However, we could just as well substitute

$$\langle \psi | \hat{H}(\hat{x}, \hat{p}) |\psi \rangle \approx \langle \psi | H(\langle \hat{x} \rangle, \langle \hat{p} \rangle) |\psi \rangle.$$  

(11)

for the energy expectation, and so obtain directly a decorrelated classical wave–equation.

There is, however, a minor subtlety to carrying out this program. In (11) it is not guaranteed that the action principle remains invariant to a re–normalization of $\psi$. Obviously we want to retain that freedom to adjust and preserve normalization. To overcome this difficulty we rescale all coordinate expectations as:

$$\langle \hat{x} \rangle = \langle \psi | \hat{x} |\psi \rangle / n \quad \text{and} \quad \langle \hat{p} \rangle = \langle \psi | \hat{p} |\psi \rangle / n,$$

(12)

where $n = \langle \psi |\psi \rangle$. Calculating variational derivatives we find

$$\frac{\delta \langle \hat{x} \rangle}{\delta \psi^*} = n^{-1}(\hat{x} - \langle \hat{x} \rangle) |\psi \rangle, \quad \text{and} \quad \frac{\delta \langle \hat{p} \rangle}{\delta \psi^*} = n^{-1}(\hat{p} - \langle \hat{p} \rangle) |\psi \rangle.$$  

(13)

Invoking now the approximate action principle

$$\delta \int i\hbar \langle \psi | \frac{d}{dt} |\psi \rangle - \langle \psi | H(\langle \hat{x} \rangle, \langle \hat{p} \rangle) |\psi \rangle dt = 0,$$

(14)
we use the chain rule
\[ \frac{\delta}{\delta \psi^*} \left[ \langle \psi | H(\langle \hat{x}, \langle \hat{p} \rangle) | \psi \rangle \right] = H(\langle \hat{x}, \langle \hat{p} \rangle) \frac{\delta n}{\delta \psi^*} + \frac{\delta \langle \hat{x} \rangle}{\delta \psi^*} H_x(\langle \hat{x}, \langle \hat{p} \rangle) + \frac{\delta \langle \hat{p} \rangle}{\delta \psi^*} H_p(\langle \hat{x}, \langle \hat{p} \rangle)), \]
to obtain the approximate equation of motion
\[ i\hbar \frac{d}{dt} |\psi\rangle = \left\{ H(\langle \hat{x}, \langle \hat{p} \rangle)) \hat{1} + H_x(\langle \hat{x}, \langle \hat{p} \rangle)(\hat{x} - \langle \hat{x} \rangle) + H_p(\langle \hat{x}, \langle \hat{p} \rangle)(\hat{p} - \langle \hat{p} \rangle) \right\} |\psi\rangle. \quad (15) \]
This is the classical Schrödinger equation, which recovers the Ehrenfest equations of motion in classical form. It propagates wave–packets neglecting dispersion and correlation. The result is that they bounce off barriers and the like just like classical particles.

One can construct exact solutions of the above nonlinear integro-differential equation. To do this we first solve the classical problem to find \( X(t) \) and \( P(t) \). Next we take any wavefunction \( \psi_0(x) \) having both position and momentum expectation values equal to zero. Then we form the time–dependent wavefunction
\[ \psi(x, t) = e^{\frac{i}{\hbar} \int_0^t L d\tau} e^{-iP(t)X(t)/2\hbar} e^{iP(t)x/\hbar} \psi_0(x - X(t)), \quad (16) \]
where the exact classical action
\[ \int_{t_0}^t L d\tau = \int_{t_0}^t \left( \frac{P \dot{X} - X \dot{P}}{2} \right) - H(X, P) d\tau \quad (17) \]
appears as the leading phase factor (showing that the Feynmann–Dirac correspondence is semi–classically exact). This argument can be made constructive, but it is much easier to verify by substitution. Alternatively, given a theory of nonlinear propagators one can set up these equations on a computer and solve them directly to verify this general solution.

V. PHYSICAL INTERPRETATION

When dealing with approximate dynamical systems we must remember that linearity is vital to the Copenhagen interpretation. However, we use nonlinear wave–equations all the time in physics. To interpret them we adopt a computational algorithm viewpoint.

We have an exact theory, and quantities that we wish to calculate — e.g. eigenvalues, stationary and time–dependent wavefunctions, expectation values, transition probabilities etc. These we could calculate exactly or approximately.

Either way we can apply a physical interpretation that presupposes linearity as an exact property of nature. To the approximately computed, i.e. nonlinearly evolved, physical
quantities we apply the Copenhagen interpretation — on the understanding that there is supposed to be an error in our treatment somewhere.[2]

For instance, in solving our approximate classical equations we have no need of $\hbar$, nor any specific wavefunction. The solution of the reduced, and thus simplified, problem requires only the initial expectation values. It is thus an approximate method for computing $\langle \hat{x}(t) \rangle$ and $\langle \hat{p}(t) \rangle$. The errors committed are identical, both numerically and conceptually, to those of the familiar Hamiltonian dynamics. Even so, it is pretty useful. One could say the existence of the classical Schrödinger equation, as an excellent semiclassical approximation, explains why classical dynamics fooled us for 300 years!

[1] K.R.W. Jones, in prep.

[2] Of course, ultimately the matter of what is correct rests with experiment.