Exact wave packet decoherence dynamics in a discrete spectrum environment

Matisse W Y Tu\(^1,2\) and Wei-Min Zhang\(^1,2\)

\(^1\) Department of Physics, National Cheng Kung University, Tainan 70101, Taiwan, Republic of China
\(^2\) National Center for Theoretical Science, Tainan 70101, Taiwan, Republic of China

E-mail: wzhang@mail.ncku.edu.tw

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Abstract

We find an exact analytical solution of the reduced density matrix from the Feynman–Vernon influence functional theory for a wave packet in an environment containing a few discrete modes. We obtain two intrinsic energy scales relating to the time scales of the system and the environment. The different relationship between these two scales alters the overall form of the solution of the system. We also introduce a decoherence measure for a single wave packet which is defined as the ratio of Schrödinger uncertainty over the delocalization extension of the wave packet and characterizes the time-evolution behaviour of the off-diagonal reduced density matrix element. We utilize the exact solution and the decoherence measure to study the wave packet decoherence dynamics. We further demonstrate how the dynamical diffusion of the wave packet leads to non-Markovian decoherence in such a microscopic environment.

1. Introduction

Wave packet dynamics has been extensively studied since the birth of quantum mechanics [1]. Studying decoherence dynamics of a wave packet still attracts attention in various research topics, from quantum dissipation dynamics, quantum cosmology, quantum measurement theory, quantum information processing, to the foundations of quantum mechanics [2]. The process of quantum decoherence is triggered by the interaction of the system with its environment. A widely used model of the environment is a set of harmonic oscillators [3, 4]. Environments with continuous distribution of oscillator frequencies have been extensively studied concerning the dissipation effects and the induced decoherence [5–18]. We shall consider in this paper an environment containing finite discrete modes.

Wave packet decoherence induced by an environment containing a few discrete modes has received attention in recent years in the study of quantum information processing using wave packets. There are many situations where the environment has a discrete spectrum. The decoherence of a molecule vibrational wave packet due to the vibrational–rotational coupling is a typical example [19, 20]. Other physical situations where environments have only a few modes being relevant include an electromagnetic field in cavity QED, molecular qubit decoherence in glassy environments [21], and electron transfer and exciton decoherence dynamics in proteins [22], to name a few. In fact, many environments associated with manipulations and measurements in quantum information processing involve a finite and discrete modes. The decoherence process under such circumstances must be studied with the back-reaction of the environment to the system being fully taken into account. The result is expected to be different from what happens with a continuous spectrum environment.

To make a comparison between the mechanisms of decoherence in a few discrete modes and a continuous spectrum environment, we take the Caldeira–Leggett model [4] with a discrete spectrum environment as a representative one. In this model, the principal system is a particle in a harmonic trap, and the environment is a set of noninteracting harmonic oscillators, each of which is linearly coupled to the principal system in their coordinates. Many researchers have studied this model; some have done research on models slightly modified from this, concerning topics not only of decoherence but many other issues of open quantum systems [5–18, 23–27]. An exact master equation to the motion of the central oscillator with a general spectral density at an arbitrary temperature was given in [10] and derived alternatively in [28]. The exact master equation lies on the dissipation dynamical equation which fully takes into account the back-reaction effects of the environment on the system. Here we present...
an analytical solution to the dissipation dynamical equation to directly describe the non-Markovian processes of the central particle. Also, the wave packet dynamics can be expressed in terms of the solution to the dissipation dynamical equation without invoking the master equation. As a result, a qualitative change of the dynamics of the central particle is directly read from the exact solution to the dissipation dynamical equation we obtained. The resulting effect can be used to analyse decoherence and instability of the system under the influence of the environment.

The paper is organized as follows. In the following section, we briefly describe the Feynman–Vernon influence functional approach to a quantum harmonic oscillator interacting linearly with a general environment of \( N \) modes. In the following section we solve analytically the reduced dynamics of the system. We obtain two intrinsic energy scales relating to the time scales of the system and the environment. We will explicitly show how the different energy scales between the system and the environment alter qualitatively the dynamics of the system. We also take the continuum limit of the environmental frequencies to the Ohmic spectrum [23] and recover the solution that was previously obtained in [4, 11]. In section 4, we study the evolution of a single wave packet. We introduce a decoherence measure for the single wave packet evolution. Non-Markovian decoherence of the wave packet in such an environment with a few discrete modes in

\[
\sum_{i} \omega_{i}^{2} X_{i}^{2}
\]

is left to the appendix.

2. Time evolution of open quantum systems

Following many works on the Caldeira–Leggett model [3, 4], we briefly review the main results obtained previously that will be used later in this work. The Hamiltonian of a particle in a harmonic trap linearly coupled with an environment is given by

\[
H = \left( \frac{p^2}{2M} + \frac{M \Omega^2 X^2}{2} \right) + \sum_{j=1}^{N} \left( \frac{p_j^2}{2m} + \frac{m \omega_j^2 q_j^2}{2} \right) + \sum_{j=1}^{N} C_j X q_j.
\]

The first two terms in the bracket are the Hamiltonian of the system, and the second term as a summation is that of the environment consisting of finite \( N \) discrete modes. The third term is the interaction Hamiltonian between the system and the environment. The notations follow convention. The requirement of finite \( N \) discrete modes in the environment makes our consideration different from the original Caldeira–Leggett model. It should be particularly noted that in the Caldeira–Leggett model an additional counter-term, \( \sum_{i=1}^{N} \frac{C_i^2}{2m \omega_i^2} X_i^2 \), is usually added to equation (1) in order to study the generic behaviour of dissipation dynamics for a particle trapped in a harmonic potential. From the theoretical point of view of understanding the quantum dissipation dynamics of a damped harmonic oscillator, such a counter-term is unavoidable since it ensures the stability of the model. However, such a counter-term exactly cancels the coupling-induced frequency-renormalization effect [6].

As has also been pointed out [6], the coupling-induced frequency-renormalization effect in many cases is a physical observable effect that has to be taken into account. In fact, the study of quantum decoherence should fully explore the environment-induced dissipation fluctuation as well as renormalization effects on the system. On the other hand, according to standard renormalization theory [30], a counter-term has to be introduced only if some ultraviolet (corresponding to the large frequency cutoff) or infrared (associated with the small frequency cutoff) divergences occur in the calculation. Since our interest lies in an environment with a finite number of discrete modes where no ultraviolet or infrared divergences exist, no counter-term is required for equation (1). Nonexistence of the counter-term for the present case of a discrete spectrum environment enables us to explore the decoherence dynamics of wave packets purely induced by the interaction with the environment without ambiguity.

Using the common assumption that the system and the environment are initially uncorrelated while the environment starts with an equilibrium state, the reduced density matrix of the system evaluated in the position basis at time \( t \) is given by

\[
\langle x | \rho_A(t) | x' \rangle = \rho_A(x, x', t) = \int \! dx_0 \int \! dx'_0 \; J(x, x', t \mid x_0, x'_0, 0) \rho_A(x_0, x'_0, 0),
\]

where \( J(x, x', t \mid x_0, x'_0, 0) \) is the propagator which includes the back-reaction effect of the environment on the system and is given by

\[
J(x, x', t \mid x_0, x'_0, 0) = \int \! D[x] D[x'] \; e^{i \int_0^t \{ \mathcal{S}_A[x] - \mathcal{S}_D[x'] \} \mathcal{F}[x, x']},
\]

in which \( \mathcal{S}_A \) is the action of the system:

\[
\mathcal{S}_A[x] = \int_0^t \! d\tau \left\{ \frac{M \dot{x}^2(\tau)}{2} - \frac{M \Omega^2 x^2(\tau)}{2} \right\},
\]

and \( \mathcal{F}[x, x'] \) is the influence functional describing the influence of the environment on the system. The explicit form of the influence functional has been solved [24]:

\[
\mathcal{F}[x, x'] = \exp \left\{ \frac{i}{\hbar} \left[ -\int_0^t \! d\tau \int_0^\tau \! d\tau' \{ x(\tau) - x'(\tau) \} K_f(\tau - \tau') \times [x(\tau') + x'(\tau')] + \int_0^\tau \! d\tau' \{ x(\tau) - x'(\tau) \} \times K_R(\tau - \tau') [x(\tau') - x'(\tau')] \right] \right\},
\]

where

\[
K_f(\tau - \tau') = -\sum_{k=1}^{N} \frac{C_k^2}{2m \omega_k^2} \sin \omega_k (\tau - \tau')
\]

3 See the discussion in [6] on pages 388–91, also in private communications with A J Leggett.
and
\[ K \beta (\tau - \tau') = \sum_{k=1}^{N} \frac{C_k^2}{2m\omega_k} \coth \frac{\hbar \omega_k \beta}{2} \cos \omega_k (\tau - \tau') \] (7)
are defined as the dissipation and fluctuation kernels, respectively, and \( \beta \) is the reciprocal of the product of the initial equilibrium temperature and Boltzmann constant.

Equations (3)–(5) show that the effective action has a quadratic form. Hence the path integral can be exactly carried out with the stationary path method [31]. By introducing the new variables \( R(\tau, r, t) \equiv \frac{\hat{x}_i(t) + \hat{x}_j(t)}{2} \) and \( r(\tau) \equiv \hat{x}(\tau) - \hat{x}(\tau) \), we rewrite the propagator \( J(x, x', t|\chi_0, \chi_0', 0) \) as \( J(R, r, t|\chi_0, \chi_0', 0, 0) \). The resulting propagator becomes [15, 32]
\[ J(R, r, t|\chi_0, \chi_0', 0, 0) = \hat{N}_0 \exp \left( \frac{i}{\hbar} \sum_{k=1}^{N} \frac{C_k^2}{2m\omega_k} \left( -\tau_0 R \hat{u}_2(0) + \hat{R} \hat{u}_1(0) + i \chi_{1i}(t) \right) r_0^2 \right) \]
(8)
where \( \chi_{ij}(t) (i, j = 1, 2) \) is defined by
\[ \chi_{ij}(t) = \int_{0}^{\tau} \int_{0}^{t} d\tau' d\tau \hat{v}_i(\tau) K_{ij}(\tau - \tau') \hat{v}_j(\tau'), \]
and \( \hat{v}_i \) and \( \hat{v}_j \) satisfy the following dissipation dynamical equations of motion:
\[ \ddot{\hat{v}}_i(\tau) + \Omega^2 \hat{v}_i(\tau) + \frac{2}{M} \int_{0}^{\tau} d\tau' K_{ij}(\tau - \tau') \hat{u}_i(\tau') = 0 \]
(10)
\[ \ddot{\hat{v}}_j(\tau) + \Omega^2 \hat{v}_j(\tau) - \frac{2}{M} \int_{0}^{\tau} d\tau' K_{ij}(\tau - \tau') \hat{u}_j(\tau') = 0 \]
(11)
subject to the boundary conditions \( v_i(0) = u_i(0) = v_2(t) = u_2(t) = 1, v_1(t) = u_1(t) = v_2(0) = u_2(0) = 0 \). \( \hat{N}_0 \) is the contribution of fluctuations around the stationary paths which is independent of the position variables for such a quadratic form of the Hamiltonian.

3. Analytical solution to the dissipation dynamics

Since equation (11) is the backward version of the forwarding equation (10), the propagator of the system, equation (8), is completely determined by solving the dissipation dynamical equation (10). The first two terms in equation (10) correspond to the classical equation of motion for the coordinate of the \( \chi_{ij}(t) \) \( (i, j \neq 11) \), and the third term with the dissipation kernel \( K_{ij} \) accounts for the non-Markovian (memory) effect of the back-reaction of the environment on the system. The fluctuation contribution from the environment is given by equation (9).

On the other hand, the propagator equation (8) is built upon the solutions of the dissipation dynamical equations (10)–(11). The solution of these equations gives rise to the full dynamics of the system. Using the fact that equation (11) is the backward version of equation (10), \( v_1(\tau) \) and \( v_2(\tau) \) are related to \( u_1(\tau) \) and \( u_2(\tau) \) by \( v_1(\tau) = u_2(t - \tau), v_2(\tau) = u_1(t - \tau) \). Furthermore, \( u_1(\tau) \) and \( u_2(\tau) \) can be expressed as \( u_1(\tau) = Z(\tau) - \frac{Z(t)}{Z(\tau)} Z(\tau) \) and \( u_2(\tau) = \frac{Z(t)}{Z(\tau)} Z(\tau) \) where \( Z(\tau) \) obeys the same equation as equation (10):
\[ \dot{Z}(\tau) + \Omega^2 Z(\tau) + \frac{2}{M} \int_{0}^{\tau} d\tau' K_{ij}(\tau - \tau') Z(\tau') = 0 \]
with the boundary conditions \( Z(0) = 0 \) and \( \dot{Z}(0) = 1 \). The solution of \( Z(\tau) \) determines the behaviours of \( u_1(\tau), u_2(\tau) \) and \( v_1(\tau), v_2(\tau) \), and all the relevant dynamics of the reduced system. \( Z(\tau) \) was solved in cases of continuous spectra of Ohmic and super-Ohmic types at the Markovian limit [32]. Here we shall give the analytical and exact solution of \( Z(\tau) \) for discrete spectra.

We found that the feature of \( Z(\tau) \) depends on a relationship between two intrinsic energy scales: \( M\Omega^2 \) and \( \sum_{k=1}^{N} \frac{C_k^2}{m\omega_k} \). The former is the intrinsic energy scale of the system in terms of the mass \( M \) of the central particle and the corresponding frequency \( \Omega \) in the harmonic trap. The latter is associated with an interaction energy scale between the system and the environment characterized by the coupling constants \( |C_k|^2; k = 1, \ldots, N \) and the intrinsic energy scales of the environmental oscillators \( m\omega_k^2; k = 1, \ldots, N \). We call \( M\Omega^2 \) the bounding strength of the system because it is just the second derivative of the harmonic potential at its valley. This strength tells how strongly the particle is bounded in this harmonic trap. We name \( \sum_{k=1}^{N} \frac{C_k^2}{m\omega_k} \) simply the spectral strength. These two energy scales indeed act as two time scales in the total system: one corresponds to the time scale of the system and the other corresponds to the time scale of the environment accompanied with the couplings between the system and the environment. Since the environment contains many different frequencies, it is not easy to figure out a definite time scale. However, the spectral strength \( \sum_{k=1}^{N} \frac{C_k^2}{m\omega_k} \) contains the contribution of every individual frequency in the environment plus the corresponding coupling to the system. It naturally provides an alternative expression to the time scale of the environment.

We will see that the different relationship between these two strengths (or equivalently between two time scales of the system and environment) alters the overall form of the solution to the dynamics of the system. The explicit forms of \( Z(\tau) \) in cases where the bounding strength of the system is stronger than, weaker than or equal to the spectral strength are quite different. We just present here the results and leave the verification of the solutions \( Z(\tau) \) to the appendix. In general, \( Z(\tau) \) has the following form:
\[ Z(\tau) = \sum_{k=0}^{N} \prod_{j=1}^{N} \left( \omega_j^2 - v_k^2 \right) \frac{\sin(v_k \tau)}{v_k} \]
(13)
where \( v_n \) satisfy
\[ M(\Omega^2 - v_n^2) \prod_{i=1}^{N} (\omega_i^2 - v_n^2) - \sum_{k=1}^{N} \frac{C_k^2}{m} \prod_{i \neq k, j=1}^{N} (\omega_j^2 - v_n^2) = 0 \]
(14)
for \( n = 0, \ldots, N \). When \( M\Omega^2 > \sum_{k=1}^{N} \frac{C_k^2}{m\omega_k} \), we have
\[ 0 < v_0 < \omega_1 < v_1 < \omega_2 < \cdots < v_N < \omega_N < v_N < \infty \]
(15)

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For a discrete spectrum, this constitutes an oscillation function in time. The continuous limit will lead this summation over sine functions to a Fourier integral that may not always be oscillatory. When \( M\Omega^2 = \sum_{k=1}^{N} \frac{C_k^2}{m_{0k}^2}, v_0 = 0 \) and the solution becomes

\[
Z_k(\tau) = \left( \prod_{k=1}^{N} \frac{\omega_k^2}{C_k^2} \right) \tau - \sum_{k=1}^{N} \frac{\prod_{j=1}^{N} (\omega_j^2 - \omega_k^2)}{v_k^2 \prod_{j=1, j\neq k}^{N} (\omega_j^2 - \omega_k^2)} \sin(v_k \tau) \quad (16)
\]

with all the other \( v_j \)'s, \( N \geq n \geq 1 \), still being located by (15).

In the case that \( M\Omega^2 < \sum_{k=1}^{N} \frac{C_k^2}{m_{0k}^2} \), \( v_0 = i\mu_0 \) where \( \mu_0 \) is a real number, and \( Z(s) \) becomes

\[
Z_k(s) = \frac{\prod_{j=1}^{N} (\omega_j^2 + \mu_0^2)}{\prod_{j=1}^{N} (\omega_j^2 - \mu_0^2)} \sin(\mu_0 s) \]

\[
- \sum_{k=1}^{N} \frac{\prod_{j=1}^{N} (\omega_j^2 - \omega_k^2)}{v_k^2 \prod_{j=1, j\neq k}^{N} (\omega_j^2 - \omega_k^2)} \sin(v_k s). \quad (17)
\]

As we have seen when the bounding strength of the system is stronger than the spectral strength, the oscillatory nature of the system is maintained although its oscillation details are completely altered. Coupling to the \( N \) oscillating modes of the environment generates \( N \) new oscillating modes to the system’s dynamics. Combining with the original oscillating mode \( \Omega \), the system now totally \( N + 1 \) oscillating modes, as shown in equation (13). Note that the existence of \( N + 1 \) new oscillating modes was also obtained by Haake and Reibold [7] through a normal mode transformation to the model Hamiltonian but the physical picture is different. In [7], the \( N + 1 \) new oscillating modes are just a hybridization to the original frequencies \( (\Omega, \omega_k, k = 1, \ldots, N) \) of the \( N + 1 \) harmonic oscillators for the system plus the environment, due to the coupling between them. Here the solution of the system, after the environment’s degrees of freedom are integrated out, contains \( N + 1 \) oscillating modes. It indicates that after the environment is traced over, the system is no longer a particle trapped in a harmonic potential, as manifested by the solution of equation (13). The \( N + 1 \) oscillating modes \( \{v_n, n = 0, \ldots, N\} \) are determined by equation (14).

Furthermore, when \( M\Omega^2 \to \sum_{k=1}^{N} \frac{C_k^2}{m_{0k}^2} \), we find from equation (14) that the frequency \( v_0 \to 0 \). In particular, the condition \( M\Omega^2 = \sum_{k=1}^{N} \frac{C_k^2}{m_{0k}^2} \) leads exactly to \( v_0 = 0 \). As we see, the first term in equation (16) comes from \( v_0 = 0 \), while the rest \( N \) mode oscillations in the solution of \( Z(\tau) \) are induced by the coupling of the system to the \( N \) modes of the environment. This solution indicates that at the critical energy condition, \( M\Omega^2 = \sum_{k=1}^{N} \frac{C_k^2}{m_{0k}^2} \), the central particle is driven out of the harmonic potential by its interaction with the environment. After a relatively long time, the solution of \( Z(\tau) \) is dominated by the linear term in time, which is responsible for an irreversible process as a sign for the possible rise of permanent loss of quantum coherence.

Now, we further consider the case of \( M\Omega^2 < \sum_{k=1}^{N} \frac{C_k^2}{m_{0k}^2} \). It is interesting to see from equation (14) that \( v_0 \) becomes an imaginary number. Although the solution of equation (17) still contains \( N \) oscillating modes induced from the coupling of the system to the \( N \) modes in the environment, the imaginary root \( v_0 = i\mu_0 \) provides the solution of \( Z(\tau) \) with a component that exponentially grows in time. The stronger the spectral strength, the larger \( \mu_0 \) will be (see appendix A.1). In other words, when the bounding strength of the system, \( M\Omega^2 \), is below a critical value of the environment’s spectral strength, the system will be pulled out from the harmonic bounding potential very quickly, and its dynamical process becomes irreversible with an exponential growth rate.

In fact, the existence of two energy scales in the Hamiltonian equation (1) and the corresponding non-Markovian dynamics resulting from the competition between the two energy scales have not attracted attention in the literature. This is mainly because a counter-term, \( \sum_{k=1}^{N} \frac{C_k^2}{m_{0k}^2} X^2 \), is usually added to equation (1) in order to study the generic behaviour of the dissipation dynamics for a damped harmonic oscillator [6], or a ‘positivity condition’, \( \Omega^2 - \sum_{k=1}^{N} \frac{C_k^2}{m_{0k}^2} \geq 0 \) (for the case \( M = m \)), is imposed on the coupling constants and the unperturbed frequencies to ensure the Hamiltonian has a finite lower bound [7]. Obviously the counter-term or the positivity condition excludes the dynamics corresponding to the case \( M\Omega^2 \leq \sum_{k=1}^{N} \frac{C_k^2}{m_{0k}^2} \). However, in the present work we deal with an environment having only a finite number of discrete modes in which no ultraviolet or infrared divergences exist. Therefore, no counter-term exists according to the standard renormalization theory [30]. Also, as Caldeira and Leggett had extensively discussed [6], the coupling-induced frequency-renormalization effect in many cases is indeed a real physical effect that has to be taken into account. There are many physical situations, such as phase transitions of the early universe in extreme environments in cosmology [36], fission of a heavy nucleus with coupling of the collective degree of freedom to the single-particle modes in nuclear physics [6], atomic tunnelling with phonon coupling in glasses [37], the instability of Bose–Einstein condensation influenced by the trapping field in cold atoms [38], etc, where the renormalization effect can be very large to reach the regime \( M\Omega^2 \leq \sum_{k=1}^{N} \frac{C_k^2}{m_{0k}^2} \) such that the system can render the original potential minimum unstable. The corresponding dynamics will undergo a catastrophic change that can be observed experimentally. Therefore, the positivity condition should also not be applicable to these physical situations, in contrast to the study of environment-induced dissipative or damped harmonic oscillation in the literature [7, 26].

In order to make a comparison between the environments with discrete and continuous spectra, we take the continuum limit of the spectrum of the environment. We first define a polynomial whose roots are those frequencies, \( \omega_k, k = 0, \ldots, N \). This is the polynomial of equation (14), \( P(v) = M\rho(v) W(v) \) where \( \rho(v) \equiv \Omega^2 - v^2 - \frac{1}{\pi} \sum_{j=1}^{N} \frac{C_j^2}{m_{0j}^2} \) and \( W(v) = \prod_{j=1}^{N} (\omega_j^2 - v^2) \). We observe that the general form of \( Z(\tau) \) can also be rewritten as \( Z(\tau) = \prod_{j=0}^{N} \frac{\omega_j^2}{v_k^2} \sin(v_k \tau) \), where \( p' \) denotes the derivative of \( p \) with respect to \( v \). By the fact that the roots of \( P(v) \) are also those of \( p(v) \) and
the roots are paired due to the evenness of the polynomials, we further rewrite $Z(\tau)$ replacing $\sin(\nu \tau)$ by $\frac{e^{\nu t} - e^{-\nu t}}{2\nu}$ as

$$Z(\tau) = -i \sum_{k=0}^{N-1} \frac{e^{\nu k \tau}}{\nu} \; \text{where} \; \nu_0 = \nu_{N+1}, \nu_1 = \nu_{N+2}, \ldots, \nu_N = \nu_{2N+1}.$$  

By the residue theorem, $Z(\tau)$ becomes \( \frac{1}{2\nu} \oint_{C} dz e^{\nu t} \), where the integration contour encloses all the roots of $p(\nu)$. Then taking the continuum limit of $p(\nu)$ that \( \sum_{j=1}^{N} C_j \left( \frac{1}{m} \right)^{\frac{1}{2} \nu^2} \to \int_{0}^{\infty} d\omega \frac{D(\omega)}{m} \) where $D(\omega)$ is the density of states in the environment and setting $D_{\text{int}}(\omega) = 2 \omega \gamma \delta(\omega - \omega_0)$ as the spectral density of an Ohmic environment (here $\Theta$ is the Heaviside function), we obtain

$$Z(\tau) = e^{-\gamma t} \frac{\sin(\Omega t)}{\Omega}$$  

(18)

as a solution to the corresponding version of dissipation dynamical equation (12): $Z(\tau) + 2\gamma_0 Z(\tau) + \Omega^2 Z(\tau) = 0$.

Here $\gamma_0$ is a constant that is usually very small in comparison to the high-frequency cutoff $\Lambda$, and $\Omega = \sqrt{\Omega_0^2 - \gamma_0^2} \simeq \Omega_0$ (for $\gamma_0 \ll \Lambda$) with the system’s renormalized frequency $\Omega'_0 \equiv \Omega_0 - \gamma_0 \Lambda / \pi$ [4, 10, 11]. As we see, whenever the environment’s spectrum becomes continuous, the form of $Z(\tau)$ as a summation over sine functions in equation (13) becomes a Fourier integral, and it may not always be oscillatory. In other words, the interaction of the system with a discrete spectral environment leads to very different results from the system interacting with a continuous spectrum environment.

Having obtained the analytical solution to the dissipation dynamical equation for an environment with discrete spectrum and reproduced the previous known results for the Ohmic bath in the continuous spectrum limit, we can now utilize this analytical solution to study the wave packet dynamics.

4. Non-Markovian wave packet dynamics

The geometry of a wave packet is well described by the covariation matrix [33]:

$$\begin{bmatrix} \Delta X^2 & \Delta \{XP\} \\ \Delta \{PX\} & \Delta P^2 \end{bmatrix},$$

where $\Delta X^2$ and $\Delta P^2$ are the widths of the wave packet in position and momentum spaces, respectively, and are defined via $\Delta X^2 = \langle X^2 \rangle - \langle X \rangle^2$, $\Delta P^2 = \langle P^2 \rangle - \langle P \rangle^2$ and $\langle P \rangle$ (with the brackets $\langle \rangle$) denoting the expectation value of an operator in the state $\rho_A$. $\Delta \{XP\}$ is a quantity that measures the internal correlation between the position and momentum observables, $\Delta \{XP\} = \frac{1}{2} \langle XP + PX \rangle - \langle X \rangle \langle P \rangle = \Delta \{PX\}$. The density matrix of the initial wave packet of the system generally takes the form

$$
\rho_A(R_0, r_0, 0) = N_0 \exp \left( -\frac{1}{2\Delta X_0^2} \left( R_0 - \frac{i}{\hbar} \Delta \{XP\} \right) \right) + \frac{1}{\hbar^2} \Delta X_0^2 \Delta P_0^2 \left( 2X_0 R_0 + \frac{2i}{\hbar} (P_0 - \Delta \{XP\} X_0) r_0 \right),
$$

(19)

where $N_0$ is the normalization constant, and the subscript ‘0’ here denotes the initial values of these quantities.

The density matrix at time $t$ is determined by the time evolution equation:

$$\rho_A(R, r, t) = \int dR_0 dr_0 J(R, r, t|R_0, r_0, 0) \rho_A(R_0, r_0, 0)$$

(20)

where the propagator $J(R, r, t|R_0, r_0, 0)$ (see equation (8)) is easy to obtain once the dynamical equations (10), (11) are solved exactly. Explicitly, the solution of equation (20) is

$$\rho_A(R, r, t) = \tilde{N} \exp \left( -\frac{1}{2\Delta X^2(t)} \left( R - \frac{i}{\hbar} \Delta \{XP\}(t) r \right) \right)$$

$$+ \frac{1}{\hbar^2} \left( \Delta X^2(t) \Delta P^2(t) \right) r^2 + 2X(t) r X + \frac{2i}{\hbar} (P(t) - \Delta \{XP\}(t) X(t)) r.$$  

(21)

which keeps the same form as the initial wave packet (19), and $\tilde{N}$ is a normalization factor. The time evolution of the wave packet is thus completely determined by the time evolution of the covariation matrix elements, which can be found from equations (8) and (20). Together with the solutions of $Z(t)$ discussed in the last section, the full information of the wave packet dynamics, in particular the decoherence process, can now be analysed.

The decoherence behaviour is mainly characterized by the decay of the off-diagonal element of the reduced density matrix. In the literature, to make the quantum coherence of wave packets manifest, one usually starts with a superposition of two well-separated Gaussian wave packets where the decoherence can be measured directly from the interference of two wave packets [2, 12, 14]. However, a single wave packet itself represents a macroscopic quantum state which has its own physical interest in many physical systems described by wave packets. A decoherence measure to a single wave packet is desirable.

Recall that $\rho_A(R, r, t) \equiv \langle x | \rho_A(t) | x' \rangle$ with $R = (x + x')/2$ and $r = x - x'$, the off-diagonal matrix element is given by the $r$-dependent part in (21) which describes the quantum coherence dynamics of the wave packet. In fact, equation (21) reveals that the dynamics of the off-diagonal matrix element is fully determined by the covariation matrix $\Delta X^2(t)$, $\Delta P^2(t)$, $\Delta \{XP\}(t)$. In particular, the correlator $\Delta \{XP\}(t)$ describes the phase dynamics of the density matrix, while the Heisenberg uncertainty, $\Delta X^2(t) \Delta P^2(t)$, measures the amplitude dynamics of its off-diagonal behaviour. Note that because of its independence on the widths $\Delta X^2(t)$ and $\Delta P^2(t)$ as well as the correlator $\Delta \{XP\}(t)$, the centre motion of the wave packet (given by $X_c$ and $P_c$) does not change the geometry of the wave packet. Without loss of generality, we may let the initial position and the momentum of the wave packet be zero, $X_0 = P_0 = 0$; then the reduced density matrix simply becomes

$$\rho_A(R, r, t) = \tilde{N} \exp \left( -\frac{R^2}{2\Delta X^2(t)} + \frac{i}{\hbar} \frac{\Delta \{XP\}(t)}{\hbar \Delta X^2(t)} \frac{R r}{2\hbar^2} \right)$$

$$- \left( \Delta X^2(t) \Delta P^2(t) - \Delta \{XP\}(t) \right) r^2.$$  

(22)
respectively. (d), (e) and (f) are the time evolution of the corresponding decoherence measure $\sum_{N}C_{k}^{2}$ of quantum coherence.

The frequencies are chosen as $\{\omega_{1}, \omega_{2}, \omega_{3}, \omega_{4}, \omega_{5}\} = \{0.48, 0.86, 1.72, 1.84, 1.89\}$. The coupling constant $\gamma$ is adjusted as 0.01, 0.39 and 0.58 to satisfy the bounding strength being larger than, equal to and smaller than the spectral strength. The wave packet delocalizes whenever its bounding strength is no larger than the spectral strength. $D_{c}$ grows monotonically when $M\Omega^{2} = \sum_{k=1}^{N}C_{k}^{2}$ results in slow diffusion of the wave packet, slow compared to that for $M\Omega^{2} < \sum_{k=1}^{N}C_{k}^{2}$, without rendering unidirectional loss of quantum coherence.

Now it becomes clear that the decay of the off-diagonal matrix element is determined by the quantity $D_{c}(t) = \frac{\Delta X^{2}(t)\Delta P^{2}(t) - \Delta \{XP\}^{2}(t)}{\Delta X^{2}(t)}$, where the denominator $\Delta X^{2}(t)\Delta P^{2}(t) - \Delta \{XP\}^{2}(t)$ is actually the Schrödinger uncertainty [34]. The minimum Schrödinger uncertainty has been used as a criterion to examine if a wave packet is a squeezed coherent state [33]. Thus $D_{c}(t)$ is a natural quantity to characterize the delocalization of a wave packet accompanied by wave packet decoherence. The degree of quantum decoherence in a wave packet can then be extracted from the off-diagonal matrix element:

$$\exp\left(-\frac{1}{2\hbar^{2}}D_{c}(t)r^{2}\right) = \exp\left(-\frac{1}{2\hbar^{2}}\frac{\Delta X^{2}(t)\Delta P^{2}(t) - \Delta \{XP\}^{2}(t)}{\Delta X^{2}(t)}r^{2}\right)$$

The larger $D_{c}(t)$, the less quantum coherence there is.

To demonstrate the non-Markovian decoherence dynamics of the wave packet, we plot the time evolutions of the wave packet width and the corresponding decoherence measure at different physical conditions. Note that for an environment with a few modes, the parameter $\beta$ reveals no sense of thermodynamics, and it is just a parameter in the initial state of the environment. We set here $M = m = \Omega = h = 1, \beta^{-1} = 1.15$ and $C_{k} = M\Omega^{2}/\sqrt{\left[(\omega_{k} - \omega_{m})^{2}\right]^{+}}$ with $\Gamma = 500$. The parameter $\gamma$ is dimensionless and is set differently according to the relationship between $M\Omega^{2}$ and $\sum_{k=1}^{N}C_{k}^{2}$. We take an initial wave packet as $\Delta X_{0} = 1/5, \Delta P_{0} = 5$ and $\Delta \{XP\}_{0} = X_{0} = P_{0} = 0$. We first fix the frequency distribution in the environment and vary only $\gamma$ to obtain the conditions $M\Omega^{2} > \sum_{k=1}^{N}C_{k}^{2}$, $M\Omega^{2} = \sum_{k=1}^{N}C_{k}^{2}$ and $M\Omega^{2} < \sum_{k=1}^{N}C_{k}^{2}$. We then fix $\gamma$ and change the frequency distributions to satisfy the above three relationships between the bounding and the spectral strengths. The results are shown in figures 1 and 2. From the plots, one can see that when the bounding strength is larger than the spectral strength; the wave packet keeps oscillating in its width as well as the decoherence measure. There is no unidirectional loss of the decoherence measure. When the two strengths balance, the wave packet starts to spread. But the decoherence measure still oscillates at some finite values. The monotonic loss of quantum coherence is seen when the spectral strength wins over the bounding strength. This happens also together with an even faster spreading of the wave packet. These phenomena are seen no matter how $\gamma$ is varied with the frequency distribution fixed or the frequency distribution is changed with $\gamma$ fixed (see figure 1, and the solid curves in figure 2). Consequently, the emergence of decoherence is subjected to the definite greatness of the spectral strength in comparison to the bounding strength of the system here. If the spectral strength is just equal to the bounding strength, delocalization dynamics occurs without necessarily leading to decoherence.
in equation (12), namely takes the history independence of the dynamical variable \( \gamma \) at 0.39 and changing the frequency distribution. (This figure is in colour only in the electronic version)

Figure 2. The solid blue lines are exact results and the dashed red lines are obtained with the Markovian approximation. (a) and (d) are for \( M\Omega^2 > \sum_{k=1}^{N} \frac{c_k^2}{m_k} \). (b) and (e) are for \( M\Omega^2 = \sum_{k=1}^{N} \frac{c_k^2}{m_k} \). (c) and (f) are for \( M\Omega^2 < \sum_{k=1}^{N} \frac{c_k^2}{m_k} \). The three conditions are achieved by fixing \( \gamma \) at 0.39 and changing the frequency distribution \( \{\omega_1, \omega_2, \omega_3, \omega_4, \omega_5\} \) to be \( [2.43, 2.66, 2.69, 2.70, 2.77] \) or \( [0.19, 0.23, 0.44, 0.89, 0.96] \) for \( M\Omega^2 > \sum_{k=1}^{N} \frac{c_k^2}{m_k} \). The balance condition uses the same set of frequencies as in figure 1. The Markovian approximation breaks down severely when \( M\Omega^2 \) is comparable to \( \sum_{k=1}^{N} \frac{c_k^2}{m_k} \).

(This figure is in colour only in the electronic version)

The non-Markovian decoherence dynamics of the wave packet (the memory effect induced from the back-reaction of the environment) can be seen by contrasting the exact solution with the Markovian approximation which is physically valid when the time scale of the environment is much smaller than that of the system and has been widely used in the literature [26, 27]. Mathematically, the Markovian approximation takes the history independence of the dynamical variable in equation (12), namely \( \int_0^\infty \text{d}\tau' K_f(\tau - \tau') Z(\tau') \simeq Z(\tau) \int_0^\infty \text{d}\tau'' K_f(\tau - \tau'') \) in solving the dissipation dynamical equation [35]. When the time scales of the environments and the system are comparable (equivalently when the values of the two strengths approach each other), we expect the dynamics of the wave packet under the Markovian approximation to deviate obviously from the exact solution. The three frequency distributions are chosen such that the time scales of the environments fall upon the regimes of interest.

As we can see from figure 2, when the environment contains only frequencies much larger than the central one, the system is located in the regime \( M\Omega^2 \gg \sum_{k=1}^{N} \frac{c_k^2}{m_k} \). We find that the Markovian approximation agrees well with the exact solution. However, when the frequencies of the environmental oscillators all lie near the central frequency (the strongest memory regime) where the two strengths are very close to each other, an apparent difference between the Markovian and non-Markovian results shows up. The exact time evolution of the wave packet width exhibits several kinks and bumps that are smeared when Markovian processes are asserted. The extension of wave packet delocalization is over estimated by the Markovian approximation. The exact time evolution of the decoherence measure in this time scale shows oscillatory features that are not seen from the Markovian approximation. The magnitude of the decoherence measure is also over-evaluated in the Markovian approximation. In other words, ignoring the history dependence smears out the subsequent features of the time evolutions of \( \Delta X^2 \) and \( D_c \) in this case. When it only consists of lower frequencies, namely when the environment has a longer time scale than that of the system, the system easily falls into the regime \( M\Omega^2 < \sum_{k=1}^{N} \frac{c_k^2}{m_k} \) where we find that the Markovian approximation over-evaluates the magnitudes of \( \Delta X^2 \) and \( D_c \) but not as severe as that in the balance case.

The wave packet dynamics that we obtained here is not limited to environments with discrete spectra. We may consider the wave packet evolution in an Ohmic bath (a continuous spectrum environment) as an example. In this case, the system undergoes an underdamping process according to (18). We find that when \( t \to \infty \) the width of the wave packet \( \Delta X^2(t) \) is given by

\[
\Delta X^2(t \to \infty) = \frac{\hbar}{\pi} \int_0^\infty \text{d}\omega \coth(\beta \omega) \left( \frac{\hbar \omega}{2} \right) \times \left( \frac{1}{M} \frac{\gamma_{\Omega} \omega}{(\Omega^2 - \omega^2)^2 + 4\gamma_{\Omega} \omega^2} \right).
\]

Note that in linear response theory, a harmonic oscillator of frequency \( \Omega_\tau \) reacts to an external force with the imaginary
part of its response being $\sigma(\omega) = \left( \frac{1}{M} (2\pi - \omega^2) + 4\gamma \frac{\omega}{2\pi} \right)$. Equation (24) can be rewritten as $\Delta X^2(N) = \frac{1}{\pi} \int_0^\infty d\omega \coth(\beta h \omega) \sigma(\omega)$, which is a well-known result of the fluctuation–dissipation theorem [4, 39]. In the extremely underdamped limit, the spread of the wave packet ultimately goes to an equilibrium value: $\Delta X^2(\infty) = \frac{1}{h\pi} \coth(\beta h \omega)$, the same result obtained in the equilibrium quantum statistical mechanics [3, 4, 40]. The numerical evaluations of $\Delta X^2(t)$ at large times under such a circumstance also accurately match the equilibrium quantum statistical result.

5. Conclusions and discussions

Here we summarize what we have done in this paper. We studied the dynamics of a particle in a harmonic trap linearly coupled to a set of noninteracting harmonic oscillators. We obtained an exact analytical solution of the system with the environment containing discrete $N$ modes. By taking the continuous spectrum limit, we examined the dynamics in an Ohmic spectral density and reproduced the solution once obtained by others. In order to visualize the dynamics more vividly, we let the system start with a wave packet. The decoherence processes are described in terms of the geometry of the wave packet. We then closely looked at the wave packet’s localization and delocalization behaviours against its decoherence measure defined by the ratio of Schrödinger uncertainty over the delocalization extension of the wave packet. We observed two intrinsic energy scales, the bounding strength $M/\Omega^2$ and the spectral strength $\Sigma_{k=1}^N C_i^2/m_i$, acting as the time scales of the system and the environment, respectively. These two energy scales were veiled in previous investigations when a counter-term was added to the Hamiltonian in the continuous spectral density where a high-frequency cutoff has to be introduced or a positivity condition is imposed on the system. However, the relationship between these two intrinsic energy scales determines the feature of the delocalization as well as decoherence dynamics of the wave packet in the cases where the environment has only a few modes so that no counter-term exists or no positivity condition can be added when decoherence dynamics is concerned.

We also numerically demonstrated the time evolution of the wave packet based on the exact solutions we obtained with an environment of a few modes satisfying a modified Drude’s spectral density. Our results show that a stronger spectral strength drives the wave packet out of the harmonic bounding potential as a consequence of the environment-induced instability, which results in strong entanglement between the system and the environment, and leads to severe decoherence, while a moderate or weaker spectral strength oscillates its decoherence measure over time. We also compared the exact results with the Markovian approximation. If the Markovian approximation is done ahead, the relationship between the two strengths still plays a determinant role in the consequent wave packet dynamics. The overall trends of wave packet dynamics are not altered by the Markovian approximation when the bounding strength is much larger than the spectral strength. But the Markovian approximation under the condition of a larger spectral strength changes the wave packet dynamics drastically from the exact solution. The critical condition that the two strengths balance each other manifests the non-Markovian wave packet dynamics most significantly. In conclusion, we have taken a few factors to explore the mechanisms of decoherence of a wave packet in a few-mode environment. One may attempt to see these issues in relevant systems mentioned above.

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Appendix. The solutions to the dissipation dynamical equations

A.1. Root property

Before we proceed to justify our solution to the dissipation dynamical equation, we first look at (14). The roots of this polynomial determine the properties of $Z(s)$. We denote the general argument of this polynomial by $\nu$ instead of $\nu_i$. For convenience of reference, we write this polynomial again:

$$P_0(\nu) = M(\Omega^2 - \nu^2) \prod_{i=1}^{N} (\omega_i^2 - \nu^2)$$

$$- \sum_{k=1}^{N} \frac{C_k^2}{m} \prod_{i=1}^{N} (\omega_i^2 - \nu^2).$$

(A.1)

It is well known that if the polynomial is evaluated at some point on the real axis to be positive and is negative at some other point, then there is a point in between at which this polynomial is evaluated to be zero as its root, denoted by $\nu_i$. We arrange $\omega_1$ through $\omega_N$ in a way that $\omega_1 < \omega_2 < \cdots < \omega_N$ and let $\nu = \omega_N$, then equation (A.1) becomes

$$P_0(\omega_N) = (-1)^n \frac{C_N^2}{m} \prod_{i=1}^{N} (\omega_i^2 - \omega_N^2) \prod_{i=n+1}^{N} (\omega_i^2 - \omega_N^2).$$

(A.2)

Clearly, the sign of the polynomial at $\omega_n$ for $n = 1, 2, \ldots, N$ is determined by $(-1)^n$, so the roots are located in the vicinity of adjacent frequencies $\omega_n$ and $\omega_{n+1}$ and we have located $N-1$ distinct roots that are all positive. Since the polynomial is even in its argument, the roots are paired. This gives another set of $N-1$ roots that are all negative. We can also see that there is a root larger than $\omega_N$ by letting $\omega_i = \alpha_i \Omega$ for $i = 1, \ldots, N$ and $\nu = (\alpha_N + f) \Omega$, that is,

$$P_0((\alpha_N + f) \Omega) = (-1)^{N+1} \prod_{j=1}^{N} \left((\alpha_N + f)^2 - \alpha_j^2\right)$$

$$\times ((\alpha_N + f)^2 - 1) \Omega^2 \left(M\Omega^2 - \sum_{k=1}^{N} \frac{C_k^2}{m} \left((\alpha_N + f)^2 + 1\right)^{-1}\right).$$

(A.3)
We can make \( P_0(\alpha_N \Omega = \omega \Omega) \) and \( P_0(\alpha_N + f)\Omega) \) differ by a sign by choosing an \( f \) which is large enough that
\[
((\alpha_N + f)^2 - 1) \left( \frac{\Omega^2}{\omega N + f} \right) > 0,
\]
and the sign of \( P_0(\alpha_N + f) \Omega) \) is \((-1)^{N+1}. \) So far by including the negative partner of this root, we have found \( 2N \) distinct roots. We know that this polynomial has \( 2 + 2 \) roots so there is still a pair of roots not yet located. Since the sign of the polynomial at \( \omega N \) is negative, if \( P_0(0) \) is positive, then there is a root lying between 0 and \( \omega N \). We see that \( P_0(0) \) is just the difference between the bounding strength of the system and the spectral strength times a positive number:
\[
P_0(0) = \left( \prod_{i=1}^{N} \alpha_i \right) \left( \frac{\Omega^2}{\omega N + f} \right)^{-1}. \tag{A.4}
\]
If \( \Omega^2 \) is larger than \( \sum_{k=1}^{N} \frac{C_k^2}{m \omega_k} \), then \( P_0(0) \) is positive and we have a root that is larger than 0 and smaller than \( \omega N \). Since \( P_0(0) \) is proportional to the product of all the roots it has, \( P_0(0) = 0 \) implies that there is a pair of roots doubly located at the origin. If \( P_0(0) \) is negative, then we have to look for roots somewhere out of the real axis. In this case, we define \( P_\gamma(y) \equiv P_i(y) \) where \( y \) is in the real domain, then \( P_\gamma(0) = P_0(0) < 0. \) If we can find a \( y \) such that \( P_\gamma(y) > 0 \), then there is a root between 0 and \( |y| \) for \( P_\gamma \) which implies a root for \( P_0 \). Let \( y = f \Omega \) where \( f \) is a positive number and we have
\[
P_\gamma(f \Omega) = \prod_{j=1}^{N} \left[ (\omega_N e_j)^2 + (f \Omega e)^2 \right] \left( \frac{f^2 + 1}{f^2 + 1} \right) \times \left( \frac{\Omega^2}{\omega N + f} \right)^{-1} \tag{A.5}
\]
Again, \( f \) can be chosen to be large enough such that
\[
(M^2 \omega^2 - \frac{1}{f^2 + 1} \sum_{k=1}^{N} \frac{C_k^2}{m \omega_k} \frac{1}{(f \Omega)^2}) > 0.
\]
This gives us a real root to \( P_\gamma \) and also an imaginary root to \( P_0 \). This root of course has a negative partner, and we find finally all the roots.

We summarize the location of half of the roots as
\[
0 \leq v_0 < \omega_1 < v_1 < \omega_2 < \cdots < \omega_{N-1} < \omega_N < \infty,
\]
for \( M^2 \omega^2 \geq \sum_{k=1}^{N} \frac{C_k^2}{m \omega_k} \) and \( v_0 = i \mu_0 \) where \( \mu_0 \) is a real number for \( M^2 \omega^2 < \sum_{k=1}^{N} \frac{C_k^2}{m \omega_k} \). The other half is negatively paired with this.

A.2. Verification of the solution

We have proved in the last subsection that \( v_0 \) through \( v_N \) are \( N + 1 \) distinct numbers. This ensures that the amplitudes of each component in the solution of \( Z(s) \) do not diverge. Now we shall check whether (13) fits (12) with the boundary conditions that \( Z(0) = 0 \) and \( \dot{Z}(0) = 1. \) Substituting (13) to (12), we have
\[
(\dot{Z}(s) + \Omega^2 Z(s)) + \frac{2}{M} \int_0^s ds' K_j(s' - s')Z(s') = \sum_{k=0}^{N} \frac{C_k^2}{m \omega_j} \sin(\omega_j s) - \frac{1}{M} \sum_{j=1}^{N} \frac{C_j^2}{m \omega_j} \sin(\omega_j s) - \frac{1}{M} \sum_{j=1}^{N} \frac{C_j^2}{m \omega_j} \sin(\omega_j s).
\]
where \( A_k \)'s are the amplitudes \( \prod_{i=1}^{N} (\omega_i - \nu_k^2 - \nu_k^2) \). We now introduce an identity,
\[
\sum_{k=1}^{N} \frac{b_k}{\prod_{i \neq k} (b_k - b_i)} = \begin{cases} 0, & 1 \leq j \leq 2 - n \\ 1, & \sum_k b_k, j = 1. \end{cases} \tag{A.8}
\]
Comparing the factor \( \sum_{k=1}^{N} \frac{\sum_{i \neq k} (\omega_i - \nu_k^2 - \nu_k^2)}{\prod_{i \neq k} (\omega_i - \nu_k^2 - \nu_k^2)} \) in the last line of (A.7) with the identity (A.8) by replacing \( b_i \) by \( \nu_k^2 + \bar{n} \) by \( N + 1 \), we can see in the numerator that the highest power of \( \nu_k^2 \) is \( N - 1 \) and \( N - 1 = (N + 1) - 2 = \bar{n} - 2. \) So this summation goes to zero, and \( Z(s) \) with the proposed form (13) fits (12). It is easy to see that the initial condition \( Z(0) = 0 \) is indeed satisfied since the sine functions are zero when their arguments are zero. To check the boundary value satisfied by its first derivative, we take
\[
\dot{Z}(0) = A_k \nu_k = \left( \prod_{i=1}^{N} \frac{\omega_i}{\nu_k^2 - \nu_k^2} \right) \frac{1}{\prod_{i=1}^{N} (\nu_k^2 - \nu_k^2)} \tag{A.9}
\]
Making use of (A.8) for the highest power in the numerator now equal \( \bar{n} - 1 \), \( \dot{Z}(0) \) becomes unity.

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