Adiabatic elimination approach to the completely positive master equation for open quantum Brownian motion

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Abstract. Open quantum Brownian motion (OQBM) was introduced as a scaling limit of discrete-time open quantum walks, providing a new class of quantum Brownian motion. In this case, the dynamics of the Brownian particle are governed by dissipative interactions with a thermal bath and depend on the quantum internal state of the Brownian particle. In this proceeding, we outline the derivation of a completely positive master equation for OQBM using the adiabatic elimination of fast variables method for a weakly driven open Brownian particle confined within a harmonic potential and dissipatively coupled to a thermal bath. We illustrate the derivation using examples of initial Gaussian and non-Gaussian distributions. For both examples, the OQBM dynamics converge to Gaussian distributions for various system-bath parameters. From the resulting dynamics, we also derive equations for the first, second, and third cumulants of the position distribution of the OQBM walker. Interestingly, we find that the third cumulant is non-zero, which reveals that the intrinsic generator of the evolution is non-Gaussian.

1. Introduction

Recently, Attal *et al.* [1] introduced the formalism of discrete-time open quantum walks (OQWs) as a new type of quantum walks (QWs) to incorporate the dissipative dynamics of open quantum systems [2]. OQWs rely entirely on the non-unitary evolutions induced by the interaction between the walker and its environment, and rest upon the implementation of appropriate completely positive trace-preserving (CPTP) maps [2, 3]. Unlike the traditional unitary QWs [4, 5], where quantum interference over the nodes of a graph determines the probability of finding the walker, in OQWs, the probability of finding the quantum walker on a particular node depends on both the structure of the underlying graph and the walker's quantum internal state. Ref. [6] demonstrated that OQWs can perform dissipative quantum computation and generate complex quantum states. Interested readers can find recent developments on this subject in [7].

Shortly after the introduction of OQWs, Bauer *et al.* [8] introduced *open quantum Brownian motion* (OQBM) as a scaling limit of discrete-time OQWs, providing a new class of quantum

Brownian motion. In this case, the dynamics of the quantum Brownian particle depends not only on the dissipative interactions with a thermal bath but also on the state of the internal degree of freedom of the quantum Brownian particle. Recently, a microscopic derivation of OQBM for a free Brownian particle subject to decoherent interaction with a thermal bath was proposed [9, 10]. In our recent work [11], we extended this framework by deriving OQBM in a generic dissipative scenario using the adiabatic elimination of fast variables technique [12, 13, 14]. However, this approach led to a master equation that is not completely positive, consistent with the limitations of the standard Caldeira-Leggett model [15]. To resolve the issue of positivity, we now apply the rotating wave approximation (RWA) [16] to the system-bath interaction Hamiltonian. This leads to a completely positive master equation for OQBM in the case of a weakly driven open Brownian particle confined within a harmonic potential and dissipatively coupled to a thermal bath.

This proceeding has the following structure: In Sec. 2, we introduce the microscopic Hamiltonian for this model and derive a completely positive Born-Markov master equation for the reduced dynamics. In Sec. 3, we write the resulting master equation in coordinate representation, and briefly outline the adiabatic elimination of fast variables method and derive a completely positive master equation for OQBM. Sec. 4 presents the numerical illustrations of the OQBM dynamics for various system-bath parameters and the equations for the cumulants of the OQBM walker. The detailed derivation and the terms and parameters omitted here will be provided in [17]. Lastly, in Sec. 5, we conclude.

2. Completely positive Born-Markov master equation

The total Hamiltonian of the system and bath can be written as

$$\hat{H} = \hat{H}_S + \hat{H}_B + \hat{H}_{SB}, \tag{1}$$

where $\hat{H}_S$, $\hat{H}_B$, and $\hat{H}_{SB}$ denote the Hamiltonians of the system, the bath, and the system-bath interaction, respectively, which reads

$$\hat{H}_S = \frac{\hat{p}^2}{2m} + \frac{m\omega^2\hat{x}^2}{2} + \frac{\hbar\omega_0}{2}\hat{\sigma}_z + \hbar\Omega\hat{\sigma}_x, \tag{2}$$

$$\hat{H}_B = \sum_n \hbar\omega_n \hat{a}_n^\dagger \hat{a}_n, \tag{3}$$

$$\hat{H}_{SB} = \hbar\big(\hat{x} + \alpha\hat{\sigma}_x\big)\sum_n g_n\big(\hat{a}_n + \hat{a}_n^\dagger\big). \tag{4}$$

Here, $\hat{x}$ and $\hat{p}$ denote the position and the momentum operators of the Brownian particle, m is the mass of the Brownian particle, and $\frac{m\omega^2\hat{x}^2}{2}$ represents the harmonic potential trapping the particle with frequency ω. The Hamiltonian for the two-level system (2LS) representing internal degree of freedom, is denoted by $\frac{\hbar\omega_0}{2}\hat{\sigma}_z$, with ω_0 being the transition frequency, and $\hbar\Omega\hat{\sigma}_x$ describes a weak classical driving of the inner degree of freedom ($\Omega \ll \omega_0$) [18, 19]. The operators $\hat{\sigma}_{i=x,y,z}$ are the standard Pauli matrices and the bath is described by the annihilation and creation operators, $\hat{a}_n$ and $\hat{a}_n^\dagger$, respectively, satisfying the standard bosonic commutation relations $[\hat{a}_n, \hat{a}_m^\dagger] = \delta_{n,m}$, and ω_n are frequencies of the corresponding oscillators. The system-bath coupling strength is denoted by g_n, and a constant α is a relative coupling strength.

To derive the reduced density matrix $\hat{\rho}_S(t)$, we assume that the system is weakly coupled to the thermal bath, allowing us to trace out the bath variables and obtain the Born–Markov master equation [2, 19]. The generic Born-Markov master equation [2, 19], when applied to our system, becomes

$$\frac{d}{dt}\hat{\rho}_S(t) = -\frac{i}{\hbar}\big[\hat{H}_S, \hat{\rho}_S\big] - \frac{1}{\hbar^2}\int_0^\infty d\tau\, \mathrm{tr}_B\Big[\hat{H}_{SB}(0), \big[\hat{H}_{SB}(-\tau), \hat{\rho}_S(t)\otimes\hat{\rho}_B\big]\Big]. \tag{5}$$

Above, $\hat{H}_{SB}(-\tau)$ denotes the system-bath interaction Hamiltonian in the interaction picture. We define the bath's density matrix at thermal equilibrium as $\hat{\rho}_B = \mathcal{Z}^{-1}\exp(-\beta\hat{H}_B)$, where the temperature is $T = (k_B\beta)^{-1}$, k_B is the Boltzmann constant and the partition function is $\mathcal{Z} = \mathrm{tr}_B[\exp(-\beta\hat{H}_B)]$. In principle, Eqn. (5) does not guarantee that the resulting dynamical equation will take the Gorini–Kossakowski–Sudarshan–Lindblad (GKSL) form [2, 20, 21]. To derive the master equation in GKSL form, one must apply the rotating-wave approximation (RWA) [16] (which corresponds to neglecting the rapidly oscillating terms) to the system-bath interaction Hamiltonian (4), which yields: $\hat{H}_{SB} = \hbar x_0 \sum_n g_n(\hat{a}^\dagger\hat{a}_n + \hat{a}\hat{a}_n^\dagger) + \hbar\alpha\sum_n g_n\big(\hat{a}_n\hat{\sigma}_+ + \hat{a}_n^\dagger\hat{\sigma}_-\big)$, where, $x_0 = \sqrt{\hbar/2m\omega}$ and $\hat{\sigma}_\pm$ are the Pauli raising and lowering operators of the 2LS, satisfying $[\hat{\sigma}_+, \hat{\sigma}_-] = \hat{\sigma}_z$. In the interaction picture, we assume that the classical driving term in the system Hamiltonian (2) is very weak, i.e., $\Omega \ll \omega_0$. By doing this, we get

$$\hat{H}_{SB}(-\tau) = x_0\sum_n g_n\hat{a}^\dagger\hat{a}_n e^{i(\omega_n-\omega)\tau} + \text{h.c.} + \alpha\sum_n g_n\hat{a}_n\hat{\sigma}_+ e^{i(\omega_n-\omega_0)\tau} + \text{h.c.} \tag{6}$$

Using the above expression (6), and choosing the spectral density of the form $\sum_n |g_n|^2 \to \int d\tilde{\omega} J(\tilde{\omega})$, we derive the following completely positive Born-Markov master equation for the reduced dynamics:

$$\frac{d}{dt}\hat{\rho}_S(t) = \mathcal{L}_{\mathrm{QHO}}\hat{\rho}_S + \mathcal{L}_{\mathrm{2LS}}\hat{\rho}_S + \mathcal{L}_{\mathrm{cross}}\hat{\rho}_S, \tag{7}$$

where $\mathcal{L}_{\mathrm{QHO}}\hat{\rho}_S$ describes the dissipator of the quantum harmonic oscillator, which reads

$$\mathcal{L}_{\mathrm{QHO}}\hat{\rho}_S(t) = -\frac{i}{\hbar}\big[\hat{H}_{\mathrm{QHO}}, \hat{\rho}_S\big] - \bar{\alpha}_1\big[\hat{x}, [\hat{x}, \hat{\rho}_S]\big] - \bar{\alpha}_2\big[\hat{p}, [\hat{p}, \hat{\rho}_S]\big] + i\bar{\alpha}_3\Big(\big[\hat{p}, \{\hat{x}, \hat{\rho}_S\}\big] - \big[\hat{x}, \{\hat{p}, \hat{\rho}_S\}\big]\Big). \tag{8}$$

Equation (8) represents a Caldeira-Leggett [15] type of master equation with an extra term $[\hat{p}, [\hat{p}, \hat{\rho}_S]]$, which allows us to write Eqn. (8) in GKSL form [20, 21]. The second term in Eqn. (7), $\mathcal{L}_{\mathrm{2LS}}\hat{\rho}_S$, has the form of the well-known quantum optical master equation for the 2LS [18, 19] and describe a dissipation of a weakly driven internal degree of freedom. The last term in Eqn. (7), $\mathcal{L}_{\mathrm{cross}}\hat{\rho}_S$, denotes a "cross-term" dissipator that captures dissipative coupling between external and internal degrees of freedom.

3. Adiabatic elimination and the OQBM master equation

In order to demonstrate that Eqn. (7) can be written as OQBM [8], we need to show that it could be represented as a diagonal representation in position, and this can be done by starting from a generic non-diagonal representation, defined as $\hat{\rho}_S(t) = \int_{-\infty}^{+\infty} dxdy\rho(x,y)\otimes|x\rangle\langle y|$. Subsequently, we make a coordinate transformation to canonical form via $u = (x+y)/2$ and $v = x - y$. In the rotated coordinate, we obtain

$$\frac{\partial}{\partial t}\rho(u,v) = \mathcal{L}_{\mathrm{QHO}}\rho + \mathcal{L}_{\mathrm{2LS}}\rho + \mathcal{L}_{\mathrm{cross}}\rho, \tag{9}$$

where

$$\mathcal{L}_{\mathrm{QHO}}\rho(u,v) = \left[\frac{i\hbar}{m}\frac{\partial^2}{\partial v\partial u} - \frac{im\omega^2}{\hbar}uv - \bar{\alpha}_1 v^2 + \bar{\alpha}_2\hbar^2\frac{\partial^2}{\partial u^2} + 2\hbar\bar{\alpha}_3\left(1 + u\frac{\partial}{\partial u}\right) - 2\hbar\bar{\alpha}_3 v\frac{\partial}{\partial v}\right]\rho, \tag{10}$$

$$\mathcal{L}_{\mathrm{2LS}}\rho(u,v) = -i\Big[\Big(\frac{\omega_0}{2} - \beta_3\Big)\hat{\sigma}_z + \Omega\hat{\sigma}_x, \hat{\rho}_S\Big] + \beta_1\mathcal{L}[\hat{\sigma}_-, \hat{\sigma}_+]\rho + \beta_2\mathcal{L}[\hat{\sigma}_+, \hat{\sigma}_-]\rho, \tag{11}$$

$$\mathcal{L}_{\mathrm{cross}}\rho(u,v) = \left(\frac{\partial}{\partial u}\hat{m}_1 + \frac{\partial}{\partial v}\hat{m}_2 + u\hat{m}_3 + v\hat{m}_4\right)\rho. \tag{12}$$

Here, $\mathcal{L}[\hat{A}, \hat{A}^\dagger]\hat{\rho} := \hat{A}\hat{\rho}\hat{A}^\dagger - (1/2)(\hat{A}^\dagger\hat{A}\hat{\rho} + \hat{\rho}\hat{A}^\dagger\hat{A})$, is the standard GKSL dissipator [20, 21] and $\hat{m}_1$, $\hat{m}_2$, $\hat{m}_3$, and $\hat{m}_4$ are the super-operators acting on the internal degree of freedom. The above system $\rho(u, v)$ involves two variables, u and v, where u denotes the slow variable and v denotes the fast variable, with the latter being the one we eliminate. Assuming $(m\omega)^2 \sim k_B T$ and that $\bar{\alpha}_1$ is larger than all the system parameters, we use the adiabatic elimination of fast variables [12, 13, 14] to derive the position distribution function $\bar{\rho}(u)$: $\bar{\rho}(u) = \int_{-\infty}^{+\infty} dv\rho(u, v)$. After performing the adiabatic elimination, we obtained that $v = 0$, which implies that $u = x$, and derive a completely positive master equation for the diagonal elements, which defines OQBM [8, 9, 10, 11]:

$$\frac{\partial}{\partial t}\bar{\rho}(x,t) \approx -\lambda_1 x\frac{\partial}{\partial x}\bar{\rho} - \lambda_2 x^2\bar{\rho} + \hat{m}_1\frac{\partial}{\partial x}\bar{\rho} + x\hat{m}_3\bar{\rho} + \lambda_3\frac{\partial^2}{\partial x^2}\bar{\rho} + \lambda_4\frac{\partial}{\partial x}(x\bar{\rho}) + \mathcal{L}_{2\mathrm{LS}}\bar{\rho}. \tag{13}$$

The diffusive term $(-\lambda_1 x\frac{\partial}{\partial x}\bar{\rho} - \lambda_2 x^2\bar{\rho} + \lambda_3\frac{\partial^2}{\partial x^2}\bar{\rho} + \lambda_4\frac{\partial}{\partial x}(x\bar{\rho}))$ describes the propagation of the Brownian particle. The Lindblad term $(\mathcal{L}_{2\mathrm{LS}}\bar{\rho})$ describes the dissipative dynamics of the internal state of the Brownian particle. The remaining term $(\hat{m}_1\frac{\partial}{\partial x}\bar{\rho} + x\hat{m}_3\bar{\rho})$ is a 'decision-making' term, describing the interaction between the external and internal degrees of freedom of the Brownian particle.

4. Numerical results and discussion

The reduced density matrix $\bar{\rho}(x, t)$ of the open quantum Brownian particle can be expressed as

$$\bar{\rho}(x,t) = \begin{pmatrix} \rho_{1,1}(x,t) & \rho_{1,2}(x,t) \\ \rho_{2,1}(x,t) & \rho_{2,2}(x,t) \end{pmatrix}, \tag{14}$$

where the diagonal elements $\rho_{1,1}(x, t)$ and $\rho_{2,2}(x, t)$ represent the probability of the system being in the first or the second quantum state, respectively, and the off-diagonal elements $\rho_{1,2}(x, t) = (\rho_{2,1}(x, t))^*$ represent quantum coherences. Using the above expression (14), the master equation (13) can be rewritten as

$$\begin{aligned}
\frac{\partial}{\partial t}\rho_+ &= \left\{\lambda_3\frac{\partial^2}{\partial x^2} + \Delta_1 x\frac{\partial}{\partial x} + \lambda_4 - \lambda_2 x^2\right\}\rho_+ - 2\delta_1\frac{\partial}{\partial x}C_I + 2\tilde{a}_2\frac{\partial}{\partial x}C_R, \\
\frac{\partial}{\partial t}\rho_- &= \left\{\lambda_3\frac{\partial^2}{\partial x^2} + \Delta_1 x\frac{\partial}{\partial x} + \Delta_2 - \lambda_2 x^2\right\}\rho_- - \bar{\beta}\rho_+ + \left\{4\tilde{a}_7 x - 4\Omega + 4\delta_2\frac{\partial}{\partial x}\right\}C_I \\
&\quad - \left\{4\tilde{a}_8 x + 4\delta_3\frac{\partial}{\partial x}\right\}C_R, \\
\frac{\partial}{\partial t}C_R &= \left\{\lambda_3\frac{\partial^2}{\partial x^2} + \Delta_1 x\frac{\partial}{\partial x} + \Delta_3 - \lambda_2 x^2\right\}C_R + \left\{\tilde{a}_8 x + \delta_3\frac{\partial}{\partial x}\right\}\rho_- + \frac{1}{2}\tilde{a}_2\frac{\partial}{\partial x}\rho_+, \\
\frac{\partial}{\partial t}C_I &= \left\{\lambda_3\frac{\partial^2}{\partial x^2} + \Delta_1 x\frac{\partial}{\partial x} + \Delta_4 - \lambda_2 x^2\right\}C_I + \left\{\Omega - \tilde{a}_7 x - \delta_2\frac{\partial}{\partial x}\right\}\rho_- - \frac{1}{2}\delta_1\frac{\partial}{\partial x}\rho_+,
\end{aligned} \tag{15}$$

where $\rho_\pm = \rho_{1,1}(x, t) \pm \rho_{2,2}(x, t)$, $C_R = \mathrm{Re}(\rho_{1,2}(x, t))$, $C_I = \mathrm{Im}(\rho_{1,2}(x, t))$. To explore the behavior of OQBM, we integrate the system of partial differential equations (15) numerically. We consider Gaussian and non-Gaussian initial distributions for the open Brownian particle and assume that the internal degree of freedom is initially a pure state described by

$$\bar{\rho}_j(x,0) = \frac{1}{2I_j}e^{-x^j} \otimes \begin{pmatrix} 2\cos^2\theta & \sin 2\theta e^{-i\phi} \\ \sin 2\theta e^{i\phi} & 2\sin^2\theta \end{pmatrix}, \tag{16}$$

where $I_j = \int_{-\infty}^{+\infty} dx e^{-x^j}$, $\theta \in [0, \pi)$, $\phi \in [0, 2\pi)$, and $j > 0$. Figure 1, shows the position probability distribution $P(x, t) = \mathrm{tr}\big(\rho_+(x, t)\big)$ of finding the open Brownian particle at position x at time t.

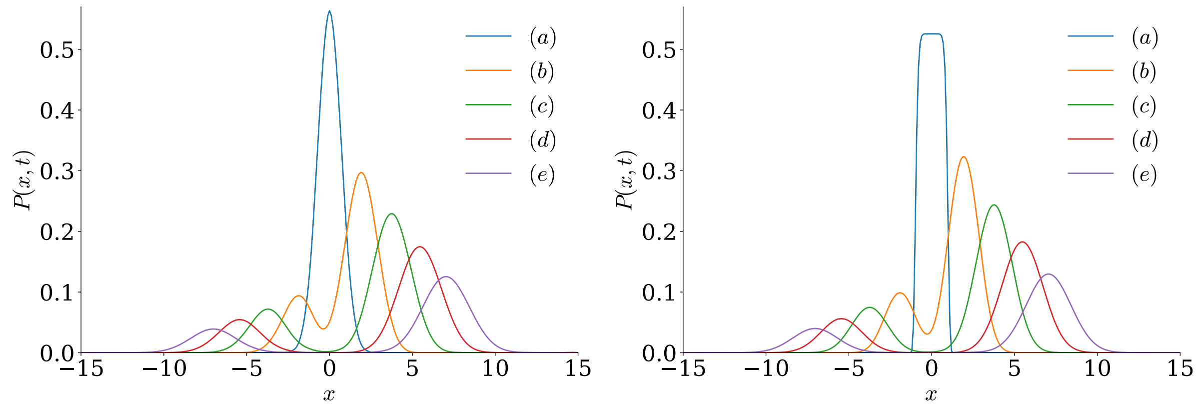

Figure 1. The position probability distribution $P(x,t)$ of the open quantum Brownian particle for different moments of time. The initial distribution is given by Eqn. (16), with $\theta = \pi/6$, $\phi = \pi/4$. The *left panel* and the *right panel* correspond to $j = 2$ and $j = 10$, respectively. Curves (a) to (e) correspond to times 0, 50, 100, 150, and 200, respectively. Other parameters are set to $\Omega = 0.3$, $\beta = \Delta_1 = \Delta_2 = \tilde{a}_7 = 10^{-3}$, $\Delta_3 = \lambda_2 = \lambda_4 = \delta_1 = \tilde{a}_8 = 10^{-4}$, $\Delta_4 = 8 \times 10^{-3}$, $\lambda_3 = 5 \times 10^{-3}$, $\delta_2 = 3 \times 10^{-2}$, $\delta_3 = 10^{-2}$, and $\tilde{a}_2 = -4 \times 10^{-2}$. For times $t \geqslant 50$, the profile splits into two Gaussians.

The *left panel* of Fig. 1 demonstrates that for the initial Gaussian distribution (for $j = 2$) and a chosen set of parameters, the OQBM walker probability distributions split into two Gaussian distributions at time $t \geqslant 50$. In the *right panel* of Fig. 1, one can see clearly that even with a non-Gaussian initial distribution (for $j = 10$), the position probability distribution of the open Brownian particle converges into a mixture of Gaussian distributions at times $t \geqslant 50$, for various parameters.

To derive the equations for the cumulants of the position distribution of the OQBM walker, we take the logarithm of the generating function of the characteristic function of the scaled reduced density matrix $\tilde{\rho}(\xi,t)$ as $\ln \bar{\rho}(k,t) = \ln\big\langle e^{-ik\xi}\big\rangle = \ln \int_{-\infty}^{+\infty} d\xi \tilde{\rho}(\xi,t) e^{-ik\xi} = \sum_{n=1}^{\infty} \frac{(-ik)^n}{n!}\langle \xi^n \rangle_c$. Assuming a Gaussian initial state of the form (16) for $j = 2$, and assuming $\langle x^4 \rangle_c = 0$. For the zeroth order $(-ik)^0$, we derive

$$0 = \bar{\lambda}_2 \langle x \rangle_c^2 + \bar{\lambda}_2 \langle x^2 \rangle_c + \Delta_1 - \lambda_4. \tag{17}$$

The above expression (17) can be written as $\langle x \rangle_c^2 + \langle x^2 \rangle_c = \langle x^2 \rangle = \frac{\hbar}{2m\omega \bar{x}_0^2}\big(2n(\omega)+1\big)$, which shows that the second moment $\langle x^2 \rangle$ of the position is related to the quantum mechanical zero-point energy and the thermal occupation $n(\omega)$.

5. Conclusion

In this contribution, we outlined the microscopic derivation of a completely positive master equation for OQBM using the adiabatic elimination of fast variables method for a weakly driven open Brownian particle confined in a harmonic potential and dissipatively coupled to a thermal bath. We numerically solve the derived master equation for a reduced density matrix of the OQBM for Gaussian and non-Gaussian initial conditions. Both examples show how the OQBM dynamics converge to Gaussian distributions even for the non-Gaussian initial distribution. We found that the third-order cumulant $\langle x^3 \rangle_c$ does not vanish, indicating deviations from Gaussianity. The OQBM master equation describes an example of quantum-classical master equations, which now seem to be finding application in various fields, including gravity

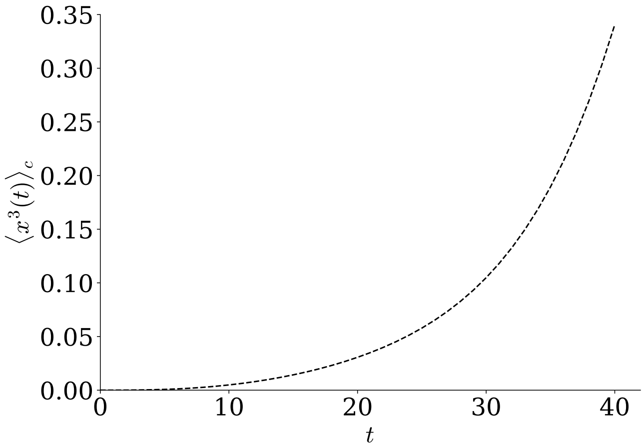

Figure 2. The evolution of the third-order cumulant $\langle x^3\rangle_c$ as functions of time. The initial distribution is given by Eqn. (16) with $\theta = \pi/8$ and $\phi = \pi/4$. Other parameters are set to $\Omega = \bar{a}_7 = 10^{-2}, \beta = 5\times10^{-3}, \chi = 0.25, \bar{\lambda}_2 = 10^{-3}, \Delta_1 = 4\times10^{-2}, \bar{\lambda}_3 = 3\times10^{-2}, \Delta_3 = \bar{\delta}_3 = \bar{a}_2 = 3\times10^{-3}, \Delta_4 = 9\times10^{-2}, \bar{a}_8 = 6\times10^{-3}, \bar{\delta}_1 = 9\times10^{-3}$, and $\bar{\delta}_2 = 2\times10^{-2}$.

theories [22, 23, 24]. Future studies along this line of research will explore the generalization of OQBM to gravity-related theories.

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