Unitary transformations depending on a small parameter

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Ongoing project in collaboration with

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I. DRAMATIS PERSONAE



Max Born
(1882-1970)

Werner Heisenberg
(1902-1976)

Pascual Jordan
(1902-1980)

Zur Quantenmechanik II, *Zeitschrift für Physik*, **35**, 557-615, 1926. [English translation in: B. L. van der Waerden, editor, Sources of Quantum Mechanics]

Dreimännerarbeit

André Deprit (1926-2006)

A.Deprit, Canonical transformations depending on a small parameter, *Celestial Mechanics* **1** 12-30, 1969

II. INTRODUCTION

The goal

- To formulate a unitary perturbation theory in quantum mechanics in the spirit of Deprit's algorithm in classical Hamiltonian mechanics.
- A problem posed to us by Deprit himself around 1992.
- On the road, some interesting connections:
  - matrix mechanics and the *dreimännerarbeit*
  - an application of geometric integrators
  - reducibility in linear differential equations
  - averaging techniques (talks by Chartier and Murua)

Canonical perturbation theory in Hamiltonian Mechanics

- $H(q, p, t; \varepsilon) = H_0(q, p) + \varepsilon H_1(q, p, t) + \varepsilon^2 H_2(q, p, t) + \cdots$, with the dynamics of H_0 solvable.
- One tries to find a symplectic near-identity transformation $(q, p) \longmapsto (Q, P)$ so that the new Hamiltonian K depends only on P: $K(P, t)$ easy to integrate
- Generating function $S(q, P, t) = qP + \varepsilon S_2(q, P, t) + \cdots$

$$K(P, t, \varepsilon) = K_0(P, t) + \varepsilon K_1(P, t) + \cdots$$

$$p = \frac{\partial S}{\partial q} = P + \varepsilon \frac{\partial S_2}{\partial q} + \cdots ; \qquad Q = \frac{\partial S}{\partial P} = q + \varepsilon \frac{\partial S_2}{\partial P} + \cdots$$

$$K = H + \frac{\partial S}{\partial t}$$

- Old *and* new variables $\Rightarrow$ solve implicit functional equations to express everything in terms of only the old or only the new variables.

Deprit algorithm in Classical Mechanics

- Modification introduced by Deprit (1969): the symplectic transformation is given by a *generator*: a function $w(q, p, \varepsilon) = w_1 + \varepsilon w_2 + \cdots$ such that the shift by 'time' ε along the trajectories of the 'Hamiltonian' w produces the required transformation $(q, p) \longmapsto (Q, P)$
- If $x \equiv (q, p)$, then $\frac{dx}{d\varepsilon} = \{x, w\}$.
- Corresponding to this transformation one has the *evolution operator* T such that $X \equiv (Q, P) = Tx$.

Deprit algorithm in Classical Mechanics

- To find T, one introduces the *Lie operator* $L \equiv \{w, \cdot\}$. Then

$$\frac{dT}{d\varepsilon} = -TL$$

- For non-autonomous systems, w, L and T are explicit functions of t, and

$$K = T^{-1}H + T^{-1}\int_0^\varepsilon d\varepsilon' \, T(\varepsilon')\frac{\partial w(\varepsilon')}{\partial \varepsilon}$$

- Everything is expanded as power series of ε.
- Very efficient computational algorithm.
- First application: Delaunay theory of the Lunar motion (1969).

Cary (1981), Lichtenberg & Lieberman (1983)

Delaunay theory

- "Delaunay worked at his theory without any assistance, by hand, for some 20 years continuously; his literal calculations cover two volumes in quarto of 400 pages each; he alone proofread them." (Deprit, Henrard & Rom)
- "Deprit and his collaborators linked it to a modern computer algebra program (MACSYMA) and reproduced Delunay's monumental calculations. The dramatic result of this double checking was that in 20 years of effort Delaunay made only one mistake —amounting to writing $147 - 90 + 9 = 46$— at the 9th order, all errors resulting from its propagation through other terms." (Michelotti)

Time-dependent perturbation theory in QM

- In QM, the time evolution of a wave function $\Psi(t)$ may described in terms of the evolution operator

$$\Psi(t) = U(t)\Psi(t_0),$$

where $U(t)$ is unitary: $U^\dagger(t) = U^{-1}(t)$, and verifies

$$i\hbar\dot{U}(t) = H(t)U(t), \qquad U(t_0) = I.$$

Schrödinger equation

- If $H(t) = H_0$, then $U(t) = \exp(-i(t - t_0)H_0/\hbar)$.

Time-dependent perturbation theory in QM

- Assume that $H(t, \varepsilon) = H_0 + H'(t, \varepsilon) \equiv H_0 + \sum_{n=1}^{\infty} \varepsilon^n H_n(t)$.
- One factorizes $U(t) = \exp(-i(t - t_0)H_0/\hbar)U_I(t)$, where the unknown operator $U_I(t)$ obeys

$$i\hbar \dot{U}_I(t) = H_I(t, \varepsilon) U_I(t), \qquad U_I(t_0) = I$$

with

$$H_I(t, \varepsilon) = \mathrm{e}^{-\frac{i}{\hbar} H_0 (t - t_0)} \, H'(t, \varepsilon) \, \mathrm{e}^{\frac{i}{\hbar} H_0 (t - t_0)}.$$

- Next we expand $U_I(t) = \sum_{n \geq 0} \varepsilon^n U_n(t)$.
- In particular

$$U_0 = I, \qquad U_1(t) = \int_{t_0}^{t} \mathrm{d}s \, H_I(s, \varepsilon).$$

- When the series is truncated, the approximation U_I is *not unitary*.

Comments

- Schemes in CM and QM are *completely* different.
- Question: is it possible to formulate a perturbation theory in QM by following the approach of CM?
- Back to 1925 and the birth of Matrix Mechanics: Born, Heisenberg and Jordan.
- Input: classical Hamiltonian mechanics, canonical transformations, old quantum theory, correspondence principle.
- Output: the first coherent formulation of Quantum Mechanics (<u>before</u> Schrödinger equation), including time-independent perturbation theory (but <u>also</u> time-dependent P.T.)

A word of caution...

"If the reader is mystified at what Heisenberg was doing, he or she is not alone. I have tried several times to read the paper that Heisenberg wrote on returning from Heligoland, and, although I think I understand quantum mechanics, I have never understood Heisenberg's motivations for the mathematical steps in his paper. Theoretical physicists in their most successful work tend to play one of two roles: they are either sages or magicians... It is usually not difficult to understand the papers of sage-physicists, but the papers of magician-physicists are often incomprehensible. In this sense, Heisenberg's 1925 paper was pure magic."

Steven Weinberg, Nobel Prize Laureate in Physics

Dreimännerarbeit: Time-independent perturbation theory

- Given $H = H_0 + \varepsilon H_1 + \varepsilon^2 H_2 + \cdots$, assume the problem defined by H_0 has been solved: we have determined Q^0 and P^0 such that $H_0(Q^0, P^0)$ is diagonal (but *not* $H(Q^0, P^0)$).
- Idea: to find a unitary transformation S ("canonical transformation") so that $P = S\,P^0 S^{-1}$, $Q = S\,Q^0 S^{-1}$ and the matrices P and Q diagonalize $K = SH(Q^0, P^0)S^{-1}$.
- Perturbative scheme: $K = K_0 + \varepsilon K_1 + \varepsilon^2 K_2 + \cdots$

$$
\begin{aligned}
S &= I + \varepsilon S_1 + \varepsilon^2 S_2 + \cdots \\
S^{-1} &= I - \varepsilon S_1 + \varepsilon^2 (S_1^2 - S_2) + \cdots
\end{aligned}
$$

- Then

$$
\begin{aligned}
K_0 &= H_0 \\
K_r &= S_r H_0 - H_0 S_r + F_r(H_0, \ldots, H_r, S_1, \ldots, S_{r-1})
\end{aligned}
$$

Dreimännerarbeit: Time-dependent perturbation theory

$$H(t, \varepsilon) = H_0 + \varepsilon H_1(t) + \varepsilon^2 H_2(t) + \cdots$$

- BHJ: "simple considerations show that the perturbation formulae ensue from those cited earlier on replacing every term of the form $H_0 S_r - S_r H_0$ by"

$$H_0 S_r - S_r H_0 - i\hbar \frac{\partial S_r}{\partial t}$$

  another magic sentence

- Same results as standard theory

Modern approach

- BHJ time-independent perturbation theory can be found in (not so) many textbooks on quantum mechanics: Tomonaga, Wu, Finkelstein, Messiah,...
- Time-dependent formalism almost completely forgotten.
- However,
  - In the mid-1990s, Scherer: "Quantum Averaging"
  - 2000, Daens *et al.*
  - 2004, Aniello

  a revival of this approach, with interesting results and applications.
- Serious limitations: the theory is not unitary; only the first orders have been explicitly obtained

III. OUR TREATMENT

Features not shared by previous schemes

- The formalism *is* unitary by construction at any order
- It is computationally well adapted (high order can be achieved)
- Flexible treatment: it can be applied to *any* linear differential equation
- It provides a natural connection with BHJ formalism and standard perturbation theory in QM

The problem

Solve the Schrödinger equation for the evolution operator $U(t)$:

$$i\hbar\dot{U} = H(t,\varepsilon)U, \qquad U(t_0) = I \tag{1}$$

where

$$H(t,\varepsilon) = H_0 + \varepsilon H_1(t) + \varepsilon^2 H_2(t) + \cdots$$

and the dynamics corresponding to H_0 (time-independent) can be obtained, i.e., we have determined

$$U_{H_0}(t,t_0) = \exp(-i(t-t_0)H_0/\hbar)$$

The procedure

We look for a unitary transformation $T(t,\varepsilon)$ such that the transformed system

$$i\hbar\dot{U}_K = K(t,\varepsilon)U_K, \qquad U_K(t_0) = I \tag{2}$$

is easier to solve than the original equation $i\hbar\dot{U} = H(t,\varepsilon)U$.

- We try to determine $T(t,\varepsilon)$ as a unitary near-identity transformation, i.e.,

$$T^\dagger(t,\varepsilon) = T^{-1}(t,\varepsilon), \qquad T(t,\varepsilon) = I + \mathcal{O}(\varepsilon).$$

- Connection between $U(t,t_0)$ and $U_K(t,t_0)$ (change of picture):

$$U(t,t_0) = T(t,\varepsilon)U_K(t,t_0)T^\dagger(t_0,\varepsilon)$$

The transformation

- It follows that
$$K = T^\dagger H T + i\hbar \frac{\partial T^\dagger}{\partial t} T \tag{3}$$
(the (t,ε) dependency has been omitted for clarity)
- Two (equivalent) options guaranteeing that T is unitary:
  - Introduce S such that $T(t,\varepsilon) = \exp(S(t,\varepsilon))$
  - Introduce a skew-Hermitian operator $L(t,\varepsilon)$ (the generator) such that $T(t,\varepsilon)$ is the solution of the operator differential equation
  $$\frac{\partial T}{\partial \varepsilon} = -T\,L, \qquad T(t,\varepsilon = 0) = I \tag{4}$$
  This is precisely Deprit's approach in classical mechanics
- Eq. (4) is a differential equation in the 'time' variable ε, the perturbation parameter.

The transformation

We follow the second approach.

- $L(t, \varepsilon)$ and $T(t, \varepsilon)$ have to be determined.
- From now on, the formalism is expressed in terms of $L(t, \varepsilon)$ (the generator of the unitary transformation)
- Once $L(t, \varepsilon)$ is obtained, we "only" have to solve the equation $\frac{\partial T}{\partial \varepsilon} = -T\,L$ to construct the transformation T.
- It is worth noticing that

$$\frac{\partial T^\dagger}{\partial \varepsilon} = L\,T^\dagger, \qquad T^\dagger(t, \varepsilon = 0) = I \tag{5}$$

so that we can write $T^\dagger(t, \varepsilon) = \mathrm{e}^{\Omega(t,\varepsilon)}$ and get $\Omega(t, \varepsilon)$ (for instance, with the Magnus expansion)

The formalism

- Deriving the relation $K = T^\dagger H T + i\hbar \frac{\partial T^\dagger}{\partial t} T$ with respect to ε and taking into account $\frac{\partial T}{\partial \varepsilon} = -T\, L$ we arrive at

$$\frac{\partial K}{\partial \varepsilon} = [L, K] + T^\dagger \frac{\partial H}{\partial \varepsilon} T + i\hbar \frac{\partial L}{\partial t} \tag{6}$$

- This is the equation we work with in the following.
- It is then clear that $T = \mathrm{e}^{-\Omega}$ and thus

$$T^\dagger \frac{\partial H}{\partial \varepsilon} T = \mathrm{e}^{\Omega} \frac{\partial H}{\partial \varepsilon} \mathrm{e}^{-\Omega} = \mathrm{e}^{\mathrm{ad}_\Omega} \frac{\partial H}{\partial \varepsilon} = \sum_{n=0}^{\infty} \frac{1}{n!} \mathrm{ad}_\Omega^n \frac{\partial H}{\partial \varepsilon}$$

The formalism

- In consequence

$$\frac{\partial K}{\partial \varepsilon} = [L, K] + \mathrm{e}^{\mathrm{ad}_\Omega} \frac{\partial H}{\partial \varepsilon} + i\hbar \frac{\partial L}{\partial t} \tag{7}$$

  an equation formulated only in terms of L, H and K, easier to handle than (6).

- Recall: We want to find a unitary transformation T generated by L such that $i\hbar \dot{U}_K = K U_K$ is easier to solve than the original equation $i\hbar \dot{U} = HU$.
- Three problems here:
  1. Choose K.
  2. Compute L.
  3. Construct T.
- It turns out that problems 1 and 2 can be solved perturbatively with (7), whereas 3 is solved independently.

Perturbative scheme

- Given

$$H(t,\varepsilon) = H_0 + \sum_{n\geq 1} \varepsilon^n H_n(t)$$

we introduce the series expansions

$$K(t,\epsilon) = \sum_{n=0}^{\infty} \epsilon^n K_n(t), \qquad L(t,\epsilon) = \sum_{n=0}^{\infty} \epsilon^n L_{n+1}(t)$$

- Then $\Omega(t,\epsilon)$ in $T = \exp(-\Omega)$ can be determined algorithmically as a power series in ϵ.
- In fact, we can use the results already obtained when designing geometric integrators from the Magnus expansion.
- By applying typical recurrences for the Magnus expansion applied to $\frac{\partial T^\dagger}{\partial \varepsilon} = LT^\dagger$ with $L = L_1 + \varepsilon L_2 + \cdots$ we get

Perturbative scheme

$$T^{\dagger}(t,\varepsilon) = \mathrm{e}^{\Omega(t,\varepsilon)}, \qquad \Omega(t,\epsilon) = \sum_{n=1}^{\infty} \epsilon^n v_n(t) \tag{8}$$

with

$$\begin{aligned}
v_1 &= L_1, \qquad v_2 = \frac{1}{2}L_2, \qquad v_3 = \frac{1}{3}L_3 - \frac{1}{12}[L_1, L_2] \\
v_4 &= \frac{1}{4}L_4 - \frac{1}{12}[L_1, L_3] \\
v_5 &= \frac{1}{5}L_5 - \frac{3}{40}[L_1, L_4] - \frac{1}{60}[L_2, L_3] + \frac{1}{360}[L_1, [L_1, L_3]] \\
&\quad - \frac{1}{240}[L_2, [L_1, L_2]] + \frac{1}{720}[L_1, [L_1, [L_1, L_2]]]
\end{aligned}$$

Thus, we can construct T once L is determined (Problem 3 solved).

On the other hand,

$$e^{\mathrm{ad}_\Omega} \frac{\partial H}{\partial \varepsilon} = \sum_{n=0}^{\infty} \epsilon^n w_n(t)$$

with

$$\begin{aligned}
w_0 &= H_1 \\
w_1 &= 2H_2 + [L_1, H_1] \\
w_2 &= 3H_3 + 2[L_1, H_2] + \frac{1}{2}[L_2, H_1] + \frac{1}{2}[L_1, [L_1, H_1]] \\
w_3 &= 4H_4 + \frac{1}{12}\Big([H_1, [L_1, L_2]] + 2[L_1, [L_1, [L_1, H_1]]] \\
&\quad +12[L_1, [L_1, H_2]] + 3[L_1, [L_2, H_1]] + 36[L_1, H_3] \\
&\quad +3[L_2, [L_1, H_1]] + 12[L_2, H_2] + 4[L_3, H_1]\Big)
\end{aligned}$$

Homological equation

- Finally, by substituting into

$$\frac{\partial K}{\partial \varepsilon} = [L, K] + \mathrm{e}^{\mathrm{ad}_\Omega} \frac{\partial H}{\partial \varepsilon} + i\hbar \frac{\partial L}{\partial t}$$

we arrive at

$$\begin{aligned} K_0 &= H_0 \\ i\hbar \frac{\partial L_n}{\partial t} + [L_n, H_0] &= n\, K_n - \tilde{F}_n, \qquad n = 1, 2, \ldots \end{aligned} \tag{9}$$

with

$$\tilde{F}_n = \sum_{j=1}^{n-1} [L_{n-j}, K_j] + w_{n-1}$$

- Next step: propose a suitable K_n and solve (9) to get L_n.
- Notice that the expressions for v_j and w_j have to be computed only once.

Choosing $K_n(t)$

- Now we have to choose appropriately $K = \sum_{n\geq 0} \varepsilon^n K_n$.
- Simplest option: $K = H_0$. Then

$$K_n = 0, \qquad n \geq 1$$

- In that case $U_K(t) = \exp\big(-iH_0(t-t_0)/\hbar\big)$ and

$$U(t) = T(t,\varepsilon)\,\mathrm{e}^{-\frac{i}{\hbar}H_0(t-t_0)} = \mathrm{e}^{-\Omega(t,\varepsilon)}\,\mathrm{e}^{-\frac{i}{\hbar}H_0(t-t_0)}.$$

- The whole ε dependency is contained in T.
- Unitary scheme.

Choosing $K_n(t)$

- Another possibility: suppose H_0 has a pure non-degenerate point spectrum. In that case we can choose K_n diagonal, and

$$U_K(t) = \mathrm{e}^{-\frac{i}{\hbar}\sum_{n\geq 0} \varepsilon^n \int_{t_0}^{t} K_n(u)du}$$

- More general situation: The solution of $i\hbar\dot{U}_K = KU_K$ is

$$U_K(t) = \mathrm{e}^{-\frac{i}{\hbar}\int_{t_0}^{t} K(u)du} \quad \Longleftrightarrow \quad \left[\int_{t_0}^{t} K(u)du, K(t)\right] = 0.$$

  This holds in particular if one takes $K_n(t)$ such that

$$[K_0, K_n(t)] = 0, \qquad [K_m(t), K_n(t)] = 0 \qquad \forall\ m, n \geq 1$$

  Finally

$$U(t) = \mathrm{e}^{-\Omega(t,\varepsilon)}\, \mathrm{e}^{-\frac{i}{\hbar}\int_{t_0}^{t} K(u)du}$$

- Notice that both T and U_K are series in ε *which have to be truncated at a given order* ε^m.

Determining $L_n(t)$

- One K_n is chosen, we have to compute L_n solution of

$$i\hbar\frac{\partial L_n}{\partial t} + [L_n, H_0] = n\,K_n - \tilde{F}_n, \qquad n \geq 1$$

- Formal solution ($t_0 = 0$):

$$\begin{aligned} L_n(t) = \quad & \exp(-itH_0/\hbar)\,L_n(0)\exp(itH_0/\hbar) \\ & -\frac{i}{\hbar}\int_0^t \mathrm{d}u\,\exp\big(-i(t-u)H_0/\hbar\big) \\ & \big(nK_n(u) - \tilde{F}_n(u)\big)\exp\big(i(t-u)H_0/\hbar\big), \end{aligned} \tag{10}$$

- Very often we will take $L_n(0) = 0$:

$$L_n(t) = -\frac{i}{\hbar}\int_0^t \mathrm{d}u\,\mathrm{e}^{-i(t-u)H_0/\hbar}\big(nK_n(u) - \tilde{F}_n(u)\big)\,\mathrm{e}^{i(t-u)H_0/\hbar}$$

BHJ perturbation theory

- We recover the BHJ perturbation theory (and therefore the standard one) by
  - Taking $K = H_0$
  - Expanding $T(t,\varepsilon) = \mathrm{e}^{-\Omega(t,\varepsilon)}$ in power series of ε (*non unitary!*)
- At first order in ε,

$$\begin{aligned} U(t) &= (I - \varepsilon L_1(t))\, \mathrm{e}^{-\frac{i}{\hbar}H_0 t} \\ L_1(t) &= \frac{i}{\hbar}\int_0^t \mathrm{d}u\, \mathrm{e}^{-i(t-u)H_0/\hbar}\, H_1(u)\, \mathrm{e}^{i(t-u)H_0/\hbar} \end{aligned}$$

- Then

$$U(t) = \mathrm{e}^{-\frac{i}{\hbar}H_0 t}\left(I - \varepsilon \frac{i}{\hbar}\int_0^t H_I(u)du\right)$$

  where

$$H_I(u) = \mathrm{e}^{iuH_0/\hbar}\, H_1(u)\, \mathrm{e}^{-iuH_0/\hbar}$$

- *This is precisely the result achieved by standard perturbation theory in the interaction picture defined by H_0.*

Time-independent perturbation

- The standard theory is also reproduced when $H \neq H(t)$.
- Then T is chosen as time-independent,

$$K(\varepsilon) = \mathrm{e}^{\Omega(\varepsilon)}\, H(\varepsilon)\, \mathrm{e}^{-\Omega(\varepsilon)}$$

and $K(\varepsilon)$ is taken so that $[H_0, K] = 0$. In this way H_0 *and* K *can be simultaneously diagonalized*.

- Equations to solve:

$$[L_n, H_0] = n\, K_n - \tilde{F}_n, \qquad [K_n, H_0] = 0, \qquad n \geq 1.$$

- Solution (averaging):

$$\begin{aligned} K_n &= \frac{1}{n} \lim_{\tau \to \infty} \frac{1}{\tau} \int_0^{\tau} du\, \mathrm{e}^{-\frac{i}{\hbar} H_0 u}\, \tilde{F}_n\, \mathrm{e}^{\frac{i}{\hbar} H_0 u} \\ L_n &= \frac{i}{\hbar} \lim_{\tau \to \infty} \frac{1}{\tau} \int_0^{\tau} dt \int_0^{t} ds \left(\mathrm{e}^{-\frac{i}{\hbar} H_0 s}\, \tilde{F}_n\, \mathrm{e}^{\frac{i}{\hbar} H_0 s} - n\, K_n \right) \end{aligned}$$

IV. AN EXAMPLE

An example from NMR

- Hamiltonian

$$H(t) = \frac{1}{2}\hbar\omega_0\sigma_3 + \varepsilon(\sigma_1 \cos\omega t + \sigma_2 \sin\omega t)$$

- Exact solution of $i\hbar\dot{U} = H(t)U$, $U(0) = I$:

$$U(t) = \mathrm{e}^{-\frac{i}{2}\omega t\sigma_3}\,\mathrm{e}^{-it\left(\frac{1}{2}(\omega_0-\omega)\sigma_3+\frac{\varepsilon}{\hbar}\sigma_1\right)}$$

- Exact transition probability between states 1 and 2:

$$|U_{21}(t)|^2 = \left(\frac{2\varepsilon}{\omega'}\sin\frac{\omega' t}{2}\right)^2$$

with $\omega' = \sqrt{(\omega_0-\omega)^2 + 4\varepsilon^2/\hbar^2}$.

Perturbative treatment

- $H(t) = H_0 + \varepsilon H_1(t)$ with

$$H_0 = \frac{1}{2}\hbar\omega_0\sigma_3, \qquad H_1(t) = \sigma_1 \cos\omega t + \sigma_2 \sin\omega t$$

- Previous formalism up to $n = 10$. Then

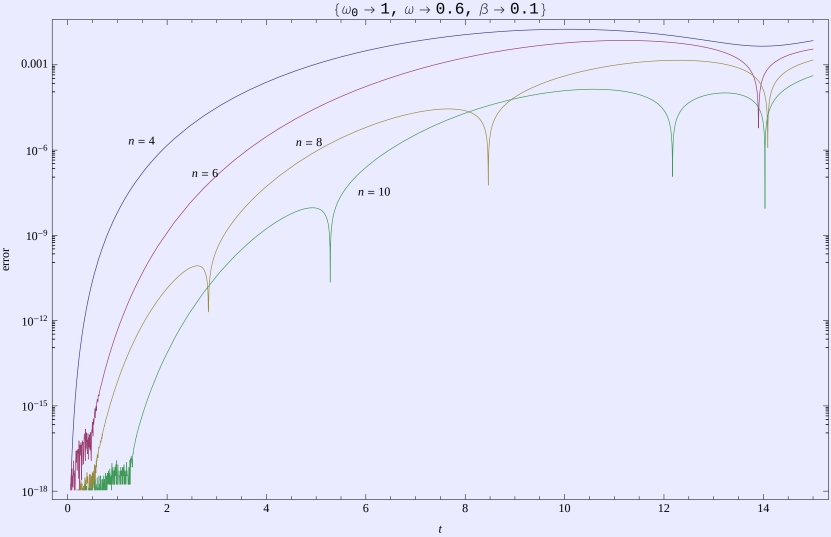
$$\begin{aligned} K &= \sum_{n=0}^{10} \varepsilon^n K_n(t) \quad \Rightarrow \quad U_K(t) = \mathrm{e}^{-\frac{i}{\hbar}\int_0^t K(u)du} \\ L &= \sum_{n=0}^{10} \varepsilon^n L_{n+1}(t) \quad \Rightarrow \quad \Omega(t,\varepsilon) \text{ such that} \\ & \quad T(t,\varepsilon) = \mathrm{e}^{-\Omega(t,\varepsilon)} \end{aligned}$$

- Finally

$$U(t) \simeq T(t,\varepsilon)U_K(t) = \mathrm{e}^{-\Omega(t,\varepsilon)}\,\mathrm{e}^{-\frac{i}{\hbar}\int_0^t K(u)du}$$

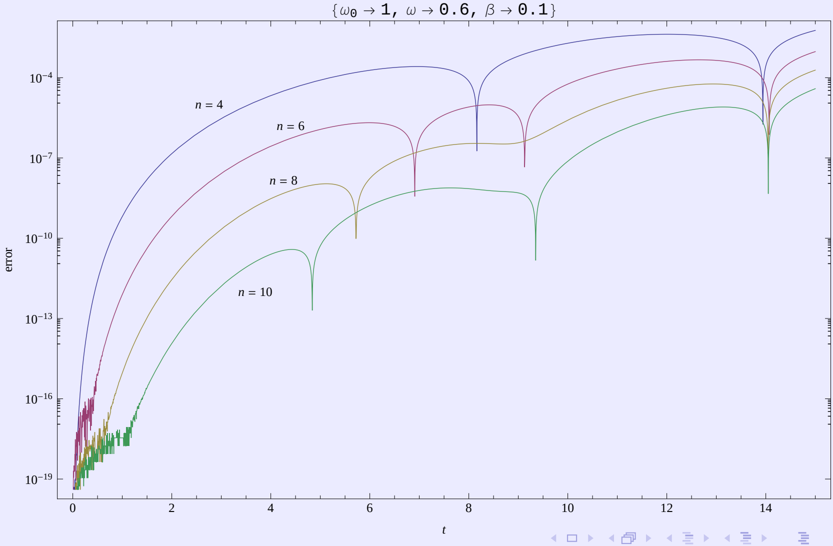
from which we compute the transition probability

First choice: $K_n(t)$ diagonal ($\beta = \varepsilon$)

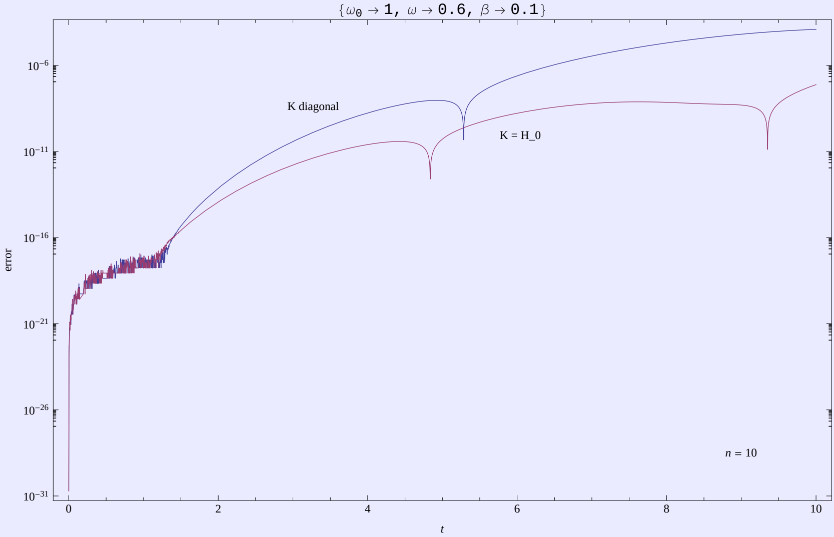


Second choice: $K_0 = H_0$, $K_n = 0$, $(n \geq 1)$. Then

$$U(t) \simeq \mathrm{e}^{-\Omega(t,\varepsilon)}\, \mathrm{e}^{-\frac{i}{\hbar} H_0 t}$$



Comparison



$\{\omega_0 \to 1, \omega \to 0.6, \beta \to 0.1\}$
error
10^{-6}
10^{-11}
10^{-16}
10^{-21}
10^{-26}
10^{-31}
K diagonal
K = H_0
$n = 10$
0
2
4
6
8
10
t

V. FURTHER DEVELOPMENTS

- The treatment is *formal*. It makes sense, then, to analyze mathematical conditions which guarantee the existence of the transformation, the existence of solutions for the homological equation, the convergence of the procedure, etc.
- The scheme can be applied to the general linear equation $\dot{Y} = (A_0 + A_I(t,\varepsilon))Y$
- Important case: when $A_I(t,\varepsilon)$ is periodic. Then Floquet theory applies. Same results as with the Floquet–Magnus expansion (C., Oteo & Ros, 2001) which *is* convergent.
- Instead of only *one* transformation, we could consider a *sequence* of transformations (*à la* KAM theory).
- Reducibility of linear equations: given $\dot{Y} = (A_0 + A_I(t,\varepsilon))Y$, when is it possible to construct a transformation T such that in the new coordinates the coefficient matrix is constant, i.e, $\dot{X} = BX$, with B constant? (Lyapunov, Erugin, Bogoliubov, etc.)