

# Determination of the external field amplitude and deviation parameter through expectation value based quantum optimal control of multiharmonic oscillators under linear control agents

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**Abstract** This work focuses on the optimal control of a quantum system composed of harmonic oscillators under linear control agents (dipole function, objective operator, and the penalty operator whose expectation value is to be suppressed). The main purpose of the work is to determine the temporal external field amplitude function. Paper recalls the formulation of the optimal control equations first. Then a set of ordinary differential equations over the expectation values of certain unknown entities is constructed. These temporal differential equations have time varying coefficients unless the weight functions appearing in the cost functional are constant. Certain accompanying conditions are needed to get unique solutions. Investigations show that one half of the conditions should be given at the initial instant and the other half should be specified at the final moment. Since the differential equations contain another unknown entity, deviation parameter, solutions must satisfy an algebraic equation derived from the definition of this parameter. Results do not involve the explicit structure of the wave function and costate function. Only the external field amplitude and the deviation parameter are determined here. The evaluation of the wave function and costate function needs additional treatments to the control equations. We report certain analytical results for external field amplitude and the deviation parameter and give certain illustrative implementations to finalize the paper.

**Keywords** Quantum optimal control · Harmonic oscillator · Matrix ODEs

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## 1 Introduction

Quantum optimal control of a system is governed by an appropriately chosen cost functional which must reflect certain behaviors of the system under control [1–5]. First of all we assume that the control over the system is provided by an interaction with an external energy source which has an electromagnetic origin. In this work we do not concern with the vector potentials. We assume that the only effect of the external system is optical type, hence, can be described by an electromagnetic field with a purely scalar potential. Multipole expansion which is basically an expansion with respect to ascending hyperpolarizabilities is used to write the scalar potential. We use weak field assumption where the interaction potential of the system is described by a dipole interaction alone. Therefore, the equation of motion of the system is governed by such potentials plus the system's Hamiltonian when it is isolated. That is,

$$H \equiv H_{is} - \mu E(t), \quad t \in [0, T] \quad (1)$$

where  $H_{is}$ ,  $\mu$ ,  $E(t)$ , and  $T$  stand for the isolated system's Hamiltonian, spatially varying dipole function, temporally varying external field amplitude function, and the interaction time period, respectively. All of these entities except the external field amplitude are given.

Second important thing is the main purpose of the control. It aims at making the deviation between the expectation value of a given operator (*objective operator*) and its target's given value which is either exactly zero (exact achievement) or close to zero as much as possible (getting smallest deviation from the target). This feature is reflected into the cost functional by considering the following additive component which may be called *objective term*.

$$J_o \equiv \frac{1}{2} (|\langle \psi(T) | \widehat{O} | \psi(T) \rangle - \widetilde{O}|)^2 \quad (2)$$

where Dirac's bracket notation is used and the symbols  $\widehat{O}$  and  $\widetilde{O}$  denote the objective operator and its expectation value's target respectively.

Third important feature to be reflected into the cost functional is about the suppressing of an undesired expectation value of an operator which may be called *penalty operator*. This reflection is done by writing the following additive component (*first penalty term*) to the cost functional

$$J_p^{(1)} \equiv \frac{1}{2} \int_0^T W_p(t) |\langle \psi(t) | \widehat{O}' | \psi(t) \rangle|^2 dt, \quad W_p(t) > 0, \quad t \in [0, T] \quad (3)$$

where  $\widehat{O}'$  and  $W_p(t)$  stand for the penalty operator and a given weight function, which is used to give different importances to different instances of suppression, respectively.

The fourth feature to be reflected into the cost functional is the demand for the finiteness of the external field amplitude. This is added to the cost functional via the following additive term (*second penalty term*)

$$J_p^{(2)} \equiv \frac{1}{2} \int_0^T W_E(t) E(t)^2 dt, \quad W_E(t) > 0, \quad t \in [0, T] \quad (4)$$

where  $W_E(t)$  denotes a weight function which is used to suppress the magnitude of the external field amplitude in different scales at different instances of the control.

Finally we need to reflect the system's dynamic into the cost functional. This can be done in two different ways. One way is to eliminate the wave function describing the system's dynamic by solving the Schrödinger's equation of the system in terms of  $E(t)$  and  $T$ . This is a quite cumbersome procedure we will avoid here. We will use the second way which uses a Lagrange multiplier. We employ the following additive component (*dynamical constraint*) in the cost functional to take the system's dynamics into consideration

$$J_{dc} \equiv \int_0^T \left\langle \lambda(t) \left| i\hbar \frac{\partial}{\partial t} - H \right| \psi(t) \right\rangle dt + \int_0^T \left\langle \psi(t) \left| -i\hbar \frac{\partial}{\partial t} - H \right| \lambda(t) \right\rangle \quad (5)$$

where  $\langle \psi(t) |$  stands for the bra of the wave function and  $\langle \lambda(t) |$  denotes a Lagrange multiplier bra (*costate function*).

Now the cost functional of the optimal control of the system under consideration can be written as the sum of the terms defined above. That is,

$$J \equiv J_o + J_p^{(1)} + J_p^{(2)} + J_{dc} \quad (6)$$

The first variation of this functional should be made zero to get the control equations for the system. Since the cost functional contains the bra and kets of the wave and costate functions together with the external field amplitude function, the coefficients of their first variations should be individually set equal to zero, the resulting equations are sufficient to determine all unknowns. By skipping the intermediate steps, the equations for the bras and kets of the wave and costate functions and also the external field amplitude are given below

$$-i\hbar \frac{\partial}{\partial t} \langle \psi(t) | = \langle \psi(t) | [H_{is} - \mu E(t)], \quad \langle \psi(0) | = \langle in | \quad (7)$$

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = [H_{is} - \mu E(t)] |\psi(t)\rangle, \quad |\psi(0)\rangle = |in\rangle \quad (8)$$

$$-i\hbar \frac{\partial}{\partial t} \langle \lambda(t) | = \langle \lambda(t) | [H_{is} - \mu E(t)] - W_p(t) \langle \psi(t) | \widehat{O}' | \psi(t) \rangle \langle \psi(t) | \widehat{O}' \\ \langle \lambda(T) | = i \frac{\eta}{\hbar} \langle \psi(T) | \widehat{O} \quad (9)$$

$$i\hbar \frac{\partial}{\partial t} |\lambda(t)\rangle = [H_{is} - \mu E(t)] |\lambda(t)\rangle - W_p(t) \langle \psi(t) | \widehat{O}' | \psi(t) \rangle \widehat{O}' |\lambda(t)\rangle, \\ |\lambda(T)\rangle = -i \frac{\eta}{\hbar} \widehat{O} |\psi(T)\rangle \quad (10)$$

$$E(t) = \frac{2}{W_E(t)} \Re e (\langle \lambda(t) | \mu | \psi(t) \rangle) \quad (11)$$

where  $\Re e$ ,  $\langle in|$  and  $|in\rangle$  stand for the real part and the given initial forms of the wave function's bra and ket respectively, and the *deviation parameter*  $\eta$  is explicitly defined below (*deviation equation*).

$$\eta \equiv \langle \psi(T) | \widehat{O} | \psi(T) \rangle - \bar{O} \quad (12)$$

As can be noticed immediately the wave function defines the system's forward evolution starting from the beginning instant of the control ( $t = 0$ ) whereas the costate function describes the backward evolution of the system from the final instant of the control ( $t = T$ ). The *field equation* (11), which determines the external field amplitude connects these two evolutions through transition matrix element between the state and costate over the dipole function and makes the problem under consideration a *boundary value problem* in time.

This work is focused on the application of these equations to a multiharmonic oscillator system and finding the possible solutions to external field amplitude  $E(t)$  and the deviation parameter  $\eta$ . We will use the expectation values of certain operators as auxiliary tools and we will not attempt to evaluate the wave and costate functions.

We have chosen multiharmonic oscillator system because of its mathematical simplicity. This does not decrease the value of the application here since many vibrational states are successfully described by elastic forces at least for low lying energy states. In the sense of actual problems in quantum chemistry elastic forces can be used to characterize the interactions between the atoms of a molecular system as the zeroth order of perturbation expansion with respect to anharmonicity.

On the other hand, this multiharmonic oscillators system may present quite strong nonlinearities depending on the structures of the control operators and the dipole function. This fact can drop more light on the mathematical structure of the quantum optimal control theory.

Paper is organized as follows. The second section involves the specifications to get the equations for a multiharmonic oscillator system. Third section covers the determination of the external field amplitude and the deviation parameter. Fourth section includes the solution of the boundary value problem obtained in the third section for constant weight functions. It also covers the construction of the accompanying conditions. Fifth section contains the concluding remarks to finalize the paper. MuPAD programs and procedures used in the implementations are given in "Appendix".

## 2 Specifications for a multiharmonic oscillator system

If we consider a multiharmonic oscillator system which is composed of  $N$  particles mutually interacting through isotropic elastic forces then we can write

$$H_{is} \equiv - \sum_{i=1}^N \frac{\hbar^2}{2m_i} \left( \frac{\partial^2}{\partial x_{3i-2}^2} + \frac{\partial^2}{\partial x_{3i-1}^2} + \frac{\partial^2}{\partial x_{3i}^2} \right) + \sum_{i=1}^{N-1} \sum_{j=i}^N \frac{k_{ij}}{2} \left[ (x_{3i-2} - x_{3j-2})^2 + (x_{3i-1} - x_{3j-1})^2 + (x_{3i} - x_{3j})^2 \right] \quad (13)$$

where  $m_i$  stands for the mass of the  $i$ th particle while  $k_{ij}$  denotes the elastic force constant between the  $i$ th and  $j$ th particles. This form of the isolated Hamiltonian contains a potential function which is a quadratic form over  $3N$  coordinates. We can rewrite the Eq. 13 in the following compact form

$$H_{is} = -\frac{\hbar^2}{2m_e} \nabla^T \mathbf{D} \nabla + \mathbf{x}^T \mathbf{K} \mathbf{x} \quad (14)$$

where  $m_e$  denotes an appropriately chosen effective mass parameter and  $\mathbf{D}$  is a  $(3N \times 3N)$  type diagonal matrix whose  $(3i - 2)$ th,  $(3i - 1)$ th, and  $3i$ th elements are all  $m_e/m_i$ ,  $(1 \leq i \leq N)$ , and the explicit form of  $\mathbf{K}$  is given below

$$\mathbf{K} \equiv \left[ \sum_{i=1}^{N-1} \sum_{j=i}^N \frac{k_{ij}}{2} (\mathbf{e}_i - \mathbf{e}_j) (\mathbf{e}_i - \mathbf{e}_j)^T \right] \otimes \mathbf{I}_3 \quad (15)$$

where  $\mathbf{e}_i$  stands for the  $N$  element cartesian unit vector whose elements are all zero except the  $i$ th one which is 1  $(1 \leq i \leq N)$  and the symbol  $\otimes$  denotes the direct product of two matrices such that each element of the left operand is multiplied by the right operand.

Since the matrix  $\mathbf{D}$  is positive definite the theory of matrices [6] dictates us that a coordinate transform can be constructed to diagonalize the matrices  $\mathbf{D}$  and  $\mathbf{K}$  at the same time. To do this we can transform the coordinates as follows

$$\mathbf{x} \equiv \mathbf{Q} \mathbf{y} \quad (16)$$

where the  $(N \times N)$  matrix  $\mathbf{Q}$  will be determined to satisfy the following conditions

$$\mathbf{Q}^{-1} \mathbf{D} \left[ \mathbf{Q}^{-1} \right]^T = \mathbf{I}_{3N} \quad (17)$$

$$\mathbf{Q}^T \mathbf{K} \mathbf{Q} = \kappa \quad (18)$$

In this formula the matrix  $\mathbf{I}_{3N}$  denotes the identity matrix of  $(3N) \times (3N)$  type and  $\kappa$  represents a diagonal matrix whose three diagonal bottommost elements vanish. The flexible parameter  $m_e$  will be chosen to satisfy the equation

$$\det \mathbf{Q} = 1 \quad (19)$$

This is because of the fact that this transformation scales the volume element of the  $3N$ -tuple integration appearing in the expectation values, and hence, affects the normalized nature of the wave function. For the moment we are not going to concern with the explicit structure of  $\mathbf{Q}$  because we do not really need it in the rest of the paper. Its explicit structure is needed only when we need the actual values of the elements of  $\kappa$ .

As a careful investigation shows that

$$\mathbf{Q} = \mathbf{D}^{\frac{1}{2}} \mathbf{R} \tag{20}$$

where  $\mathbf{R}$  is a  $(3N) \times (3N)$  type orthonormal matrix diagonalizing the matrix  $\mathbf{D}^{\frac{1}{2}} \mathbf{K} \mathbf{D}^{\frac{1}{2}}$  and corresponding to a hyperrotation in  $(3N)$ -dimensional Euclid space of the position variables. Its columns are assumed to be organised such that its determinant becomes 1 ( $-1$  is the other possibility).

Equation (20) together with (19) allows us to get the following value for  $m_e$

$$m_e \equiv \left( \prod_{i=1}^N m_i \right)^{\frac{1}{N}} \tag{21}$$

We are now ready to express the system’s isolated Hamiltonian in  $y$  coordinates. We can write

$$H_{is} = -\frac{\hbar^2}{2m_e} \sum_{i=1}^{3N} \frac{\partial^2}{\partial y_i^2} + \sum_{i=1}^{3N} \kappa_i y_i^2 \tag{22}$$

where  $\kappa_i$  stands for the  $i$ th diagonal element of  $\kappa$  whose explicit definition is given below

$$\kappa \equiv \mathbf{R}^T \mathbf{D}^{\frac{1}{2}} \mathbf{K} \mathbf{D}^{\frac{1}{2}} \mathbf{R} \tag{23}$$

As can be noticed without difficulty  $\kappa_{3N-2} = \kappa_{3N-1} = \kappa_{3N} = 0$ . We do not explicitly show these vanishing values in (22) for convenience. As a matter of fact  $\kappa_i$ s appear as an  $N$ -triple because of the direct product structure in the related matrix. This feature may help us for certain simplifications later.

The specification of the system’s Hamiltonian has been completed now. The next items to be specified are dipole function, objective and penalty operators, respectively. We take the dipole function linear in position whereas the objective and penalty operators will be linear in both position and momentum. That is, they can be expressed in certain linear forms of the position (and momentum) operators. Since the above transformations are linear the bilinear form structure of these entities will be conserved under these transformations. Therefore, we can write

$$\mu \equiv \sum_{i=1}^{3N} \mu_i y_i \tag{24}$$

$$\widehat{O} \equiv \sum_{i=1}^{3N} \left[ \alpha_i y_i + \beta_i \left( -i\hbar \frac{\partial}{\partial y_i} \right) \right] \tag{25}$$

$$\widehat{O}' \equiv \sum_{i=1}^{3N} \left[ \alpha'_i y_i + \beta'_i \left( -i\hbar \frac{\partial}{\partial y_i} \right) \right] \tag{26}$$

where  $\mu_i, \alpha_i, \alpha'_i, \beta_i, \beta'_i, (1 \leq i \leq 3N)$ , represent given scalars.

These complete the specifications for an isotropic multiharmonic oscillator system. We do not specify the weight functions for the moment not to lose the chance of observing their roles in the evaluational complexities of the solution to the quantum optimal control problem under consideration.

### 3 Determination of the external field amplitude and deviation parameter for a multiharmonic oscillator system

The field equation can be explicitly written as follows after the above specifications

$$W_E(t)E(t) = \sum_{i=1}^{3N} \mu_i s_i(t), \quad 1 \leq i \leq 3N \quad (27)$$

where

$$s_i(t) \equiv 2\Re e (\langle \lambda(t) | y_i | \psi(t) \rangle), \quad 1 \leq i \leq 3N \quad (28)$$

We can now construct the following equation by simple differentiation and then using the Eqs. 7 and 8

$$\begin{aligned} \frac{d}{dt} [\langle \lambda(t) | y_i | \psi(t) \rangle] &= \langle \lambda(t) | \{H_{is} - \mu E(t), y_i\} | \psi(t) \rangle \\ &\quad - \frac{i}{\hbar} W_p(t) \langle \psi(t) | \widehat{O}' | \psi(t) \rangle \langle \psi(t) | \widehat{O}' y_i | \psi(t) \rangle, \quad 1 \leq i \leq 3N \end{aligned} \quad (29)$$

This equation can be put into the following form after taking real part of its both sides

$$\begin{aligned} \dot{s}_i(t) &= -2\Re e \langle \lambda(t) | \{H_{is} - \mu E(t), y_i\} | \psi(t) \rangle \\ &\quad + W_p(t) \langle \psi(t) | \widehat{O}' | \psi(t) \rangle \langle \psi(t) | \{\widehat{O}', y_i\} | \psi(t) \rangle, \\ \{\widehat{O}', y_i\} &\equiv -\frac{i}{\hbar} (\widehat{O}' y_i - y_i \widehat{O}'), \quad 1 \leq i \leq 3N \end{aligned} \quad (30)$$

where dot represents the temporal differentiation and the Poisson's brackets whose definitions are given in the second part of the above equation can be explicitly evaluated by using (24)–(26). Results are given below

$$\{H_{is} - \mu E(t), y_i\} = -\frac{1}{m_e} \left( -i\hbar \frac{\partial}{\partial y_i} \right), \quad \{\widehat{O}', y_i\} = -\beta'_i \mathcal{I}, \quad 1 \leq i \leq 3N \quad (31)$$

which imply

$$\dot{s}_i(t) = \frac{1}{m_e} r_i(t) - \beta'_i W_p(t) \sum_{i=1}^N [\alpha'_i q_i(t) + \beta'_i p_i(t)], \quad 1 \leq i \leq 3N \quad (32)$$

where in (31)  $\mathcal{I}$  stands for the unit operator and the new unknowns  $q_i(t)$ ,  $p_i(t)$ , and  $r_i(t)$  are explicitly defined below

$$q_i(t) \equiv \langle \psi(t) | y_i | \psi(t) \rangle, \quad 1 \leq i \leq 3N \quad (33)$$

$$p_i(t) \equiv \left\langle \psi(t) \left| -i\hbar \frac{\partial}{\partial y_i} \right| \psi(t) \right\rangle, \quad 1 \leq i \leq 3N \quad (34)$$

$$r_i(t) \equiv 2\Re e \left( \left\langle \lambda(t) \left| -i\hbar \frac{\partial}{\partial y_i} \right| \psi(t) \right\rangle \right), \quad 1 \leq i \leq 3N \quad (35)$$

The first order ordinary differential equation in (32) requires a condition to get unique solution. Since  $t$  varies between 0 and  $T$  inclusive either  $t = 0$  or  $t = T$  can be considered as the instant to specify a value for  $s_i(t)$ . We can show that most convenient instant is  $t = T$ , that is,  $s_i(T)$  value should be given. However, as a careful investigation shows that

$$s_i(T) \equiv -\eta \langle \psi(T) | \{ \widehat{O}, y_i \} | \psi(T) \rangle = \beta_i \eta, \quad 1 \leq i \leq 3N \quad (36)$$

Now we require an ordinary differential equation and accompanying boundary condition for  $r_i(t)$ . To get that condition we can follow the steps mentioned above and obtain the below equation

$$\begin{aligned} \dot{r}_i(t) = & -\Re e \left( \left\langle \lambda(t) \left| \left\{ H_{is} - \mu E(t), -i\hbar \frac{\partial}{\partial y_i} \right\} \right| \psi(t) \right\rangle \right) \\ & + W_p(t) \langle \psi(t) | \widehat{O}' | \psi(t) \rangle \left\langle \psi(t) \left| \left\{ \widehat{O}', -i\hbar \frac{\partial}{\partial y_i} \right\} \right| \psi(t) \right\rangle, \quad 1 \leq i \leq 3N \end{aligned} \quad (37)$$

where

$$\left\{ H_{is} - \mu E(t), -i\hbar \frac{\partial}{\partial y_i} \right\} = \kappa_i y_i - \mu_i E(t) \mathcal{I}, \quad \left\{ \widehat{O}', -i\hbar \frac{\partial}{\partial y_i} \right\} = \alpha'_i \mathcal{I}, \quad 1 \leq i \leq 3N \quad (38)$$

hence

$$\dot{r}_i(t) = -\kappa_i s_i(t) + \mu_i E(t) I(t) + \alpha'_i W_p(t) \sum_{j=1}^{3N} (\alpha'_j q_j(t) + \beta'_j p_j(t)), \quad 1 \leq i \leq 3N \quad (39)$$



where

$$I(t) \equiv \langle \lambda(t) | \mathcal{I} | \psi(t) \rangle, \quad 1 \leq i \leq 3N \quad (40)$$

and the accompanying condition should be given as  $r_i(T) = -\alpha_i \eta$ . A careful investigation shows that  $\dot{I}(t) = 0$ . Since  $I(T) = 0$  we conclude that  $I(t) \equiv 0$ . Therefore,

$$\dot{r}_i(t) = -\kappa_i s_i(t) + \alpha'_i W_p(t) \sum_{j=1}^{3N} \left( \alpha'_j q_j(t) + \beta'_j p_j(t) \right), \quad 1 \leq i \leq 3N \quad (41)$$

By skipping intermediate steps similar to the abovementioned ones we can show that the new unknown entities  $(q_i(t), p_i(t), 1 \leq i \leq 3N)$  satisfy the following equations

$$\dot{q}_i(t) = \frac{1}{m_e} p_i(t), \quad q_i(0) = \langle in | y_i | in \rangle \equiv q_i^{(in)}, \quad 1 \leq i \leq 3N \quad (42)$$

$$\dot{p}_i(t) = -\kappa_i q_i(t) + \frac{\mu_i}{W_E(t)} \sum_{j=1}^{3N} \mu_j s_j(t), \quad p_i(0) = \left\langle in \left| -i\hbar \frac{\partial}{\partial y_j} \right| in \right\rangle \equiv p_i^{(in)},$$

$$1 \leq i \leq 3N \quad (43)$$

If we define the  $(3N)$ -element vectors  $\mathbf{p}, \mathbf{q}, \mathbf{r}, \mathbf{s}, \boldsymbol{\mu}, \boldsymbol{\alpha}, \boldsymbol{\alpha}', \boldsymbol{\beta}, \boldsymbol{\beta}'$  such that their  $i$ th elements  $(1 \leq i \leq 3N)$  are  $p_i(t), q_i(t), r_i(t), s_i(t), \mu_i(t), \alpha_i, \alpha'_i, \beta_i, \beta'_i$ , respectively then we can put the Eqs. (32), (39), (42), and (43) into the following compact form

$$\dot{\mathbf{z}}(t) = \mathbf{A}(t)\mathbf{z}(t) \quad (44)$$

where

$$\mathbf{z}^T \equiv [\mathbf{p}(t), \mathbf{q}(t), \mathbf{r}(t), \mathbf{s}(t)] \quad (45)$$

$$\mathbf{A}(t) = \begin{bmatrix} \mathbf{B} & W_E(t)^{-1} \mathbf{u}_1 \mathbf{u}_2^T \\ -W_p(t) \mathbf{u}_3 \mathbf{u}_4^T & \mathbf{B} \end{bmatrix} \quad (46)$$

$$\mathbf{B} = \begin{bmatrix} \mathbf{0} & -\kappa \\ \frac{1}{m_e} \mathbf{I}_{3N} & \mathbf{0} \end{bmatrix}, \quad \mathbf{u}_1 = \begin{bmatrix} \boldsymbol{\mu} \\ \mathbf{0} \end{bmatrix}, \quad \mathbf{u}_2 = \begin{bmatrix} \mathbf{0} \\ \boldsymbol{\mu} \end{bmatrix}, \quad \mathbf{u}_3 = \begin{bmatrix} \boldsymbol{\alpha}' \\ -\boldsymbol{\beta}' \end{bmatrix}, \quad \mathbf{u}_4 = \begin{bmatrix} \boldsymbol{\beta}' \\ \boldsymbol{\alpha}' \end{bmatrix} \quad (47)$$

Equation (44) may have regular or/and irregular singular points in the interval  $[0, T]$  depending on the weight functions  $W_E(t)$  and  $W_p(t)$ . If these functions are assumed to be positive and continuous in a region including this interval in the complex plane of  $t$  then we can conjecture that all points of the interval are regular points of

the differential equation in (44). This means that the solution can be expanded into an infinite series of nonnegative powers of  $t$ . This urges us to write

$$\mathbf{z}(t) = \mathbf{Z}(t)\mathbf{c} \tag{48}$$

where  $\mathbf{c}$  is a constant vector undetermined yet and  $\mathbf{Z}(t)$ , which may be called *Evolution Operator* or *Propagator*, is analytic over the interval  $[ 0, T ]$  and satisfies

$$\dot{\mathbf{Z}}(t) = \mathbf{A}(t)\mathbf{Z}(t), \quad \mathbf{Z}(0) = \mathbf{I} \tag{49}$$

To determine  $\mathbf{c}$  we can use the boundary conditions. We can write first

$$\mathbf{Z}(t) \equiv \begin{bmatrix} \mathbf{Z}_{11}(t) & \mathbf{Z}_{12}(t) \\ \mathbf{Z}_{21}(t) & \mathbf{Z}_{22}(t) \end{bmatrix}, \quad \mathbf{c} \equiv \begin{bmatrix} \mathbf{c}_1 \\ \mathbf{c}_2 \end{bmatrix} \tag{50}$$

where  $\mathbf{c}_1$  and  $\mathbf{c}_2$  are  $(6N)$ -element vectors, and  $\mathbf{Z}_{11}(t), \mathbf{Z}_{12}(t), \mathbf{Z}_{21}(t), \mathbf{Z}_{22}(t)$  are  $(6N) \times (6N)$  blocks to satisfy

$$\mathbf{Z}_{ij}(0) = \delta_{ij}\mathbf{I}, \quad i, j = 1, 2 \tag{51}$$

Here,  $\delta_{ij}$  stands for the Kroenecker’s symbol. By taking  $t = 0$  in (48) we can obtain

$$\mathbf{c}_1^T = \left[ p_1^{(in)}, \dots, p_{3N}^{(in)}, q_1^{(in)}, \dots, q_{3N}^{(in)} \right] \equiv \mathbf{v}_1^T \tag{52}$$

which enables us to write the following equation after taking  $t = T$  in (48) and solving the second one of the resulting partitioned equations

$$\mathbf{c}_2 = \eta \mathbf{Z}_{22}(T)^{-1} \mathbf{v}_2 - \mathbf{Z}_{22}(T)^{-1} \mathbf{Z}_{21}(T) \mathbf{v}_1 \tag{53}$$

where

$$\mathbf{v}_2^T = [ -\alpha_1, \dots, -\alpha_{3N}, \beta_1, \dots, \beta_{3N} ] \tag{54}$$

Now we have everything explicitly in terms of known entities except the deviation parameter  $\eta$ . To evaluate  $\eta$  we rewrite (12) first as follows

$$\eta = \mathbf{v}_3^T \mathbf{z}_1(T) - \tilde{O} \tag{55}$$

where  $\mathbf{z}_1(t)$  is the block containing first  $6N$  elements of  $\mathbf{z}(t)$  and

$$\mathbf{v}_3^T \equiv [ \boldsymbol{\beta}^T, \boldsymbol{\alpha}^T ] \tag{56}$$

These equalities urges us to write (55) more explicitly as below

$$\begin{aligned} \eta = & \mathbf{v}_3^T \mathbf{Z}_{11}(T) \mathbf{v}_1 - \mathbf{v}_3^T \mathbf{Z}_{12}(T) \mathbf{Z}_{22}(T)^{-1} \mathbf{Z}_{21}(T) \mathbf{v}_1 \\ & + \left( \mathbf{v}_3^T \mathbf{Z}_{12}(T) \mathbf{Z}_{22}(T)^{-1} \mathbf{v}_2 \right) \eta - \tilde{O} \end{aligned} \quad (57)$$

which produces

$$\eta = \frac{\mathbf{v}_3^T \mathbf{Z}_{11}(T) \mathbf{v}_1 - \mathbf{v}_3^T \mathbf{Z}_{12}(T) \mathbf{Z}_{22}(T)^{-1} \mathbf{Z}_{21}(T) \mathbf{v}_1 - \tilde{O}}{1 - \mathbf{v}_3^T \mathbf{Z}_{12}(T) \mathbf{Z}_{22}(T)^{-1} \mathbf{v}_2} \quad (58)$$

Now Eq. (27) can be reexpressed as follows

$$E(t) = W_E(t)^{-1} \mathbf{u}_2^T z_2(t) = W_E(t)^{-1} \mathbf{u}_2^T [ \mathbf{Z}_{11}(t) \mathbf{c}_1 + \mathbf{Z}_{12}(t) \mathbf{c}_2 ] \quad (59)$$

where everything is known as  $\mathbf{c}_2$  vector can be explicitly obtained after plugging known value  $\eta$  into its expression. This completes the analytical determination of the external field amplitude and deviation parameter. Everything can be explicitly found as long as  $\mathbf{Z}(t)$  is evaluated. Its differential equation is accompanied by unit matrix initial value as we have seen above. However, this is the case only when the weight functions are positive. Otherwise certain singularities may arise and make it impossible to impose unit matrix initial condition because of the singularity of  $\mathbf{Z}(t)$  at  $t = 0$ . On the other hand,  $\mathbf{Z}_{22}(t)$  may not be invertible when the weight functions are not positive. We do not deal with these extraordinary circumstances here. We only focus on the cases where the weight functions are positive during the control.

Another important point to be mentioned is the constraints in the definition of the multiharmonic system. We assumed that the system is isotropic, that is, not depending on the direction in the three dimensional physical space. Of course, this can be relaxed, and then the direct-product with  $\mathbf{I}_3$  structure is lost. The other important constraint was the lack of interaction with the origin. We assumed that the whole system's particles are mutually interacting through linear forces. Then we selected one of the oscillators as the new origin of the system's coordinates. However, we could assume that entire system is fixed around the origin where another harmonic oscillator is located and not freely moving in space. If this could happen then one would be able to prove that all  $\kappa$  values would be positive. And furthermore, we would not be enforced to use the multiples of 3 as the degree of the freedom for the system. Hence, we may comfortably use a positive integer  $N$  as the dimension and a positive definite  $\kappa$  matrix to describe the multiharmonic oscillator. In the remaining part of the paper we are going to use this rather generalized form of the definition for the multiharmonic oscillator.

#### 4 Implementations for constant weight cases

Let us consider the case where the weight functions  $W_E(t)$  and  $W_p(t)$  are given constants and the number of the oscillators is denoted by  $N$ . We can rewrite (46) and the first one of the equations in (47) as follows

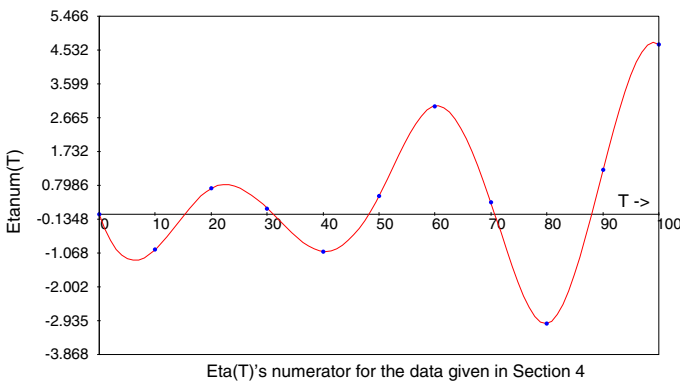
$$\mathbf{A} = \begin{bmatrix} \mathbf{B} & W_E^{-1} \mathbf{u}_1 \mathbf{u}_2^T \\ -W_p \mathbf{u}_3 \mathbf{u}_4^T & \mathbf{B} \end{bmatrix}, \quad \mathbf{B} = \begin{bmatrix} \mathbf{0} & -\kappa \\ \frac{1}{m_e} \mathbf{I}_N & \mathbf{0} \end{bmatrix} \tag{60}$$

where  $\kappa$  may be a nonnegative or positive definite diagonal matrix. If it is nonnegative then its zero eigenvalues correspond to freely moving particles. Otherwise entire system can be considered as if it is composed of oscillators interacting with the origin via elastic forces.

Evolution matrix of the system,  $\mathbf{Z}(t)$ , can be analytically evaluated as follows

$$\mathbf{Z}(t) = e^{t\mathbf{A}} \tag{61}$$

which enables us to evaluate all intermediate terms and finally external field amplitude and the deviation parameter. We are not going to give explicit structures since the inverse of  $\mathbf{Z}_{22}(t)$  can not be analytically found in simple form unless very specific structure is given for the system under consideration. Even if we have the analytical forms for the expressions they may not be convenient for actual computations. For this reason, instead of using explicit expressions, it is better to use symbolic and/or numeric interpreters for the calculations in computers. We prefer to use MuPAD which is an Open Computer Algebra System developed at Paderborn University in Germany. We give more details about MuPAD and its utilization in our implementations in Appendix. Now we consider Eq. (58) where the deviation parameter  $\eta(T)$  is given as a ratio of two  $T$  dependent expressions. If the numerator of that expressions vanishes at certain  $T$  values for which denominator remains nonzero then the deviation parameter becomes zero. That is, the expectation value of objective operator achieves its prescribed target value. This reveals the fact that there may be some specific interaction time values leading us to exact achievement cases. This situation is plotted in Fig. 1 by using the data given in the first MuPAD code of Appendix. If there is a signal of the fact that the numerator and the denominator have common factor(s) vanishing at some nonnegative  $T$  values then it is better to eliminate them to get better numerical stability. As can be noticed from Fig. 1, the numerator of  $\eta(T)$  vanishes at  $T$  values of 13.86772, 35.74048, 43.76518, 75.88353, 89.42919, respectively. These roots are



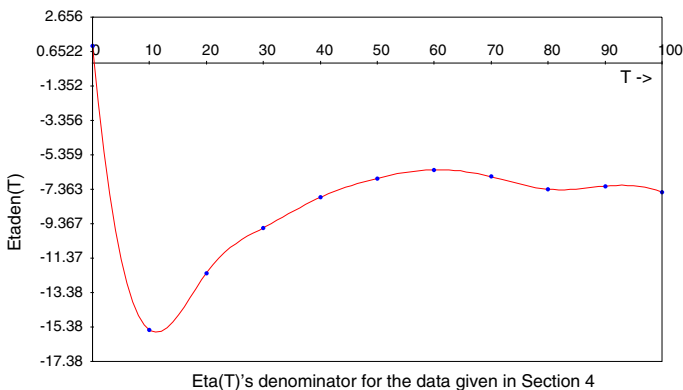
**Fig. 1** The variation of deviation parameter’s numerator with respect to control time

evaluated by MuPAD facilities and Regula–Falsi Method within seven decimal digit accuracy. The roots in Fig. 1 may seem to be a little bit shifted from these values. This comes from the utilization of cubic splines to create plot from a finite number of data. The roots are not evaluated from these splines. Instead, own structure of  $\eta(T)$ 's numerator is used in the Regula–Falsi method. We are not going to give the MuPAD code for finding roots although we did not use the MuPAD's root finding methods but construct a numerical algorithm based on Regula–Falsi Method. The  $T$  values annihilating the numerator of  $\eta(T)$  are appearing between 0 and 100.0 here. However, the number of these critical values are in fact infinite because of the sinusoidal and cosinusoidal dependence on  $T$ . This behavior comes from the pure imaginary eigenvalues of  $\mathbf{B}$  in this case.

If the denominator in (58) vanishes for certain  $T$  values which do not make numerator zero at the same time then the worst case is encountered. The deviation of the objective operator's expectation value from its target value becomes infinite. These types of  $T$  values should be avoided in control. The variation of  $\eta(T)$ 's denominator with  $T$  is given in Fig. 2. As seen from figure there is just a single root for denominator in  $T$ 's range between 0 and 100. Although there is oscillation in the denominator of  $\eta(T)$  with respect to  $T$  there seem not to be any tendency to vanish in other  $T$  values. This is because of the amplitude of the oscillation. It is not sufficiently large to intersect the horizontal axis. This smallness comes from the initial values. One can find some other set of initial values for which the denominator of  $\eta(T)$  vanishes infinitely many times.

The discussions above imply that  $\eta(T)$  may have finitely or infinitely many zeros and poles depending on  $\kappa$  and initial values. Because of the high number of control parameters in our case we do not give explicit conditions to or not to get poles or zeros here. A norm and spectral analysis may reveal criteria for this purpose. We keep this beyond the scope of the paper.

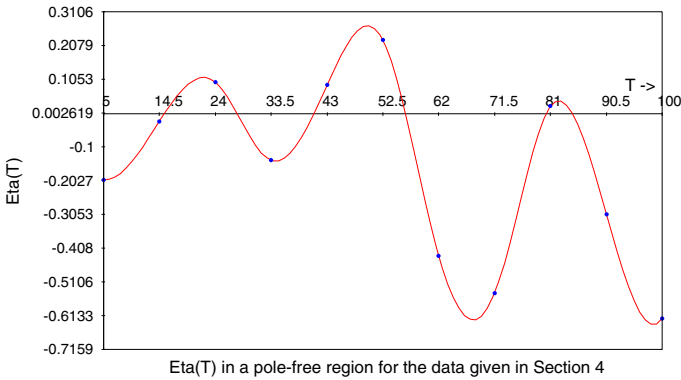
Deviation parameter can be evaluated as a function of control time by using MuPAD's symbolic capabilities. However, this is a time and memory consuming procedure. Although the stack size of MuPAD can be increased from its default, 250 KB,



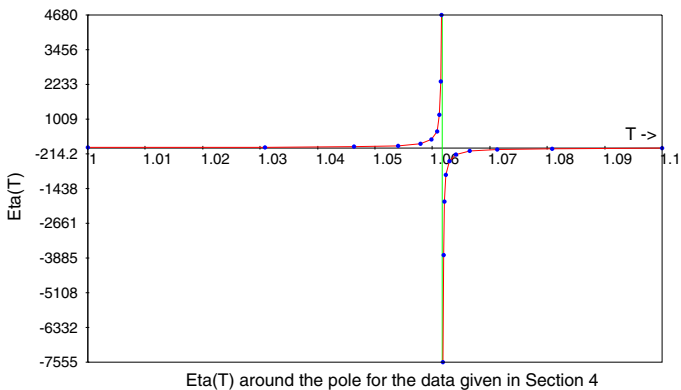
**Fig. 2** The variation of deviation parameter's denominator with respect to control time

we do not recommend to use symbolic evaluations unless a real need arises to see symbolical structures of the entities to be evaluated. Here we have used numerical facilities.  $\eta(T)$  is evaluated at certain finite number of  $T$  values and then the plots are created from this finite data by interpolation like using cubic splines. However, this procedure may hide the poles unless their locations are given as interpolation points and this latter case may cause a lot of problems because of the sudden change of the function in the vicinity of the pole. Hence, the variation of  $\eta$  around a pole is depicted separately. Figures 3 and 4 show the variation of  $\eta(T)$  in a pole free region and in the vicinity of the pole, respectively.

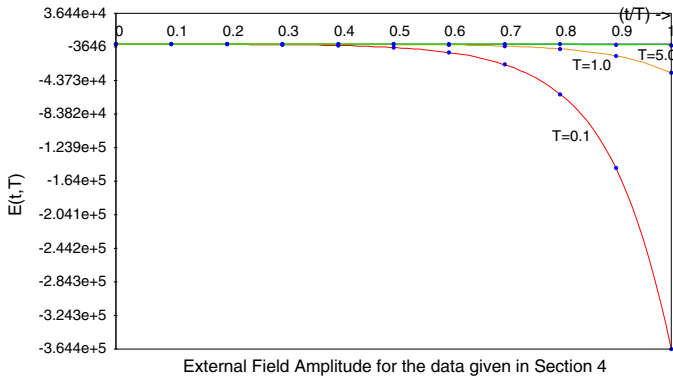
The external field amplitude,  $E(t, T)$  can be evaluated by using (59). Its variation with time,  $t$ , is given in Fig. 5 for three different values of  $T$ , 0.1, 1.0, and 5.0, respectively. As can be seen from the figure external field amplitude’s variation in time becomes flattened as the control time  $T$  increases. However, this does not reflect real situation because of the different scaling of three cases and the use of interpolation. In the calculations of  $E(t, T)$  we have scaled time  $t$  such that new  $t$  remains between



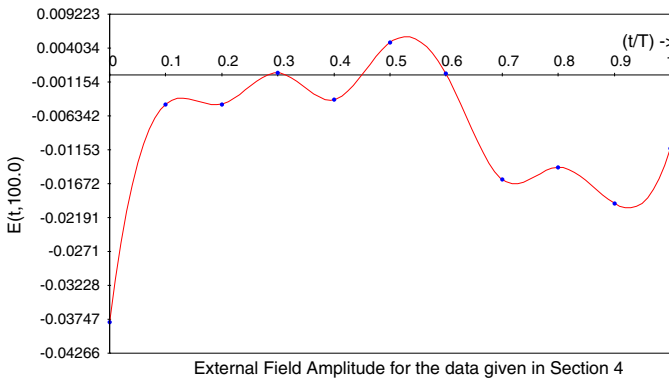
**Fig. 3** The variation of deviation parameter with respect to control time in an interval which does not contain any pole for  $\eta(T)$



**Fig. 4** The variation of deviation parameter with respect to control time in an interval which contains a pole for  $\eta(T)$



**Fig. 5** The variation of deviation parameter with respect to control time in an interval which contains a pole for  $\eta(T)$



**Fig. 6** The variation of deviation parameter with respect to control time in an interval which contains a pole for  $\eta(T)$

0 and 1 inclusive without depending on the value of  $T$ . This scaling results in a linear structure in  $\mathbf{A}$  when  $W_E$  and  $W_p$  are assumed to be proportional to  $T$  and  $\frac{1}{T}$ , respectively. This means that the frequency of the sinusoidal and cosinusoidal oscillations is proportional to  $T$  when  $T$  tends to infinity. This, however, implies that the oscillations of  $E(t, T)$  in  $t$  becomes more appearable as  $T$  increases. Figure 6 shows this fact.

The entities to evaluate the external field amplitude and the deviation parameter are defined by using MuPAD's procedure facility. They are gathered into a single file and may be called in an `xmupad` session by using `fread` command. It must be called after the initial value assignments mentioned above are done. The matrix  $\mathbf{A}$  appearing in the argument of exponential matrix depends on the interaction time,  $T$ , and given through the second code of Appendix.

After the definition of  $\mathbf{A}$  one can define the  $2N \times 2N$  type partitions of  $\mathbf{Z}(t, T)$  as one of the procedure definitions for these four matrices is given in Appendix.

The definitions of the numerator, denominator and itself of  $\eta(T)$  and finally external field amplitude can be done through the relevant MuPAD procedures in Appendix.

The creation of the figures are done by using the `plot` library of MuPAD. We do not give the codes written for this purpose anywhere in this paper.

## 5 Concluding remarks

In this work we have concerned with a quantum multiharmonic oscillator system's optimal control under linear dipole interaction and linear objective operator together with linear penalty operator. We have used expectation values of certain appropriately defined operators as unknowns instead of the wave and accompanying costate functions. We could have been able to construct ordinary differential equations for these expectation values. These equations are linear and can be put into matrix form where the coefficient matrix is time variant unless the weight functions are constants in time. We have shown that these equations are accompanied by certain boundary conditions whose first half are given at the beginning of the control while the remaining half should be given at the final instant of the control. In this sense, the equations describe a forward and a backward evolution which are related to each other via boundary conditions.

We could get analytical results in terms of the evolution matrix of the set of ordinary differential equations and certain constant vectors appearing in the definitions of dipole function, objective operator, and penalty operator. The results also depend on the duration of the control, that is, the parameter  $T$ .

The actual evaluation of the evolution matrix of the system may not be always possible depending on the time dependence of the weight functions. Hence the general results include somehow implicity. We may not write actually explicit results. This implicity continues to survive even if the weight functions are constants in time. Because, an exponential matrix arises in the structure of the evolution matrix. Although there are several methods to evaluate it, actual evaluation can not be analytic in general. It requires numerical methods to get the result unless some specific nature exists in the argument of the exponential matrix.

Here, we have solved the quantum optimal control problem of a multiharmonic oscillator system. Time dependent cases of the weight functions can not be solved analytically in terms of exponential matrices. However, a lot of numerical approximation methods can be developed to this end.

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## Appendix: MuPAD utilization in implementations

MuPAD has a public licence for all individuals and organisations dealing with education and scientific research. It can be used either in standalone terminals of Linux or under X. The commands corresponding to these mediums are respectively `mupad` and `xmupad`. It can be used in either interactive or batch mode. In batch mode, the commands to be interpreted are written into a file which called "script". If we assume that the name of that file is `prog1.mu` then the the unix redirectioning command



`mupad < prog1.mu` can be used. MuPAD takes the commands from the lines of the file `prog1.mu`, executes them sequentially, and sends the outputs to the standard output stream. Hence, the outputs are displayed on the screen by default. If one wants to store this output into a file whose name is, say, `prog1.out` then the unix redirection command `mupad < prog1.mu > prog1.out` can be used. Same kind of actions can be taken in `xmupad` without using redirectioning. When `xmupad` is invoked, a window for interactive utilization is created and the prompt `>` is displayed. As soon as a command is written and entered at this prompt, it is executed and the output is displayed on this window. The commands can be taken from a batch file whose name is, say, `prog1.xmu`, by using `fread("prog1.xmu")` command. All commands in `prog1.xmu` should be terminated by a delimiter either `:` or `;` and file must not have the session finishing command `quit`. The following lines are taken from an input file to assign values to system's parameters for the quantum optimal control of a nine harmonic oscillator system. Precision is set to environmental parameter `DIGITS` by the assignment operator `:=`. It is set to twenty decimal digit accuracy. The values of the same type entities except `kappas` are taken equal and the common value is denoted by a corresponding word terminating with `com`. The letters `a`, `b`, `ap`, and `bp` stands for  $\alpha$ ,  $\beta$ ,  $\alpha'$ , and  $\beta'$  parameters. The vectors are named with the words ending with `v`. The vector or matrix natures of corresponding entities are given by the `matrix(m,n,List,Type)` command whose first two arguments are for the dimension and the third argument is a single list or list of list to specify the elements while the last argument specifies the type of entity if it has a special nature like diagonality. `linalg::` prefix means that the following command is taken from the linear algebra library. The command `substitute` embeds the vector or matrix given in its second argument into the matrix given in its first argument at location specified in its last two arguments.

```

DIGITS:=20: me:=1: Otilde:=0: WE:=1.0: WP:=1.0:
pcom:=1.0: qcom:=0.0: acom:=1.0: bcom:=0.0: apcom:=0.0:
    bpcom:=1.0:
Kappa:=matrix(9,9,[1.0,0.9,0.8,0.7,0.6,0.5,0.4,0.3,0.2,
    0.1],Diagonal):
Unit9mat:=matrix(9,9,[1,1,1,1,1,1,1,1,1],Diagonal):
muv:=matrix(9,1,[1,1,1,1,1,1,1,1,1]):
pinv:=pcom*matrix(9,1,[1,1,1,1,1,1,1,1,1]):
qinv:=qcom*matrix(9,1,[1,1,1,1,1,1,1,1,1]):
alphav:=acom*matrix(9,1,[1,1,1,1,1,1,1,1,1]):
betav:=bcom*matrix(9,1,[1,1,1,1,1,1,1,1,1]):
alphapriv:=apcom*matrix(9,1,[1,1,1,1,1,1,1,1,1]):
betapriv:=bpcom*matrix(9,1,[1,1,1,1,1,1,1,1,1]):
v1v:=matrix(18,1): v1v:=linalg::substitute(v1v,pinv,1,1):
v1v:=linalg::substitute(v1v,qinv,10,1): v2v:=matrix(18,1):
v2v:=linalg::substitute(v2v,-alphav,1,1):
v2v:=linalg::substitute(v2v,betav,10,1):
v3v:=matrix(18,1): v3v:=linalg::substitute(v3v,betav,
    1,1):

```

```

v3v:=linalg::substitute(v3v, alphav, 10, 1) :
u1v:=matrix(18, 1) : u1v:=linalg::substitute(u1v, muv, 1, 1) :
u2v:=matrix(18, 1) : u2v:=linalg::substitute(u2v, muv, 10, 1) :
u3v:=matrix(18, 1) : u3v:=linalg::substitute(u3v, alphapr,
    1, 1) :
u3v:=linalg::substitute(u3v, -betapr, 10, 1) :
u4v:=matrix(18, 1) : u4v:=linalg::substitute(u4v, betapr,
    1, 1) :
u4v:=linalg::substitute(u4v, alphapr, 10, 1) :

```

The following MuPAD code is written as a procedure to create the **A** matrix for three harmonic oscillators system mentioned above.

```

A:=proc(T)
    begin
        temp:=matrix(36, 36) :
        temp1:=(1/WE)*u1v*linalg::transpose(u2v) :
        temp2:=WP*u3v*linalg::transpose(u4v) :
        temp:=linalg::substitute(temp, temp1, 1, 19) :
        temp:=linalg::substitute(temp, -temp2, 19, 1) :
        temp:=linalg::substitute(temp, -T*Kappa, 1, 10) :
        temp:=linalg::substitute(temp, -T*Kappa, 19, 28) :
        temp:=linalg::substitute(temp, (T/me)*Unit9mat,
            10, 1) :
        temp:=linalg::substitute(temp, (T/me)*Unit9mat,
            28, 19) :
        float(temp) :
    end_proc :

```

The uppermost and leftmost block element of the evolution matrix is evaluated via the following simple MuPAD procedure.

```

Z11:=proc(t, T) begin (numeric::expMatrix(t*A(T)))
    [1..18, 1..18] : end_proc :

```

where `numeric::` means that the numeric library of MuPAD will be used. The function `expMatrix` evaluates an exponential matrix. Computations are done at purely numerical level. Symbolical calculations may take quite long times as we emphasized before.

The following procedures are also used in the numerical implementations of this paper.

```

numer1:=proc(T) begin (linalg::transpose(v3v)*Z11(1, T)*
    v1v)[1, 1] : end_proc :
numer2:=proc(T) begin (linalg::transpose(v3v)*Z12(1, T)*
    numeric::inverse(Z22(1, T))*Z21(1, T)*v1v)[1, 1] :
    end_proc :
etanum:=proc(T) begin numer1(T)-numer2(T) : end_proc :

```

```

etadenom:=proc(T) begin 1-(linalg::transpose(v3v)*
    Z12(1,T)*numeric::inverse(Z22(1,T))*v2v)[1,1]:
end_proc:
eta:=proc(T)
    begin
        (etanum(T)-Otilde)/etadenom(T):
    end_proc:
extfield:=proc(t,T)
    begin
        temp1:=(linalg::transpose(u2v)*Z21(t,T)*
            v1v)/(T*WE):
        temp2:=(linalg::transpose(u2v)*Z22(t,T)*
            numeric::inverse(Z22(1,T))*v2v)/
            (T*WE):
        temp3:=(linalg::transpose(u2v)*Z22(t,T)*
            numeric::inverse(Z22(1,T))*
            Z21(1,T)*v1v)/(T*WE):
        temp:=temp1[1,1]+eta(T)*temp2[1,1]-temp3
            [1,1]:
    end_proc:

```

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