Master equations for a damped nonlinear oscillator and the validity of the Markovian approximation

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(Received 18 July 1988)

The different conditions that could be imposed on a Markovian master equation for a nonlinear oscillator weakly coupled to a thermal reservoir are formulated. They concern preservation of trace and positivity of a density matrix, return to a proper equilibrium state, and the detailed balance condition. It is shown that only one of the known master equations satisfies all of these conditions. Then the validity of the Markovian approximation is reanalyzed using certain non-Markovian weak-coupling approximations, and the existence of different stages of evolution associated with different time scales of the Hamiltonian dynamics is predicted. The consequences of these facts for the description of a damped nonlinear oscillator are discussed.

I. INTRODUCTION

This paper is motivated by a recent interest in the dynamics of the nonlinear oscillator with a Hamiltonian

$$H=\omega a^{\dagger}a+\chi(a^{\dagger}a)^2,\quad [a,a^{\dagger}]=1,\quad \hbar\equiv 1 \tag{1.1}$$

weakly coupled to a heat bath at temperature $T\geq 0$.[1,2] This system may serve as a relatively simple but nontrivial model for analyzing different approximation schemes used in the theory of quantum open systems. One of the most important problems is the validity of the Markovian approximation and a proper form of the associated master equation. In contrast to the exactly soluble case of a harmonic oscillator coupled to a bosonic heat bath,[3] the dynamics of a nonlinear oscillator weakly interacting with an environment can be treated only approximately. Even the best estimations involve perturbation expansions which can be controlled for finite time intervals only. Moreover, different master equations may yield asymptotically equivalent results. Hence it is worthwhile to formulate some additional criteria which may help to fix a form of the proper master equation.[4] These conditions are both of mathematical and phenomenological origin. They are consistent with the weak-coupling and Markovian approximations for the long-time evolution and allow application of powerful mathematical tools such as spectral decomposition of the Heisenberg evolution, ergodic theory for completely positive one-parameter semigroups, or the H theorem for the relative entropy.[5] On the other hand, some of them correspond to the usual phenomenological picture of a return to equilibrium, a detailed balance condition, and a kinetic description in terms of the Pauli master equation.

In Sec. III we discuss three types of master equations for a nonlinear oscillator. The first one (I) is obtained by adding the term $-i[\chi(a^{\dagger}a)^2,\rho(t)]$ to the well-known equation for a damped harmonic oscillator. The second one (II) was derived by Haake *et al.*,[2] and the third one (III) is obtained by a direct application of the Davies rigorous weak-coupling limit.[6,7] Obviously master equation I drives the system into an improper stationary state, which is an equilibrium state for a harmonic oscillator. We shall show that master equation II does not preserve the positivity of a density matrix. Master equation III satisfies all required conditions but it involves a kind of rotating-wave approximation which is valid for $t\gg\max\{1/\omega,1/\chi,\tau_R\}$ (τ_R is the decay time of the reservoir's correlations). Hence master equation III is meaningful for rather strong nonlinearities $\chi\gg 1/\kappa$ (κ is the damping rate). All these difficulties suggest that one analyze more carefully the Markovian approximation in the weak-coupling regime. It is done in Sec. IV using a non-Markovian weak-coupling approximation obtained by means of a certain cumulant expansion. Particularly, the interplay of different time scales τ_R, $1/\omega$, $1/\chi$, and $1/\kappa$ is studied in detail. In Sec. V we evaluate the time evolution of the mean value $\langle a(t)\rangle$ for the master equations I, II, and III (with $T=0$), which could be, in principle, compared with experimental results.

Finally, one should mention that in this paper the mathematical consistency of the approximative dynamics is strongly advocated, with special emphasis on complete positivity. However, there may exist practically useful examples of evolution equations that meet these requirements only approximately and/or are for the restricted domain of possible initial states.

II. PROPERTIES OF MASTER EQUATIONS

We formulate now some desired conditions which might be imposed on the Markovian master equation for the nonlinear quantum oscillator (1.1).

(a) The master equation of the form

$$\frac{d}{dt}\rho(t)=L\rho(t),\quad t\geq 0 \tag{2.1}$$

is derived using certain weak-coupling and Markovian approximations from the reduced dynamics of a nonlinear oscillator with a bare Hamiltonian

$$H_0=\omega_0 a^{\dagger}a+\chi_0(a^{\dagger}a)^2+\cdots . \tag{2.2}$$

The oscillator is weakly coupled to a heat bath by means of the interaction Hamiltonian

$$H_{\rm int}=\lambda(a\otimes\Gamma^{\dagger}+a^{\dagger}\otimes\Gamma)\ , \qquad (2.3)$$

and the initial state is taken to be the product of an arbitrary density matrix $\rho(0)$ of the oscillator and the canonical operator for the bath

$$\rho(0)\otimes e^{-H_B/kT}/Z,\quad T>0\ . \qquad (2.4)$$

In the limit case $T=0$, we replace the canonical operator by the ground state of the bath.

(b) The propagator $\{e^{Lt},\ t\geq 0\}$ for the master equation (2.1) preserves trace and satisfies the condition of complete positivity,[5] which assures that $\rho(t)=e^{Lt}\rho(0)$ is a density matrix (positive operator, trace equal to 1) for any density matrix $\rho(0)$. These conditions imply the following form of L:

$$L\rho=-i[H,\rho]+\tfrac{1}{2}\sum_{k,l}c_{kl}([F_k\rho,F_l^{\dagger}]+[F_k,\rho F_l^{\dagger}]) \qquad (2.5)$$

with $H=H^{\dagger}$, (c_{kl}) is the positively defined matrix, or equivalently,

$$L\rho=-i[H,\rho]+\tfrac{1}{2}\sum_{m}([V_m\rho,V_m^{\dagger}]+[V_m,\rho V_m^{\dagger}])\ . \qquad (2.6)$$

(c) The Gibbs state $\rho_{\rm eq}=e^{-H/kT}/Z$, defined by the renormalized Hamiltonian (1.1), is a stationary state for Eq. (2.1) and, moreover, for any initial state $\rho(0)$ and any observable A

$$\lim_{t\to\infty}{\rm tr}[\rho(t)A]={\rm tr}(\rho_{\rm eq}A)\ . \qquad (2.7)$$

(d) The generator L may be decomposed as $L=L_H+L_D$ where $L_H=-i[H,\dots]$, $[L_H,L_D]=0$, and L_D satisfies the quantum detailed balance condition[8,9] in the form

$$(X,L_D^{*}Y)=(L_D^{*}X,Y)\ . \qquad (2.8)$$

Here $(X,Y)={\rm tr}(\rho_{\rm eq}X^{\dagger}Y)$ and L_D^{*} is the Heisenberg picture generator, i.e., ${\rm tr}[(L_D\rho)X]={\rm tr}(\rho L_D^{*}X)$.

(e) The diagonal matrix elements of $\rho(t)$ in the basis of the occupation number states $\{|n\rangle,\ a^{\dagger}a|n\rangle=n|n\rangle,\ n=0,1,2,\dots\}$ evolve independently of the off-diagonal ones and their evolution is governed by the Pauli master equation

$$\frac{d}{dt}p_n(t)=\sum_{m=n\pm1}[a_{nm}p_m(t)-a_{mn}p_n(t)]\ , \qquad (2.9)$$

with $p_n(t)=\langle n|\rho(t)|n\rangle$; the transition probabilities satisfy the classical detailed balance condition

$$a_{n+1,n}=a_{n,n+1}e^{-(E_{n+1}-E_n)/kT}\ , \qquad (2.10)$$

where $E_n=\omega n+\chi n^2$.

III. THREE EXAMPLES OF MASTER EQUATION

We present now three examples of the master equation (I, II, and III) for the nonlinear oscillator. All of them satisfy condition (a) but their properties are different.

(I) This is a simple modification of the well-known master equation for a harmonic oscillator (see Ref. 1 for the case $T=0$) which leads to

$$L_{\rm I}\rho=-i[\omega a^{\dagger}a+\chi(a^{\dagger}a)^2,\rho]+\tfrac{1}{2}\kappa([a,\rho a^{\dagger}]+e^{-\omega/kT}[a^{\dagger},\rho a]+{\rm H.c.})\ . \qquad (3.1)$$

Obviously, master equation I satisfies conditions (a) and (b), while (c), Eq. (2.8), and (e) are fulfilled for $H=\omega a^{\dagger}a$ ($E_n=\omega n$) being the Hamiltonian of a harmonic oscillator.

(II) This equation was derived by Haake *et al.*,[2] and the generator takes form

$$L_{\rm II}\rho=-i[\omega_0a^{\dagger}a+\chi_0(a^{\dagger}a)^2,\rho]+\frac{i}{2}{\rm P}\int_{-\infty}^{+\infty}d\nu\,A(\nu)(\{[1+n_{\rm th}(\nu)][(\phi-\nu)^{-1}a\rho,a^{\dagger}]+n_{\rm th}(\nu)[a^{\dagger},\rho(\phi-\nu)^{-1}a]\}-{\rm H.c.})$$
$$+\kappa(\{[[1+n_{\rm th}(\phi)]a\rho,a^{\dagger}]+[a^{\dagger},\rho n_{\rm th}(\phi)a]\}+{\rm H.c.})\ , \qquad (3.2)$$

where $\kappa>0$ and $A(\nu)$ depend on the bath's parameters, $n_{\rm th}(\nu)$ is the thermal number of quanta $n_{\rm th}(x)=(e^{x/kT}-1)^{-1}$, and ϕ is an operator given by $\phi=\omega_0+\chi_0+2\chi_0a^{\dagger}a$, where ω_0 and χ_0 are the bare parameters of the oscillator.

Master equation II satisfies condition (a) and conditions (c) and (e), with H replaced by $H_0=\omega_0a^{\dagger}a+\chi_0a^{\dagger}a^2$, which is rather a shortcoming because, for all fundamental interactions, the bare Hamiltonian is a not uniquely defined cutoff-dependent quantity.[10] The importance of the mathematical consistency condition (b) is not satisfied by $L_{\rm II}$. The proof of this fact is the following. Assume that e^{Lt}, $t\geq0$ preserves positivity of a density matrix. Then for arbitrary orthogonal vectors $|a\rangle,|b\rangle$ $\langle a|b\rangle=0$, we have

$$0\leq\lim_{t\searrow0}\frac{1}{t}\langle a|(e^{Lt}|b\rangle\langle b|)|a\rangle=\langle a|(L|b\rangle\langle b|)|a\rangle\ . \qquad (3.3)$$

Let $|a\rangle\equiv|a_z\rangle=|n-1\rangle+z|m-1\rangle$ and $|b\rangle=|n\rangle+|m\rangle$, with $z\in\mathbb{C}$ and $m>n+1$. Then $J(z)=\langle a_z|(L_{\rm II}|b\rangle\langle b|)|a_z\rangle$ may be easily evaluated:

$$J(z)=|z|^2m\{2\,{\rm Re}[g(m-1)]\}+z[g(n-1)+\bar{g}(m-1)]\sqrt{nm}+\bar{z}[\bar{g}(n-1)+g(m-1)]\sqrt{nm}+2n\,{\rm Re}[g(n-1)]\ , \qquad (3.4)$$

where

$$g(n)=\kappa[1+n_{\rm th}(\omega_0+\chi_0(2n+1))] + \frac{i}{\pi}{\rm P}\int_{-\infty}^{+\infty}d\nu\, A(\nu)[\omega_0+\chi_0(2n+1)-\nu]^{-1} \times[1+n_{\rm th}(\omega_0+\chi_0(2n+1))] \ .$$

$J(z)$ reaches its minimum for

$$z_0=-[\bar{g}(n-1)+g(m-1)]/2\sqrt{m/n}\ {\rm Re}[g(m-1)]$$

and

$$J(z_0)=-\frac{n}{2\,{\rm Re}[g(m-1)]}|g(n-1)-g(m-1)|^2\le 0 \tag{3.5}$$

is always negative, except for the trivial case $\chi_0=0$.

(III) The form of $L_{\rm III}$ is uniquely determined by conditions (b), (c), (d), and (e):[8]

$$L_{\rm III}\rho=-i[\omega a^\dagger a+\chi(a^\dagger a)^2,\rho] +\tfrac{1}{2}\sum_{n=0}^{\infty}\gamma_n([A_n,\rho A_n^\dagger] +\exp\{-[\omega+(2n+1)\chi]/kT\} \times[A_n^\dagger,\rho,A_n]+{\rm H.c.}) \tag{3.6}$$

with $\gamma_n>0$, $A_n=|n\rangle\langle n+1|$.

In order to satisfy condition (a), one may use the rigorous weak-coupling limit proposed by Davies which leads to (3.6) with

$$\gamma_n=\lambda^2(n+1)\int_{-\infty}^{+\infty}dt\langle\Gamma_t^\dagger\Gamma\rangle_B e^{i[\omega+2(n+1)\chi]t} \ , \tag{3.7}$$

and links the bare and renormalized Hamiltonians

$$H=\omega a^\dagger a+\chi(a^\dagger a)^2=H_0+\lambda^2 w(a^\dagger a) \ ,$$

$$w(n)=(n+1)\{s[\omega+(2n-1)] +s[-\omega-(2n+1)\chi]\} \ , \tag{3.8}$$

$$s(x)={\rm Im}\int_0^\infty dt\, e^{ixt}\langle\Gamma_t^\dagger\Gamma\rangle_B \ ,$$

where $s(x)$ is the cutoff-dependent quantity.

In contrast to $L_{\rm I}$ and $L_{\rm II}$, the generator $L_{\rm III}$ does not converge to the generator for a damped harmonic oscillator when $\chi(\chi_0)\searrow 0$. This is due to the fact that $L_{\rm III}$ was derived using a particular averaging procedure that eliminates oscillating terms in the integral version of the equation of motion.[5-7] Therefore the master equation with the generator $L_{\rm III}$ provides a good approximation for $t\gg\max\{1/\omega,1/\chi,\tau_R\}$ (here τ_R is the decay time of the correlations $\langle\Gamma_t^\dagger\Gamma\rangle_B$), which makes the limit $\chi\searrow 0$ meaningless. As a consequence, $L_{\rm III}$ may be used for damping rates $\kappa=\gamma_0\ll\min(\omega,\chi)$. These restrictions are, however, inevitable. One cannot expect that an equation of the type (2.1) with a fixed L driving the system to the proper equilibrium state will be valid for times $t\lesssim\max\{1/\omega,1/\chi\}$. Due to the indeterminancy relations $\Delta t\Delta\omega\gtrsim 1$, the whole system needs this time to "recognize" the action of the Hamiltonian part $-i[H,\dots]$ and to "adapt" the dissipation mechanism to the ultimate equilibrium state $\rho_{\rm eq}=e^{-H/kT}/Z$. We shall discuss this problem in Sec. IV.

IV. VALIDITY OF THE MARKOVIAN APPROXIMATION

We consider an open system S with a bare Hamiltonian

$$H_0=\sum_k E_k^0|k\rangle\langle k| \tag{4.1}$$

weakly coupled to a heat bath B, with a free Hamiltonian H_B and the interaction of the form

$$\lambda H_{\rm int}=\lambda A\otimes F,\quad A=A^\dagger,\ F=F^\dagger \ . \tag{4.2}$$

We take as an initial state the product state

$$\rho(0)\otimes\sigma_B \ , \tag{4.3}$$

where σ_B is an equilibrium or a ground state of the bath. One can always redefine H_0 and F such that

$$\langle F\rangle_B=0 \ , \tag{4.4}$$

where

$$\langle X\rangle_B\equiv{\rm tr}(\sigma_B X) \ .$$

The reduced dynamics of S in the interaction picture is given by

$$\rho(t)=W_t\rho(0) ={\rm tr}_B\left[T\exp\left[-i\lambda\int_0^t ds[\tilde{H}_{\rm int}(s),\dots]\right] \times\rho(0)\otimes\sigma_B\right] \ . \tag{4.5}$$

Here the interaction picture is taken with respect to $H+H_B$, where H is a renormalized Hamiltonian of S. $H=H_0-H_c$ and H_c consists of counterterms which cancel the cutoff-dependent terms generated by an interaction with the bath,

$$H_c=\lambda H_c^{(1)}+\lambda^2 H_c^{(2)}+\cdots,\quad [H_0,H_c^{(k)}]=0 \ . \tag{4.6}$$

Here

$$\tilde{H}_{\rm int}(s)=A(s)\otimes F_s+H_c \ , \tag{4.7}$$

with

$$A(s)=e^{iHs}Ae^{-iHs},\quad F_s=e^{iH_Bs}Fe^{-iH_Bs} \ .$$

Introducing a kind of cumulant expansion[11-13]

$$W_t=\exp\left[\sum_{n=1}^{\infty}\lambda^n K^{(n)}(t)\right] \ , \tag{4.8}$$

we obtain for the first two terms

$$K^{(1)}(t)=0 \tag{4.9}$$

[$H_c^{(1)}=0$, a consequence of (4.3)]

$$K^{(2)}(t)\rho=-it[H_c^{(2)},\rho]-\tfrac{1}{2}\,\mathrm{tr}_B\int_0^t ds\int_0^s dw[\tilde{H}_{\rm int}^{(1)}(s),[\tilde{H}_{\rm int}^{(1)}(w),\rho\otimes\sigma_B]]$$
$$=-i[B(t),\rho]+\tfrac{1}{2}\sum_{\omega,\omega'} b_{\omega\omega'}(t)([A_\omega\rho,A_{\omega'}^\dagger]+\mathrm{H.c.})\,, \tag{4.10}$$

where

$$A(t)=\sum_\omega A_\omega e^{-i\omega t},\quad \tilde{H}_{\rm int}^{(1)}(s)=A(s)\otimes F_s\,, \tag{4.11}$$

$$b_{\omega\omega'}(t)=\int_0^t ds\int_0^t dw\langle F_sF_w\rangle_B e^{i(\omega's-\omega w)}\,, \tag{4.12}$$

and $b_{\omega\omega'}(t)$ is a positively defined matrix for all $t\geq 0$.

$$B(t)=B^\dagger(t)=\sum_{\omega,\omega'} s_{\omega'\omega}(t)A_{\omega'}^\dagger A_\omega+tH_c^{(2)}\,,$$
$$s_{\omega'\omega}(t)=-(i/2)\int_0^t ds\int_0^s dw(\langle F_sF_w\rangle_B \times e^{-i(\omega w-\omega's)}-\mathrm{H.c.})\,, \tag{4.13}$$

Comparing (4.8)–(4.13) with (2.5), one concludes that

$$W_t^{(2)}=\exp[\lambda^2K^{(2)}(t)],\quad t\geq 0 \tag{4.14}$$

is a one-parameter family of completely positive trace-preserving maps and provides mathematically consistent weak-coupling non-Markovian approximation for the reduced dynamics W_t. We analyze qualitatively the time dependence of $b_{\omega\omega'}(t)$. Generally,

$$\langle F_sF_w\rangle_B=\int_{-\infty}^{+\infty}dE\,h(E)e^{-iE(s-w)}\,, \tag{4.15}$$

with $h(E)\geq 0$ and $h(-E)=e^{-E/kT}h(E)$. The function $h(E)$ usually grows with $E\nearrow\infty$ [typical behavior for a bosonic reservoir is $h(E)\sim E^3$] up to a certain cutoff parameter $E_{\max}\gg\{\omega\}$ and then falls to zero. Hence one may write

$$b_{\omega\omega'}(t)=4\pi^2e^{-(i/2)(\omega-\omega')t}\times\int_{-E_{\max}}^{E_{\max}}dE\,h(E)\frac{\sin(E-\omega)t}{\pi(E-\omega)}\,\frac{\sin(E-\omega')t}{\pi(E-\omega')}\,.$$

For $t\ll E_{\max}^{-1}$, we may set

$$b_{\omega\omega'}(t)\cong\left[4\int_{-E_{\max}}^{E_{\max}}dE\,h(E)\right]t^2\,.$$

This strongly cutoff-dependent and highly non-Markovian stage of the evolution is due to the initial choice of the state (2.4). The assumption (2.4) is rather unphysical for fundamental interactions (e.g., electromagnetic ones) because one cannot switch them off at the moment $t=0$, while for an interaction with a medium (e.g., the interaction of electrons with phonons in crystal) such a state could, in principle, be realized.

For $t\gg E_{\max}^{-1}$, the functions $\sin[(E-\omega)t]/\pi(E-\omega)$ and $\sin^2[(E-\omega)t]/\pi(E-\omega)^2t$ behave like the approximations of $\delta(E-\omega)$ in the integral (4.16). For fixed ω,ω' $(\omega\neq\omega')$, we may distinguish two time scales.

(i) For $E_{\max}^{-1}\ll t\ll|\omega-\omega'|^{-1}$, we have

$$b_{\omega\omega'}(t)\cong b_{\omega\omega}(t)\cong b_{\omega'\omega'}(t)\cong 4\pi h(\omega)t\,.$$

(ii) For $t\gg|\omega-\omega'|^{-1}$, we obtain

$$b_{\omega\omega}(t)=4\pi h(\omega)t,\quad b_{\omega'\omega'}(t)\cong 4\pi h(\omega')t,\quad b_{\omega\omega'}(t)\cong 0\,.$$

Similar results may be shown for $s_{\omega\omega'}(t)$. The main difference is that for

$$t\gg\max_{\omega\neq\omega'}|\omega-\omega'|^{-1}\,,$$
$$\sum_{\omega',\omega}s_{\omega'\omega}(t)A_{\omega'}^\dagger A_\omega$$

is cutoff dependent and cancels with the counterterm $tH_c^{(2)}$.

The consequences of the above estimations for the nonlinear damped oscillator are the following. For

$$t\gg\max\{1/\omega,1/\chi,\tau_R\cong E_{\max}^{-1}\}\,,$$

the reduced dynamics may be approximated by the solution of the master equation (2.1) with the generator $L_{\rm III}$, which describes a "detailed balanced" return to the equilibrium state $\rho_{\rm eq}=e^{-H/kT}/Z$, $H=\omega a^\dagger a+\chi(a^\dagger a)^2$. However, for small nonlinearities and initial conditions such that $\bar{n}\chi\ll\omega$, $\bar{n}=\mathrm{tr}[\rho(0)a^\dagger a]$, the time scale $\omega^{-1}\ll t\ll(\bar{n}\chi)^{-1}$ might be relevant. On that time scale and with the above conditions, the evolution is more precisely described by the master equation with the generator of the type $L_{\rm I}$.

V. TIME-DEPENDENT SOLUTIONS

We compare the time-dependent averages $\mathrm{tr}[\rho(t)a]$ for the dynamics governed by $L_{\rm I}$, $L_{\rm II}$, and $L_{\rm III}$ under the following conditions: (a) $T=0$ and (b) $\rho(0)=|\alpha\rangle\langle\alpha|$, where $|\alpha\rangle$ is a coherent state and $a|\alpha\rangle=\alpha|\alpha\rangle$. Moreover, we assume for $L_{\rm II}$ the validity of the following linear approximation:

$$f(n)=\tfrac{1}{2}\mathrm{P}\int_{-\infty}^{+\infty}d\nu\,A(\nu)[\nu-\omega_0-\chi_0(2n+1)]^{-1}\cong A+Bn\,, \tag{5.1}$$

and for $L_{\rm III}$ the simplifying relation $\gamma_n=(n+1)\gamma_0$. The straightforward but tedious calculations lead to the final results:

$$\mathrm{tr}[\rho(t)a]=\alpha\exp[-i(\omega+\chi)t-\tfrac{1}{2}\gamma_0t-|\alpha|^2\xi(1-e^{(-i2\chi-\gamma_0)t})]\,, \tag{5.2}$$

where, for $L_{\rm I}$ (see Ref. 1),

$$\xi=(1-i\gamma_0/2\chi)^{-1}\,,$$

for L_{II},

$$\omega=\omega_0+(A-B),\quad \chi=\chi_0+B\ ,$$

$$\xi=[1-i\gamma_0/(2\chi_0+B)]^{-1}\ ,$$

and for L_{III},

$$\xi=1\ .$$

VI. CONCLUSION

A mathematically consistent master equation in the weak-coupling regime can be unambiguously defined if the time scale of the Hamiltonian motion is well separated from the time scale of the dissipative one. If this is not the case, then different stages of evolution governed approximatively by different master equations may appear. Only the last stage is described by the generator obtained using the (renormalized) Davies weak-coupling limit which satisfies the detailed balance condition with respect to a proper equilibrium state. The damped nonlinear oscillator is a good illustration of this phenomenon because its Hamiltonian defines two independent time scales $1/\omega$ and $1/\chi$. As proposed in Ref. 1, this system may be realized as an intracavity electromagnetic mode interacting with a nonlinear crystal and hence the theoretical predictions might be verified experimentally.

ACKNOWLEDGMENTS

This work is partially supported by the Polish Ministry of Education, project No. CPBP 01.03.3.3.

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