Extended Feynman Formula for the Harmonic Oscillator by the Discrete Time Method

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Abstract
We calculate the Feynman formula for the harmonic oscillator beyond and at caustics by the discrete formulation of path integral. The extension has been made by some authors, however, it is not obtained by the method which we consider the most reliable regularization of path integral. It is shown that this method leads to the result with, especially at caustics, more rigorous derivation than previous.

1 Introduction
In optics it is known as the Guoy phase shift [1] that when light waves pass through a focal point, the phase jumps $-\pi/2$ discontinuously. This point is called the caustic point, in which the intensity of light beam goes to infinity classically. In quantum mechanics this is the point in which two or more classical paths join. So phenomena at caustics are observed in many systems which are in the similar structure. In path integral formula they make a change in the phase and this effect is known as the Maslov correction [2].

The harmonic oscillator is one of the most important systems because it is solved exactly, it gives the first order approximations of various systems and so on. Path integral formula for the harmonic oscillator was obtained by Feynman himself [3]. It is given by

$$K(x_F, x_I; T) = \sqrt{\frac{m\omega}{2\pi i\hbar \sin \omega T}} \exp \left[ i \frac{m\omega}{2\hbar \sin \omega T} \left( (x_I^2 + x_F^2) \cos \omega T - 2x_I x_F \right) \right]$$ (1)

where $x_I$ ($x_F$) is the initial (final) position with the Hamiltonian

$$H = \frac{1}{2m} p^2 + \frac{1}{2} \omega^2 x^2.$$ 

However it is known that this formula is valid only for a half-period. In every half-period, infinite classical paths join at $x_I$ or $x_F$, so the harmonic oscillator is the system in which caustics

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appear. The extension for any time interval was made by Souriau [4] first. For \( \omega T / \pi \neq [\omega T / \pi] \), it is given by

\[
K(x_F, x_I; T) = \sqrt{\frac{m \omega}{2\pi i \hbar \sin \omega T}} e^{-i\omega T/2\pi} \exp\left[i \frac{m \omega}{2\hbar} (x_I^2 + x_F^2) \cos \omega T - 2x_I x_F \right]
\] (2)

and for \( \omega T / \pi = [\omega T / \pi] \), by

\[
K(x_F, x_I; T) = e^{-i\omega T/2\pi} \delta(x_F - (-1)^{[\omega T / \pi]} x_I)
\] (3)

where \([x]\) means the maximum integer not greater than \(x\). Later Horváthy [5] derived them by modifying Feynman’s original method and Liang and Morandi [6] by using the eigenfunction expansion for the propagator. However there seems to be no derivation by the discrete time formulation of path integral (the discrete time method). Therefore we derive the extended Feynman formula by this method.

Path integral is a powerful quantization method and has plain idea, however, in practical calculation some difficulties arise, for example, integral measure is not necessarily given. The discrete time method is one of the regularizations of path integral and in some cases it is indispensible [7–9]. The outline of this formulation is as follows. Path integral formula is defined by

\[
K(x_F, t_F; x_I, t_I) = \langle x_F | e^{-i\hat{H}(t_F-t_I)} | x_I \rangle
\]

or, if the Hamiltonian has time translation invariance, it is given by

\[
K(x_F, x_I; T) = \langle x_F | e^{-i\hat{H}T} | x_I \rangle
\] (4)

where \(T\) is the time interval. Then we write [4] as

\[
K(x_F, x_I; T) = \lim_{N \to \infty} \langle x_F | (1 - \frac{i}{\hbar} \Delta t \hat{H})^N | x_I \rangle
\]

\[
= \lim_{N \to \infty} \int \prod_{i=1}^{N-1} dx_i \prod_{j=1}^{N} \langle x_j | (1 - \frac{i}{\hbar} \Delta t \hat{H}) | x_{j-1} \rangle
\]

where we have successively inserted the completeness relation

\[
\int dx_i |x_i\rangle\langle x_i| = 1
\]

and put \( \Delta t = T/N, x_j = x(j\Delta t), x_N = x_F, x_0 = x_I \). In the harmonic oscillator, by making use of

\[
\langle x_j | p_j \rangle = \int \frac{dp_j}{\sqrt{2\pi\hbar}} e^{\pi p_j x_j},
\]

the matrix element is given by

\[
\langle x_j | (1 - \frac{i}{\hbar} \Delta t \hat{H}) | x_{j-1} \rangle = \int \frac{dp_j}{2\pi\hbar} \langle x_j | p_j \rangle \langle p_j | x_{j-1} \rangle \left[ 1 - \frac{i}{\hbar} \Delta t \left( \frac{p_j^2}{2m} + \frac{m}{2} \omega^2 x_j^2 \right) \right]
\]

\[
= \int \frac{dp_j}{2\pi\hbar} e^{\pi p_j x_j} \exp\left[ -\frac{i}{\hbar} \Delta t \left( \frac{p_j^2}{2m} + \frac{m}{2} \omega^2 x_j^2 \right) \right] + O(\Delta t^2).
\] (5)
Then carrying out the $p_j$-integrals, we obtain

$$K(x_F, x_I; T) = \lim_{N \to \infty} \left( \frac{m}{2\pi i \hbar \Delta t} \right)^{N/2} \int \prod_{i=1}^{N-1} dx_i \exp \left[ \frac{i}{\hbar} S \right],$$  

$$S = \Delta t \sum_{j=1}^{N} \left\{ \frac{m}{2} \left( \frac{\Delta x_j}{\Delta t} \right)^2 - \frac{1}{2} m \omega^2 \pi_j^2 \right\}$$

where we have put $\Delta x_j = x_j - x_{j-1}$, $\pi_j = (x_j + x_{j-1})/2$ and omitted $O(\Delta t^2)$ terms to disappear in $N \to \infty$. This is the path integral formula for the harmonic oscillator by the discrete time method. Naive integration of (6) leads to the original Feynman formula (1). In §2 we calculate (6) carefully to derive the extended Feynman formula (2) and (3).

### 2 The Extended Feynman formula

At first we write (7) by matrix notation as

$$S = \frac{m}{2\Delta t} (xA + 2bx + c)$$

$$A = \begin{pmatrix} 2\alpha & -\beta & 0 & 0 & \ldots & 0 \\ -\beta & 2\alpha & -\beta & 0 & \ldots & 0 \\ 0 & -\beta & 2\alpha & \ddots & & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & \ldots & 0 & -\beta & 2\alpha \end{pmatrix}, \quad b = -\beta(x_I, 0, \ldots, 0, x_F), \quad c = \alpha(x_I^2 + x_F^2)$$

$$\alpha = 1 - \frac{\omega^2 \Delta t^2}{4}, \quad \beta = 1 + \frac{\omega^2 \Delta t^2}{4}$$

where $t$ means transposition. The $x_i$-integrals in (6) are the Fresnel integrals and they are evaluated by

$$\int_{-\infty}^{\infty} e^{i ax^2} dx = e^{i \frac{\pi}{2}} \sqrt{\frac{\pi}{a}}, \quad \int_{-\infty}^{\infty} e^{-i ax^2} dx = e^{-i \frac{\pi}{2}} \sqrt{\frac{\pi}{a}} \quad (\alpha > 0).$$

So we need to know numbers of positive eigenvalues and negative one. By easy calculation we find the eigenvalues of $A$ are

$$\lambda_k = 2(\alpha - \beta \cos \frac{k\pi}{N}) \quad (k = 1, 2, \ldots, N - 1)$$

or

$$\lambda_k = 4 \cos^2 \frac{k\pi}{2N} \left( -\frac{\omega^2 \Delta t^2}{4} + \tan^2 \frac{k\pi}{2N} \right)$$

without $\alpha$ and $\beta$ and the corresponding normalized eigenvectors are

$$(\psi_k)_l = \sqrt{\frac{2}{N}} \sin \frac{lk\pi}{N} \quad (k, l = 1, 2, \ldots, N - 1)$$
where \((v_k)_l\) means the \(l\)th element of \(v_k\).

Since cosine decreases monotonously on \(0 \leq x \leq \pi\), we find \(\lambda_k\)'s are ordered according to \(k\). So if we obtain the zero point \(x_0(N)\) of

\[
f(x) = 2(\alpha - \beta \cos \frac{\pi}{N} x) \in \mathbb{C}^0[0, N],
\]

then \(k\) less than \([x_0(N)]\) corresponds to negative eigenvalues. Since \(f(x)\) increases monotonously and \(f(0) < 0\) and \(f(N) > 0\), \(f(x) = 0\) has a unique solution

\[
x_0(N) = \frac{N}{\pi} \cos^{-1} \frac{\alpha}{\beta} = \frac{2N}{\pi} \tan^{-1} \frac{\omega T}{2N}
\]

where we have used \(\cos^{-1} x = 2 \tan^{-1} \sqrt{\frac{1-x}{1+x}}\). Further by the Maclaurin expansion of arctangent, (13) is evaluated by

\[
x_0(N) = \frac{\omega T}{\pi} \left(1 - \frac{1}{3} \left(\frac{\omega T}{2N}\right)^2 + \cdots\right)
\]

so we find

\[
x_0(N) \uparrow \frac{\omega T}{\pi}.
\]

Now we can count number of eigenvalues of each sign. Two cases arise whether \(\omega T / \pi\) is integer or not. We put \(M = \lfloor \omega T / \pi \rfloor\) for simplicity.

(i) \(\omega T / \pi \neq M\)

Because \(M < \omega T / \pi < M + 1\), for sufficiently large \(N\)

\[
M < x_0(N) < M + 1.
\]

So \(M\) of \(N - 1\) eigenvalues are negative and \(N - M - 1\) are positive.

(ii) \(\omega T / \pi = M\)

Because \(x_0(N) < M\) and \(x_0(N) \uparrow M\), for large but finite \(N\), \(M - 1\) of \(N - 1\) eigenvalues are negative and \(N - M\) are positive and in \(N \to \infty\), \(M - 1\) remain negative and the \(M\)th goes to 0 and \(N - M - 1\) are positive.

In both cases, for sufficiently large \(N\), \(\lambda_k \neq 0\) and so det \(A \neq 0\). To deal with both cases together, we put

\[
L = \begin{cases} M & (\omega T \neq M\pi) \\ M - 1 & (\omega T = M\pi) \end{cases}.
\]

We proceed to calculate (13). We put \(x_c\) as the solution of \(Ax + b = 0: Ax_c + b = 0\). Then making use of the translation \(x = y + x_c\), we obtain

\[
S = \frac{m}{2\Delta t} (yAy - bA^{-1}b + c).
\]

Further making use of the orthogonal transformation \(y = Pz\) with \(P = (v_1, v_2, \ldots, v_{N-1})\), we obtain

\[
K(x_F, x_I; T) = \lim_{N \to \infty} Q \exp \left[ i \frac{1}{\hbar} S_c \right]
\]
so we find these into (16), we obtain Frensel integrals (9) by signs of eigenvalues, where we have written ingredients which are unnecessary for later calculations as where we have rewritten to (11), we immediately find Making use of the well-known formulas to (11), we immediately find

\[
Q = \left( \frac{m}{2\pi i\Delta t} \right)^{N/2} \left\{ \prod_{k=1}^{N-1} \int dx_k e^{\frac{i}{2\pi} k\omega x_k^2} \right\}, \quad S_c = \frac{m}{2\Delta t} (-bA^{-1}b + c)
\]

where we have rewritten \(z\) to \(x\). First we calculate \(Q\). Taking account of the difference of the Frensel integrals (9) by signs of eigenvalues, \(Q\) is evaluated by

\[
Q = \left( \frac{m}{2\pi i\Delta t} \right)^{N/2} \left( \prod_{k=1}^{L} \int dx_k e^{\frac{i}{2\pi} k\omega x_k^2} \right) \left( \prod_{k=L+1}^{N-1} \int dx_k e^{\frac{i}{2\pi} k\omega x_k^2} \right) = \sqrt{\frac{m}{2\pi i\Delta t}} e^{-i\frac{\pi}{2}} \prod_{k=1}^{N-1} |\lambda_k|^{1/2N}
\]

Making use of the well-known formulas

\[
\prod_{r=1}^{n-1} \cos \frac{r\pi}{2n} = \frac{\sqrt{n}}{2^{n-1}}, \quad \prod_{r=1}^{n-1} \left( x^2 + \tan^2 \frac{rx}{2n} \right) = \frac{1}{4nx} \left( (x + 1)^2 - (x - 1)^2 \right)
\]

we find

\[
\prod_{k=1}^{N-1} |\lambda_k| = \frac{N}{\omega T} \left| \frac{\sigma^2(N) - \overline{\sigma}^2(N)}{2i} \right|
\]

Putting (18) into (17), we obtain

\[
Q = \sqrt{\frac{m\omega}{2\pi i\Delta t}} e^{-i\frac{\pi}{2}} \prod_{k=1}^{N-1} |\lambda_k|^{1/2N}
\]

Next we calculate \(S_c\). We write the determinant of the “\(N - 1\)” dimensional matrix \(A\) as \(D_{N-1}\). Then \(D_n\)’s satisfy

\[
D_{n+1} = 2\alpha D_n - \beta^2 D_{n-1}, \quad D_0 = 1, \quad D_1 = 2\alpha
\]

so we find

\[
D_{N-1} = \frac{N}{\omega T} \frac{\sigma^2(N) - \overline{\sigma}^2(N)}{2i}
\]

and

\[
A^{-1} = \frac{1}{D_{N-1}} \begin{pmatrix}
D_{N-2} & \beta D_{N-3} & \cdots & \beta^{N-3} D_1 & \beta^{N-2} \\
\vdots & \vdots & \ddots & \vdots & \vdots \\
\beta^{N-2} & \beta^{N-3} D_1 & \cdots & \beta D_{N-3} & D_{N-2}
\end{pmatrix}
\]

where we have written ingredients which are unnecessary for later calculations as *. Putting these into (16), we obtain

\[
S_c = \frac{m}{2\Delta t} \left\{ (\alpha - \beta^2 \frac{D_{N-2}}{D_{N-1}})(x_t^2 + x_F^2) - \frac{\beta^N}{D_{N-1}} 2x_t x_F \right\}
\]

\[
= \frac{m\omega (\sigma^2(N) + \overline{\sigma}^2(N))(x_t^2 + x_F^2) - \sigma(N)\overline{\sigma}(N)4x_t x_F}{\sigma^2(N) - \overline{\sigma}^2(N)}.
\]

(20)
By (19) and (20), the Feynman formula (16) is expressed as

\[
K(x_F, x_I; T) = \lim_{N \to \infty} \frac{m \omega}{2 \pi i \hbar} \frac{e^{-i \frac{\omega}{2 \hbar} \pi}}{\sqrt{\sigma^2(N) - \overline{\sigma}^2(N)}} \times \exp \left[ -\frac{m \omega}{2 \hbar} \sigma^2(N) - \overline{\sigma}^2(N) \right] 
\times \left\{ (\sigma^2(N) + \overline{\sigma}^2(N))(x_I^2 + x_F^2) - \sigma(N)\overline{\sigma}(N)4x_Ix_F \right\}.
\]  

(21)

Because \( \sigma(N) \to e^{i \omega T/2} \) \( (N \to \infty) \), if \( \omega T/2 \in \mathbb{N} \cup \{0\} \) then \( \sigma^2(N) - \overline{\sigma}^2(N) \to 0 \) \( (N \to \infty) \), so we need to classify whether \( \omega T/2 \in \mathbb{N} \cup \{0\} \) or not.

(i) \( \omega T/\pi \notin \mathbb{N} \cup \{0\} \)

In this case no divergence appears. Each factor converges:

\[
\sigma^2(N) - \overline{\sigma}^2(N) \to 2i \sin \omega T, \sigma^2(N) + \overline{\sigma}^2(N) \to 2 \cos \omega T, \sigma(N)\overline{\sigma}(N) \to 1 \quad (N \to \infty)
\]

and \( L = M \), so (21) is

\[
K(x_F, x_I; T) = \sqrt{\frac{m \omega}{\pi i \hbar}} \frac{e^{-i \frac{\omega}{2 \hbar} \pi}}{\sqrt{|\sigma(N)|^2}} \exp \left[ i \frac{m \omega}{2 \hbar} \frac{x_I^2 + x_F^2}{1 - z^2(N)} \right] \times \exp \left[ \frac{m \omega}{2 \hbar} (x_I^2 + x_F^2) + \frac{m \omega}{\hbar} (x_I^2 + x_F^2 - 2z(N)x_Ix_F) \right].
\]

(22)

This is in accordance with (2).

(ii) \( \omega T/\pi \in \mathbb{N} \cup \{0\} \)

In this case \( L = M - 1 \) and now divergence appears. To handle divergence we slightly rewrite (21) as

\[
K(x_F, x_I; T) = \lim_{N \to \infty} \frac{m \omega}{\pi i \hbar} \frac{e^{-i \frac{\omega}{2 \hbar} \pi}}{\sqrt{|\sigma(N)|^2}} \times \exp \left[ i \frac{m \omega}{2 \hbar} \frac{x_I^2 + x_F^2}{1 - z^2(N)} \right] \times \exp \left[ \frac{m \omega}{2 \hbar} (x_I^2 + x_F^2) - \frac{m \omega}{\hbar} (x_I^2 + x_F^2 - 2z(N)x_Ix_F) \right].
\]

(23)

where we have put \( z(N) = \overline{\sigma}(N)/\sigma(N) \) for simplicity. Further we put

\[
u = \sqrt{\frac{m \omega}{2 \hbar}} (x_I + x_F), \quad v = \sqrt{\frac{m \omega}{2 \hbar}} (x_I - x_F),
\]

(24)

then we can rewrite (24) to

\[
K(x_F, x_I; T) = \lim_{N \to \infty} \sqrt{\frac{m \omega}{\pi i \hbar}} \frac{e^{-i \frac{\omega}{2 \hbar} \pi}}{\sqrt{|\sigma(N)|^2}} \times \frac{e^{-\frac{\pi^2}{4(1 - i/2 \omega)}}}{\sqrt{1 + z(N)}} \times \frac{e^{-\frac{\pi^2}{4(1 - i/2 \omega)}}}{\sqrt{1 - z(N)}}
\]

(25)

For sufficiently large \( N \)

\[
\arg \sigma(N) = N \tan^{-1} \left( \frac{M \pi}{2N} \right) = \frac{M \pi}{2} - \frac{1}{3} \left( \frac{M \pi}{2} \right)^3 \frac{1}{N^2} + \cdots
\]
so we can put
\[ \arg \sigma(N) = \frac{M\pi}{2} - \varepsilon(N), \quad \varepsilon(N) > 0, \quad \varepsilon(N) \to 0 \quad (N \to \infty) \]

and then we immediately obtain
\[ z(N) = e^{-2i\arg \sigma(N)} = (-1)^M e^{2i\varepsilon(N)}. \quad (26) \]

By (26) we find there are two cases of divergence in (25).

(a) \( M \in 2\mathbb{N} \cup \{0\} \)

In this case
\[ 1 - z(N) = 2 \sin \varepsilon(N) e^{-i(\frac{\pi}{2} - \varepsilon(N))} \]

and
\[ z(N) \to 1, \quad \arg(1 - z(N)) = -\frac{\pi}{2} \quad (N \to \infty), \]

so the denominator and the numerator of the last factor in (25) diverge.

To handle this divergence we consider not \( K(x_F, x_I; T) \) itself but
\[ \int_{-\infty}^{\infty} K(x_F, x_I; T) f(x_I) \, dx_I \quad (27) \]

where \( f(x_I) \) is a well-behaved function because path integral formula has essentially meaning within integral. The explicit expression of (27) is
\[ (27) = \int_{-\infty}^{\infty} \lim_{N \to \infty} \frac{m\omega}{\pi i \hbar} e^{-\frac{\Delta^2}{4\hbar}} \frac{e^{-\frac{i\Delta \frac{M}{2} \pi}{\hbar}}}{\sqrt{[\sigma(N)]^2}} \exp \left[ \frac{u^2(x_I) + v^2(x_I)}{2} \right] \frac{\exp \left[ -\frac{u^2(x_I)}{1 + z(N)} \right]}{\sqrt{1 + z(N)}} \frac{\exp \left[ -\frac{v^2(x_I)}{1 - z(N)} \right]}{\sqrt{1 - z(N)}} f(x_I) \, dx_I \]
\[ = \int_{-\infty}^{\infty} \lim_{N \to \infty} \frac{\sqrt{2}}{i\pi} \frac{e^{-\frac{i\Delta \frac{M}{2} \pi}{\hbar}}}{\sqrt{[\sigma(N)]^2}} \exp \left[ \frac{u^2(x_I(v)) + v^2}{2} \right] \frac{\exp \left[ -\frac{u^2(x_I(v))}{1 + z(N)} \right]}{\sqrt{1 + z(N)}} \frac{\exp \left[ -\frac{v^2}{1 - z(N)} \right]}{\sqrt{1 - z(N)}} f(x_I(v)) \, dv \quad (28) \]

where we have made a change of the integral variable \( x_I \) to \( v \). Making use of the formula
\[ \int_{-\infty}^{\infty} e^{-ux^2} f(x) \, dx = e^{-\frac{1}{2} \arg w} \int_{-\infty}^{\infty} e^{-\frac{1}{2} |w| x^2} f(xe^{-\frac{i}{2} \arg w}) \, dx \quad (29) \]
with \( w \in \mathbb{C}, \ |\arg w| < \pi/2 \), we rewrite (28) to
\[ (28) = \lim_{N \to \infty} e^{-\frac{i}{2} \arg \sigma(N)} \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} \sqrt{2} e^{-\frac{i\Delta \frac{M}{2} \pi}{\hbar}} e^{\frac{v^2}{2}} \frac{1}{\sqrt{1 + z(N)}} \frac{1}{\sqrt{1 - z(N)}} f(x_I) \, dv \quad (30) \]

where \( v \) in arguments has become \( v e^{\frac{i}{2} \arg(1 - z)} \). By using one of the expression of the \( \delta \)-function
\[ \lim_{r \to \infty} \frac{1}{\sqrt{\pi r}} e^{-\frac{x^2}{r}} = \delta(x), \]
with \( r = |1 - z(N)| \), we obtain
\[
(30) = \int_{-\infty}^{\infty} e^{-\frac{M\pi}{2} \delta(v)} f(x_I(v)) dv
\] (31)
where \( x_I(v) \) is \( x_I(v e^{-i\frac{\pi}{4}}) \) actually, but because of the nature of the \( \delta \)-function, \( x_I(v e^{-i\frac{\pi}{4}}) \) is the same with \( x_I(v) \). Making a change of variable \( v \) to \( x_I \), we finally obtain
\[
(31) = \int_{-\infty}^{\infty} e^{-\frac{M\pi}{2} \delta(x_F - x_I)} f(x_I) dx_I
\]
so we find
\[
K(x_F, x_I; T) = e^{-i\frac{M\pi}{2} \delta(x_F - x_I)} = e^{-i\frac{M\pi}{2} \delta(x_F - (-1)^M x_I)} \tag{32}
\]
(b) \( M \in \mathbb{N} \setminus 2\mathbb{N} \)
In this case
\[
1 + z(N) = 2 \sin \varepsilon(N) e^{-i(\frac{\pi}{4} - \varepsilon(N))}
\]
and
\[
z(N) \to -1, \quad \arg(1 + z(N)) = -\frac{\pi}{2} \quad (N \to \infty).
\]
In the similar way with (a), we obtain
\[
K(x_F, x_I; T) = e^{-i\frac{M\pi}{2} \delta(x_F + x_I)} = e^{-i\frac{M\pi}{2} \delta(x_F - (-1)^M x_I)} \tag{33}
\]
Putting (32) and (33) together, we obtain
\[
K(x_F, x_I; T) = e^{-i\frac{M\pi}{2} \delta(x_F - (-1)^M x_I)} \quad (M \in \mathbb{N} \cup \{0\}) \tag{34}
\]
This is in accordance with (3).

3 Discussion

In this paper we have derived the extended Feynman formula by the discrete time formulation of path integral. As stated in [10], we can observe clearly that when time passes over every caustic point, number of negative eigenvalues increases and the phase correction is multiplied in the Feynman formula.

As pointed out in [11], if we integrate (6) formally to
\[
\frac{1}{\sqrt{\det A}} = \frac{1}{\sqrt{(-1)^M \det A}},
\]
we do not know which branch of \( \sqrt{-1} \) should be chosen. The Frensel integral seems to be indispensable to obtain correct number of eigenvalues in each sign.

The extensions of the Feynman formula for other systems like a forced harmonic oscillator have been made [12–17]. The extensions by the discrete time method will be applicable to these systems.

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