Perturbative approach to the time evolution of periodic quantum systems

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Analytic and algebraic methods in physics XXII

Outline for section 1

Introduction

Consider the Schrödinger's equation with an initial condition

$$H(t)\,|\psi(t)\rangle = i\hbar\frac{d}{dt}\,|\psi(t)\rangle\,, \qquad |\psi(t=t_0)\rangle = |\psi_0\rangle\,, \tag{1}$$

and an unitary operator $U(t,t_0)$ such that $|\psi(t)\rangle = U(t,t_0)\,|\psi_0\rangle$.
Then, we arrive to the time evolution equation.

$$\frac{d}{dt'}U(t',t_0) = -iH(t')U(t',t_0), \qquad U(t',t_0)|_{t_0} = I. \tag{2}$$

Here, $t' = t/\hbar$. Advantage that the parameter t' is mute.

$$U(t,t_0) = -i\int_{t_0}^{t} H(t_1)U(t_1,t_0)dt_1. \tag{3}$$

Introduction

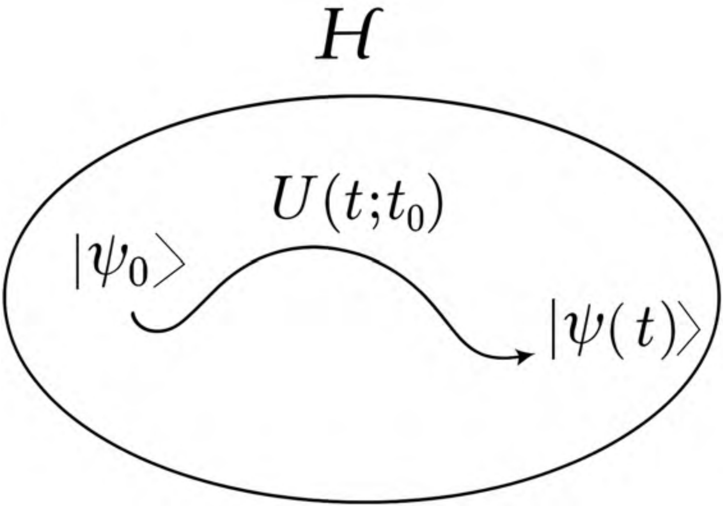


Figure: Dynamics of a state in the Hilbert space.

Outline for section 2

Stationary system

Let H_0 be a stationary Hamiltonian and U_0 the generator of the evolution. Consider a basis $\{\left|u_n^0\right\rangle\}_{n=1}^N$ with a g-fold degenerate eigenvalue, such that

$$\left\langle u_i^0 \middle| u_j^0 \right\rangle = \delta_{ij}, \qquad \sum_n \left|u_n^0\right\rangle \left\langle u_n^0\right| = \mathbb{I}, \tag{4}$$

and

$$H_0 \left|u_n^0\right\rangle = E_n^0 \left|u_n^0\right\rangle, \tag{5}$$

$$U_0(t, t_0) \left|u_n^0\right\rangle = \lambda_n^0 \left|u_n^0\right\rangle. \tag{6}$$

Here, $U_0(t, t_0) = e^{-iH_0(t-t_0)}$, $\lambda_n^0 = e^{-iE_n^0(t-t_0)}$.

The perturbation

When the stationary system interacts with a classical field, the Hamiltonian is [1].

$$\mathscr{H}(t) = H_0 + \varepsilon\gamma(t)V. \qquad (7)$$

Under the hypotheses:

- ε is the smallness parameter ($|\varepsilon\gamma(t)| << 1$).
- $\gamma(t+T) = \gamma(t)$ is the time-dependent function of period T.
- V is the interaction potential comparable with H_0.

Here, both H_0 and V must be Hermitian.

[1] V. K. Thankappan, Quantum Mechanics. Wiley Eastern Limited, 1985, isbn: 0-470-20072-3.

The eigenvalue equation

Through the Floquet theorem [2], let $\{u_n\}_{n=1}^{N}$ be an orthonormal basis of Floquet states that fulfil

$$\langle u_i | u_j \rangle = \delta_{ij}, \qquad \sum_n |u_n\rangle \langle u_n| = \mathbb{I}, \tag{8}$$

and the generator of the evolution satisfies the eigenvalue equation

$$U(\varepsilon)\,|u_n\rangle = \lambda_n\,|u_n\rangle\,. \tag{9}$$

Here, the elements of equation (9) are given by:

$$U(\varepsilon) = U_0(T) + \varepsilon U_1(T) + \varepsilon^2 U_2(T) + \ldots \tag{10}$$

$$|u_n\rangle = |n\rangle + \varepsilon\,|u_n^1\rangle + \varepsilon^2\,|u_n^2\rangle + \ldots \tag{11}$$

$$\lambda_n = \lambda_n^0 + \varepsilon\lambda_n^1 + \varepsilon^2\lambda_n^2 + \ldots \tag{12}$$

[2] S. P. Eastham, B. M. Brown and K. M. Schmidt, Quantum Mechanics, Springer Basel, 2013, isbn: 978-3-0348-0527-8.

Expressions for the corrections

Through the equations from (9) to (12), we get

$$\varepsilon^0 : \left(U_0 - \lambda_n^0\right)|n\rangle = 0, \tag{13}$$

$$\varepsilon^1 : \left(U_0 - \lambda_n^0\right)\left|u_n^1\right\rangle = -\left(U_1 - \lambda_n^1\right)|n\rangle\,, \tag{14}$$

$$\varepsilon^2 : \left(U_0 - \lambda_n^0\right)\left|u_n^2\right\rangle = -\left(U_2 - \lambda_n^2\right)|n\rangle - \left(U_1 - \lambda_n^1\right)\left|u_n^1\right\rangle\,, \tag{15}$$

$$\vdots$$

$$\varepsilon^k : \left(U_0 - \lambda_n^0\right)\left|u_n^k\right\rangle = -\left(U_k - \lambda_n^k\right)|n\rangle - \ldots - \left(U_1 - \lambda_n^1\right)\left|u_n^{k-1}\right\rangle. \tag{16}$$

Thus, our goal is to calculate the corrections $U_i, \lambda_n^i, \left|u_n^i\right\rangle$, $i = 1, 2$.

Factorization method

In order to know $U(T)$ up to the second order correction, we propose

$$U(t) = U_0(t, t_0)W(t). \tag{17}$$

Substituting in equation (2) and fitting the Magnus expansion[3][4]

$$\begin{aligned} U(T) = U_0(T,0)\Bigg\{ & \mathbb{I} - \varepsilon i \int_0^T dt_1 \gamma(t_1) V(t_1) \\ & - \varepsilon^2 \frac{1}{2}\left[\int_0^T dt_2 \int_0^{t_2} dt_1 \gamma(t_2)\gamma(t_1)[V(t_2), V(t_1)] \right. \\ & \left. + \left(\int_0^T dt_1 \gamma(t_1) V(t_1) \right)^2 \right] \Bigg\} + \dots, \quad V(t) = U_0^\dagger(t) V U_0(t) \end{aligned} \tag{18}$$

[3] D. J. Tannor. Introduction to Quantum Mechanics: A Time-Dependent Perspective. Maple Vail Book Manufacturing Group, 1958. isbn: 1-891389-23-8.

[4] S. Blanes, F. Casas, J.A. Oteo, J. Ros. The Magnus expansion and some of its applications. Physics Reports 470,2009, 151–238, doi: 0375-9601/97/17.00

$U(T)$ corrections

Immediately we obtain

$$\varepsilon^0: \; U_0(T) = e^{-iH_0 T} \tag{19}$$

$$\varepsilon^1: \; U_1(T) = -iU_0(T) \int_0^T dt_1 \gamma(t_1) V(t_1) \tag{20}$$

$$\begin{aligned} \varepsilon^2: \; U_2(T) = -\frac{1}{2} \Bigg[\int_0^T dt_2 \int_0^{t_2} dt_1 \gamma(t_2)\gamma(t_1) [V(t_2), V(t_1)] \\ + \left(\int_0^T dt_1 \gamma(t_1) V(t_1) \right)^2 \Bigg] \Bigg\} \end{aligned} \tag{21}$$

Outline for section 3

State correction of k-order

The basis $\{|u_n^0\rangle\}_{n=1}^N$ has no degenerations. Then, by projecting $\langle u_n^0|$ over equation (16), we obtain the correction to k-order

$$\left|u_n^k\right\rangle = \left\langle u_n^0\middle|u_n^k\right\rangle |u_n^0\rangle + \sum_{m\neq n} \frac{|u_m^0\rangle\langle u_m^0|}{\lambda_n^0-\lambda_m^0}\Big[(U_1-\lambda_n^1)\left|u_n^{k-1}\right\rangle + (U_2-\lambda_n^2)\left|u_n^{k-2}\right\rangle + \ldots + \left(U_k-\lambda_n^k\right)|u_n^0\rangle\Big]. \tag{22}$$

with the conditions,

$$\langle u_n^1|u_n^0\rangle = \langle u_n^0|u_n^1\rangle = 0, \tag{23}$$

$$\langle u_n^2|u_n^0\rangle = \langle u_n^0|u_n^2\rangle = -\frac{1}{2}\langle u_n^1|u_n^1\rangle, \ldots, \tag{24}$$

$$\left\langle u_n^k\middle|u_n^0\right\rangle = \left\langle u_n^0\middle|u_n^k\right\rangle = -\frac{1}{2}\left[\left\langle u_n^{k-1}\middle|u_n^1\right\rangle + \ldots + \left\langle u_n^1\middle|u_n^{k-1}\right\rangle\right]. \tag{25}$$

Corrections of 1st order

For $k = 1$ in equation (22) and projecting $\left\langle u_n^0 \right|$ over equation (14), we obtain

$$\left| u_n^1 \right\rangle = -i \sum_{m \neq n} \lambda_m^0 \frac{\int_0^T \gamma(t_1) e^{-i\omega_{nm} t_1} dt_1}{\lambda_n^0 - \lambda_m^0} \left\langle u_m^0 \right| V \left| u_n^0 \right\rangle \left| u_m^0 \right\rangle, \qquad (26)$$

$$\lambda_n^1 = -i\lambda_n^0 \int_0^T \gamma(t_1) dt_1 \left\langle u_n^0 \right| V \left| u_n^0 \right\rangle. \qquad (27)$$

With $\omega_{nm} = E_n^0 - E_m^0$. Expressing λ_n as an exponential

$$\lambda_n = \lambda_n^0 + \varepsilon \lambda_n^1 = \lambda_n^0 (1 - \varepsilon i \alpha T) \approx e^{-i\left(E_n^0 + \varepsilon\alpha\right) T}, \qquad (28)$$

where $\lambda_n^1 = -i\alpha T \lambda_n^0$.

Corrections of 2nd order

For $k=2$ in equation (22), we obtain

$$\begin{aligned}\left|u_n^2\right\rangle = &-\frac{1}{2}\left\langle u_n^1\middle|u_n^1\right\rangle\left|u_n^0\right\rangle \\ &+\sum_{m\neq n}\frac{\left|u_m^0\right\rangle}{\lambda_n^0-\lambda_m^0}\left\{\sum_{s\neq n}(\alpha-\beta)\left\langle u_s^0\right|V\left|u_n^0\right\rangle\left\langle u_m^0\right|V\left|u_s^0\right\rangle\right. \\ &\left.-\left[\left(i\frac{\lambda_n^0\lambda_m^0}{\lambda_n^0-\lambda_m^0}-1\right)\phi+\eta\right]\left\langle u_n^0\right|V\left|u_n^0\right\rangle\left\langle u_m^0\right|V\left|u_n^0\right\rangle\right\},\end{aligned} \tag{29}$$

with

- $\alpha = i\lambda_m^0 cot\left(\omega_{ns}\frac{T}{2}\right)\int_0^T\gamma(t_1)e^{-i\omega_{ns}t_1}dt_1\int_0^T\gamma(t_2)e^{-i\omega_{sm}t_2}dt_2.$
- $\beta = \frac{1}{2}\lambda_m^0\int_0^T\int_0^{t_2}\gamma(t_2)\gamma(t_1)\left[e^{-i\left(\omega_{ns}t_1+\omega_{sm}t_2\right)}-e^{-i\left(\omega_{ns}t_2+\omega_{sm}t_1\right)}\right]dt_1dt_2.$
- $\phi = \int_0^T\gamma(t_1)dt_1\int_0^T\gamma(t_2)e^{-i\omega_{nm}t_2}dt_2.$
- $\eta = \frac{1}{2}\lambda_m^0\int_0^T\int_0^{t_2}\gamma(t_2)\gamma(t_1)\left[e^{-i\omega_{nm}t_2}-e^{-i\omega_{nm}t_1}\right]dt_1dt_2.$

Corrections of 2nd order

Projecting $\left\langle u_n^0 \right|$ over the equation (15), we get

$$\lambda_n^2 = -\lambda_n^0 \Big[i \textstyle\sum_{m\neq n} \Big(cot\big(\omega_{nm}\frac{T}{2}\big) \Big| \int_0^T \gamma(t_1) e^{-i\omega_{nm}t_1} dt_1 \Big|^2 + \int_0^T \int_0^{t_2} \gamma(t_2)\gamma(t_1) sin(\omega_{nm}(t_2 - t_1)) dt_1 dt_2 \Big) \left| \left\langle u_n^0 \right| V \left| u_m^0 \right\rangle \right|^2 + \frac{1}{2} \Big(\int_0^T \gamma(t_1) dt_1 \Big)^2 \Big(\left\langle u_n^0 \right| V \left| u_n^0 \right\rangle \Big)^2 \Big], \tag{30}$$

Expressing the eigenvalue as an exponential,

$$\lambda_n \approx exp\Big\{ -i \Big(E_n^0 + \varepsilon \frac{1}{T} \int_0^T \gamma(t_1) dt_1 \left\langle u_n^0 \right| V \left| u_n^0 \right\rangle + \varepsilon^2 \frac{1}{T} \textstyle\sum_{m\neq n} \eta \left| \left\langle u_n^0 \right| V \left| u_m^0 \right\rangle \right|^2 \Big) T \Big\}, \tag{31}$$

with $\eta = cot\big(\omega_{nm}\frac{T}{2}\big) \Big| \int_0^T \gamma(t_1) e^{-i\omega_{nm}t_1} dt_1 \Big|^2 + \int_0^T \int_0^{t_2} \gamma(t_2)\gamma(t_1) sin(\omega_{nm}(t_2 - t_1)) dt_1 dt_2$.

Outline for section 4

Constructing the degenerate case

Consider the basis $\{|u_n^0\rangle\}_{n=1}^N$ with a g-fold degenerate eigenvalue, such that for $i \leq g$

$$H_0 |u_i^0\rangle = E^0 |u_i^0\rangle, \quad E^0 = E_1^0 = \ldots = E_i^0 \tag{32}$$

$$U_0(t, t_0) |u_i^0\rangle = \lambda^0 |u_i^0\rangle, \quad \lambda^0 = \lambda_1^0 = \ldots = \lambda_i^0 \tag{33}$$

Constructing the basis $\{|n\rangle\}_{n=1}^N$ in such a way that

$$|n\rangle = \begin{cases} \sum_i^g S_{in} |u_i^0\rangle, & n \leq g, \quad S_{in} \in [0, 1] \\ |u_n^0\rangle, & n > g \end{cases} \tag{34}$$

and each $|n\rangle$ is normalized in the same way that each $|u_n^0\rangle$.

S_{in} coefficients for the first order correction

Projecting $\left\langle u_j^0 \right|$ $(j \leq g)$ over equation (14),

$$\sum_{i=1}^{g} \left[\left\langle u_j^0 \right| U_1 \left| u_i^0 \right\rangle - \lambda_n^1 \delta_{ij} \right] S_{in} = 0. \tag{35}$$

As a matrix equation

$$\left[\mathbf{U_1} - \lambda_n^1 \mathbb{I}_g \right] S_n = 0, \tag{36}$$

$$\mathbf{U_1} = \begin{bmatrix} U_{11} & U_{12} & \dots & U_{1g} \\ U_{21} & U_{22} & \dots & U_{2g} \\ \vdots & \vdots & \ddots & \vdots \\ U_{g1} & U_{g2} & \dots & U_{gg} \end{bmatrix}, \quad S_n = \begin{bmatrix} S_{1n} \\ S_{2n} \\ \vdots \\ S_{gn} \end{bmatrix}, \quad \lambda_n^1 = \langle n | U_1 | n \rangle . \tag{37}$$

K-order correction for the states

Projecting $\langle m|$ $(m > g)$ over equation (16),we obtain

$$\left|u_n^k\right\rangle = \sum_{m\leq g} \left\langle m\middle|u_n^k\right\rangle |m\rangle + \sum_{m>g} \frac{|m\rangle\langle m|}{\lambda_n^0 - \lambda_m^0}\Bigg[\left(U_1 - \lambda_n^1\right)\left|u_n^{k-1}\right\rangle + \left(U_2 - \lambda_n^2\right)\left|u_n^{k-2}\right\rangle + \ldots + \left(U_k - \lambda_n^k\right)|n\rangle \Bigg]. \tag{38}$$

Where the new conditions are

$$\left\langle u_n^1\middle|m\right\rangle = \left\langle m\middle|u_n^1\right\rangle = 0, \tag{39}$$

$$\left\langle u_n^2\middle|m\right\rangle = \left\langle m\middle|u_n^2\right\rangle = -\frac{1}{2}\left\langle u_n^1\middle|u_m^1\right\rangle, \ldots, \tag{40}$$

$$\left\langle u_n^k\middle|m\right\rangle = \left\langle m\middle|u_n^k\right\rangle = -\frac{1}{2}\left[\left\langle u_n^{k-1}\middle|u_m^1\right\rangle + \ldots + \left\langle u_n^1\middle|u_m^{k-1}\right\rangle\right]. \tag{41}$$

Correction to the 1st order

Evaluating $k = 1$ in (38) and projecting $\langle n|$ over equation (14),we obtain

$$\left|u_n^1\right\rangle = -i \sum_{i=1}^{g} S_{in} \sum_{m>g} \frac{\lambda_m^0}{\lambda_n^0 - \lambda_m^0} \int_0^T \gamma(t_1) e^{-i\omega_{nm}t_1} dt_1 \left\langle u_m^0\right| V \left|u_i^0\right\rangle \left|u_m^0\right\rangle, \tag{42}$$

$$\lambda_n^1 = -i\lambda_n^0 \int_0^T \gamma(t_1) dt_1 \sum_{i,j=1}^{g} S_{in} S_{jn} \left\langle u_i^0\right| V \left|u_j^0\right\rangle. \tag{43}$$

So, the eigenvalue is given by

$$\lambda_n \approx e^{-i\left(E_n^0 + \varepsilon \frac{1}{T} \int_0^T \gamma(t_1) dt_1 \sum_{i,j=1}^{g} S_{in} S_{jn} \left\langle u_i^0\right| V \left|u_j^0\right\rangle\right) T}. \tag{44}$$

Outline for section 5

Two-levels system

Consider the basis $\{|0\rangle, |1\rangle\}$ and an external interaction with an oscillatory field. The Hamiltonian is given by

$$H(t) = -\frac{\omega_0}{2}\sigma_3 + \varepsilon cos(\omega t)\sigma_1. \tag{45}$$

The evolution operator up to the first order in ε is

$$U(T,0) = U_0\left\{1 - \varepsilon\frac{i}{2}\left[\left(\frac{1}{\omega_-}sin(\omega_- T) + \frac{1}{\omega_+}sin(\omega_+ T)\right)\sigma_1 \right.\right.$$
$$\left.\left. + \left(-\frac{1}{\omega_-}\left(cos(\omega_- T) - 1\right) + \frac{1}{\omega_+}\left(cos(\omega_+ T) - 1\right)\right)\sigma_2\right]\right\}. \tag{46}$$

Here, $\omega_- = \omega - \omega_0$ and $\omega_+ = \omega + \omega_0$.

Two-levels system

Also, let $|\psi_0\rangle \in \mathbb{H}$ an arbitrary state and $a, b \in \mathbb{C}$ such that

$$|\psi_0\rangle = a|0\rangle + b|1\rangle = \begin{bmatrix} a \\ b \end{bmatrix}, \quad \||\psi_0\rangle\|^2 = |a|^2 + |b|^2 = 1. \tag{47}$$

Evolving the state

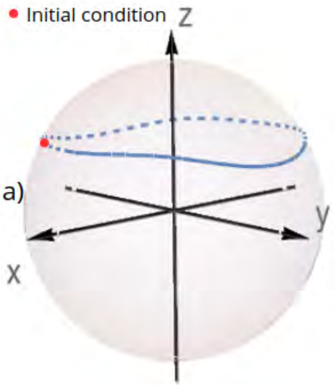
$$|\psi(T)\rangle = U(T,0)|\psi_0\rangle = \begin{bmatrix} a(T) \\ b(T) \end{bmatrix}, \tag{48}$$

and taking $\xi(T) = \frac{a(T)}{b(T)} \in \mathbb{C}$. Using the mapping $\beta : \mathbb{C} \longrightarrow S_1$ such that $\forall \mathbf{r} = (x, y, z) \in S_1$

$$x(T) = 2\mathbf{Re}\{a(T)\bar{b}(T)\}, \tag{49}$$
$$y(T) = 2\mathbf{Im}\{a(T)\bar{b}(T)\}, \tag{50}$$
$$z(T) = |a(T)|^2 - |b(T)|^2. \tag{51}$$

Two-levels system: non-resonant case

Not much changes on the path[5]



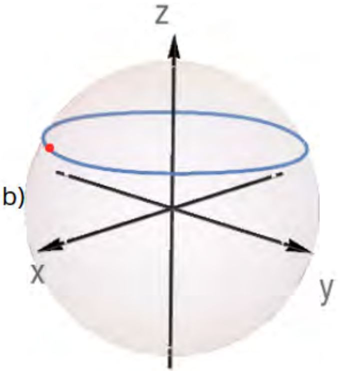
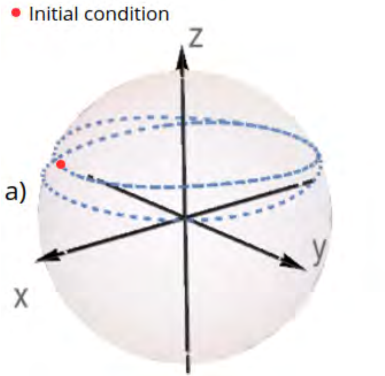


Figure: a) $|\psi_0\rangle = \sqrt{3}/2\,|0\rangle + 1/2\,|1\rangle$, $\varepsilon = 0.1\ eV$, $\omega_0 = 1\ eV$, $\omega = 3\ eV$. b) $|\psi_0\rangle = \sqrt{3}/2\,|0\rangle + 1/2\,|1\rangle$, $\varepsilon = 0.5\ eV$, $\omega_0 = 15\ eV$, $\omega = 30\ eV$.

[5] S. Cruz y Cruz, B. Mielnik. "Quantum control with periodic sequences of non resonant pulses", Rev. Mex. Fis. 53, 4, 20027, 37-41. PACS: 03.65.Ta; 32.80.Qk

Two-levels system: resonant case

Great changes on the path[6]



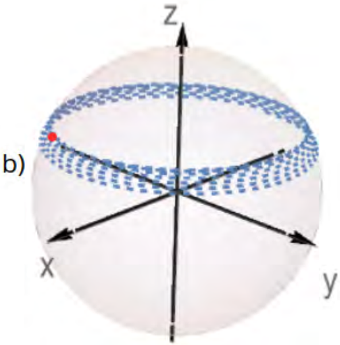


Figure: a) $|\psi_0\rangle = \sqrt{3}/2\,|0\rangle + 1/2\,|1\rangle$, $\varepsilon = 0.1\ eV$, $\omega_0 = 2\ eV$, $\omega = 3\ eV$.
b) $|\psi_0\rangle = \sqrt{3}/2\,|0\rangle + 1/2\,|1\rangle$, $\varepsilon = 0.1\ eV$, $\omega_0 = 20\ eV$, $\omega = 19\ eV$

[6] O. Rosas-Ortiz. D. J. Fernandez C. "Inverse techniques and evolution of spin-1/2 systems". In: PHYSICS LETTERS A 236 (1997), p. 5. doi: 0375-9601/97/17.00.

Outline for section 6

Conclusions

- The perturbative formulation is an alternative way to solve the time-evolution equation for regular potentials for systems with degeneration.
- We can study the evolution of the external and the inner freedom degrees under these frameworks.
- Resonant systems are more useful to control transitions to specific states. Whereas the non-resonant systems maintain the evolution almost without path changes.
- Calculate approximately the Floquet states and the quasi-energies.
- The interpretation of quasi-energies in the energetic sense is still an open problem.

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Thank you for your attention.