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Optimal control of classical molecular dynamics: A perturbation formulation and the existence of multiple solutions

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This paper considers the prospect for there being multiple solutions to the control of classically modelled molecular dynamical systems. The research presented here follows up on a parallel study based on quantum mechanics. For polyatomic molecules it is generally expected that a classical mechanical model will be adequate and necessary as a means for designing optical fields for molecular control. The prospect for multiple control field solutions existing in this domain is important to establish in terms of ultimate laboratory realization of molecular control. A general formulation of the multiplicity problem is considered and the existence of a denumerably infinite number of solutions for the control field amplitude is shown to be the case under certain mild limitations on the physical variables.

1. Introduction

In recent years there has been considerable activity in designing, and attempts to implement, optical fields for manipulating molecular motion. Interest in this area arises for fundamental reasons as well as possible practical applications. One of the most promising general approaches to the design of optical fields is based on the introduction of optimal control techniques [1–5] at the molecular scale [6–11]. These techniques provide a rigorous foundation for designing optical fields in an environment where desired physical objectives, such as bond breaking, will inevitably be pitted against other competitive product channels and the desire to achieve the goals at the performance of minimal optical work. The design problem is posed by presenting an optimizing cost functional which contains the objectives and penalties as well as the natural constraint that the physical equations of motion must be satisfied [12–23]. The cost functional depends on the unknown desired optical field, and equations for the latter quantity are obtained by minimizing the cost

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functional. Except for the weak field linear regime, this molecular field design process is inherently nonlinear and the prospect exists for possibly finding multiple solutions (i.e., optical fields) with each satisfactorily meeting the desired objectives.

The latter prospect was recently explored within the domain of a quantum mechanical description of molecular systems [24,25]. The curious fact that the optimizing equations are two-point boundary value problems in *time* suggests that a type of underlying eigen problem may be present. This situation was confirmed and it was proved that a denumerably infinite multiplicity of solutions exist according to the eigenstructure of the control equations [24,25].

Although molecular dynamics is properly described by quantum mechanics, much successful modelling for many molecular purposes is done with classical mechanics. Classical mechanics often gives quite reliable results and secondly it is the only viable means for treating polyatomic molecules with more than even a few atoms. Thus, for these reasons, classical mechanics has already been introduced into the molecular control domain for designing and manipulating optical fields [26–28]. Just as with quantum mechanics a very fundamental issue is whether multiple solutions exist to the classically modelled control equations. The cursory similarity between the classically and quantum mechanically modelled control problems suggest that multiple solutions might once again exist but this matter needs to be established on rigorous grounds. The latter objective is the purpose of the present paper and indeed it will be shown that a denumerably infinite number of multiple control solutions can exist to the classical control equations in the presence of rather mild assumptions on the variables of interest. Although this conclusion is essentially the same as found for quantum mechanical control, some essential differences arise. In particular, the mathematical formulations within classical and quantum mechanics are distinct and some subtleties concerning the existence of the multiple solutions also differ. The conclusion of this paper has practical and computational consequences for future classically modelled control design efforts.

Section 2 of the paper will briefly summarize the optimal control formulation by defining the cost functional and obtaining the resultant variational equations. Section 3 deals with the linearization of the variational equations in the weak field regime. Section 4 includes the proof of the existence of the multiple solutions in the linearized case while section 5 considers the effect of the nonlinear terms on the multiplicity of the solutions. Concluding remarks finalize the paper in section 6.

2. The variational design equations

Consider a molecular system whose classical free motion is completely described through its time-independent Hamiltonian $H_0(\mathbf{p}, \mathbf{q})$ and its initial state characterized by the momenta, $\tilde{\mathbf{p}}$, and coordinates $\tilde{\mathbf{q}}$. Although the explicit struc-

ture of $H_0(\mathbf{p}, \mathbf{q})$ is not necessary to formulate the equations of optimally controlled molecular motion, an analysis of the solutions may be facilitated by certain simplifying structure. In particular we shall assume that cartesian coordinates are used allowing the kinetic energy term to be expressed as a quadratic form in the momenta, $\mathbf{p}$, with an inverse mass matrix, $\mathbf{P}$, whose elements are constants. The use of other well-known coordinate systems like curvilinear coordinates, or unusual non-orthogonal frames may cause the appearance of spatial coordinate dependence in the inverse mass matrix. The potential term, $V(\mathbf{q})$, is purely a function of spatial coordinates, $\mathbf{q}$. Therefore, the time-independent Hamiltonian of free molecular motion can be expressed as follows:

$$H_0(\mathbf{p}, \mathbf{q}) = \tfrac{1}{2}\mathbf{p}^{\mathrm{T}}\mathbf{P}\mathbf{p} + V(\mathbf{q}), \tag{2.1}$$

where the number of degrees of freedom for the system is assumed to be N. Thus, $\mathbf{p}, \mathbf{q}$ are vectors of length N and $\mathbf{P}$ is a $(N \times N)$-matrix with constant components. The potential function, $V(\mathbf{q})$ is assumed to be continuous and bounded everywhere except possibly at a finite number of points in configuration space without a serious loss of generality.

If we apply an electric field, whose scalar amplitude is denoted by $\mathcal{E}(t)$, to the molecule, then its evolution will deviate from its classical free molecular motion. The path of the motion can be manipulated by changing the field's frequency or temporal structure. In this way, it may be possible to break certain bonds in the molecular or otherwise control its dynamical evolution. We can write the Hamiltonian of the molecule in the presence of the field as follows:

$$H(\mathbf{p}, \mathbf{q}, t) = H_0(\mathbf{p}, \mathbf{q}) + \mu(\mathbf{q})\mathcal{E}(t), \tag{2.2}$$

where $\mu(\mathbf{q})$ stands for the time-independent dipole function of the molecule and the field amplitude varies only with time. The vector nature of the dipole and field is implicitly understood. We could equivalently consider a purely magnetic or electromagnetic field, with the only change being in the structure of the field–molecule interaction. The formulation in eqs. (2.1) and (2.2) encompasses electronic, vibrational or rotational degrees of freedom, and appropriate terms for nonlinear field effects could also be added [29]. However, our attention will be focused here on vibrational and rotational motion which often can be adequately described by classical dynamics.

Standard methods of classical dynamics can be used, in principle, to determine the trajectories, $\mathbf{p}(t), \mathbf{q}(t)$ of the molecular system described via $H(\mathbf{p}(t), \mathbf{q}(t), t), \tilde{\mathbf{p}}, \tilde{\mathbf{q}}$, as long as $\mathcal{E}(t)$ is given. However, the character of the problem abruptly changes when we want to *design* a field such that the molecular motion follows a new route or achieves a final state which is as close as possible to one we desire. The process for designing an appropriate field can be realized through optimal control theory [1–6]. Optimal control theory is implemented by the selection of an appropriate cost functional and the derivation of the corresponding Euler equations. Here, we

will draw a parallel to the optimally controlled quantum dynamical case in our previous work [24,25].

We now assume that the field-molecule interaction exists over the time interval $0<t\leqslant T$, and consider an observable which is characterized by $\hat{O}(\mathbf{p}(T),\mathbf{q}(T))$, as a function of momentum and space coordinates at the target time T. If we desire that $\hat{O}(\mathbf{p}(T),\mathbf{q}(T))$ becomes as close as possible to a given target value represented by $\tilde{O}$, then the following objective term can be chosen as a part of the cost functional

$$\mathcal{J}_0 = \tfrac{1}{2}(O(\mathbf{q}(T),\mathbf{p}(T)) - \tilde{O})^2 . \tag{2.3}$$

The next step is the definition of the penalty terms. For this purpose, we consider only two different penalty terms in this work, one of which, is aimed to suppressing an undesired observable function denoted by $O'(\mathbf{q}(t),\mathbf{p}(t))$ during the field-molecule interaction via an appropriately chosen weight function denoted by $W_p(t)$. This penalty term can be expressed as

$$\mathcal{J}_p^{(1)} = \tfrac{1}{2}\int_0^T \mathrm{d}t\; W_p(t)O'(\mathbf{q}(t),\mathbf{p}(t))^2 , \quad W_p(t)>0, \quad t\in[0,T] . \tag{2.4}$$

The second penalty term allows for the possibility of minimizing the field fluence. This term also includes an appropriate weight function denoted by $W_{\mathcal{E}}(t)$ and is given as follows:

$$\mathcal{J}_p^{(2)} = \tfrac{1}{2}\int_0^T \mathrm{d}t\; W_{\mathcal{E}}(t)\mathcal{E}(t)^2, \quad W_{\mathcal{E}}(t)>0 , \quad t\in[0,T] . \tag{2.5}$$

Until now, the momentum and space coordinates have directly or indirectly entered the cost terms. These variables must satisfy the fundamental equations of classical dynamics. The Hamiltonian equations may be introduced explicitly into the cost functional through a constraint term, via temporally varying costate Lagrange multipliers, $\lambda_j^{(q)}(t)$, $\lambda_j^{(p)}(t)$, $1\leqslant j\leqslant N$. Therefore, we can write the following constraint term:

$$\mathcal{J}_{c,d} = \int_0^T \mathrm{d}t \sum_{j=1}^{N} \lambda_j^{(q)}(t)\left[\dot{q}_j - \frac{\partial H}{\partial p_j}\right] + \int_0^T \mathrm{d}t \sum_{j=1}^{N} \lambda_j^{(p)}(t)\left[\dot{p}_j + \frac{\partial H}{\partial q_j}\right] . \tag{2.6}$$

Now, we are at a point where the total cost functional can be written as a sum of these individual terms,

$$\mathcal{J} = \mathcal{J}_0 + \mathcal{J}_p^{(1)} + \mathcal{J}_p^{(2)} + \mathcal{J}_{c,d} . \tag{2.7}$$

Although the first three terms were given explicit forms above, in practice, there is additional flexibility to build in a variety of other physical cost terms. The dynamical equations of the optimally controlled system are obtained by the stationary variational condition of $\mathcal{J}$

$$\delta\mathcal{J} = 0 . \tag{2.8}$$

The independent variation of $\lambda_j(t), p_j(t), q_j(t), 1 \leqslant j \leqslant N$, and the field amplitude $\mathcal{E}$, leads to the following set of equations:

$$\dot{q}_j = \sum_{k=1}^{N} P_{jk} p_k(t), \quad q_j(0) = \tilde{q}_j, \quad 1 \leqslant j \leqslant N, \tag{2.9a, b}$$

$$\dot{p}_j(t) = -\frac{\partial V(\mathbf{q}(t))}{\partial q_j(t)} - \mathcal{E}(t) \frac{\partial \mu(\mathbf{q}(t))}{\partial q_j(t)}, \quad p_j(0) = \tilde{p}_j, \quad 1 \leqslant j \leqslant N, \tag{2.10a, b}$$

$$\begin{aligned} \dot{\lambda}_j^{(q)}(t) = & W_p(t) O'(\mathbf{q}(t), \mathbf{p}(t)) \frac{\partial O'(\mathbf{q}(t), \mathbf{p}(t))}{\partial q_j(t)} + \sum_{k=1}^{N} \frac{\partial^2 V(\mathbf{q}(t))}{\partial q_j(t) \partial q_k(t)} \lambda_k^{(p)}(t) \\ & + \mathcal{E}(t) \sum_{k=1}^{N} \frac{\partial^2 \mu(\mathbf{q}(t))}{\partial q_j(t) \partial q_k(t)} \lambda_k^{(p)}(t), \quad 1 \leqslant j \leqslant N, \end{aligned} \tag{2.11a}$$

$$\lambda_j^{(q)}(T) = -\eta \frac{\partial O(\mathbf{q}(T), \mathbf{p}(T))}{\partial q_j(T)}, \quad 1 \leqslant j \leqslant N, \tag{2.11b}$$

$$\dot{\lambda}_j^{(p)}(t) = W_p(t) O'(\mathbf{q}(t), \mathbf{p}(t)) \frac{\partial O'(\mathbf{q}(t), \mathbf{p}(t))}{\partial p_j(t)} - \sum_{k=1}^{N} P_{jk} \lambda_k^{(q)}(t), \quad 1 \leqslant j \leqslant N, \tag{2.12a}$$

$$\lambda_j^{(p)}(T) = -\eta \frac{\partial O(\mathbf{q}(T), \mathbf{p}(T))}{\partial p_j(T)}, \quad 1 \leqslant j \leqslant N, \tag{2.12b}$$

$$\mathcal{E}(t) = -\frac{1}{W_{\mathcal{E}}(t)} \sum_{k=1}^{N} \lambda_k^{(p)}(t) \frac{\partial \mu(\mathbf{q}(t))}{\partial q_k(t)}, \tag{2.13}$$

$$O(\mathbf{q}(T), \mathbf{p}(T)) = \tilde{O} + \eta, \tag{2.14}$$

where the constant variable η is defined by eq. (2.14) and is introduced to facilitate the further analysis.

When the control problem is well posed we can demand the exact achievement of the goal $O(\mathbf{q}(T), \mathbf{p}(T)) = \tilde{O}$ at $t = T$. In this case we replace the objective cost term given by eq. (2.3) with the following objective constraint term:

$$\mathcal{J}_{c,o} = \eta \big(O(\mathbf{q}(T), \mathbf{p}(T)) - \tilde{O} \big), \tag{2.15}$$

where η is now a constant Lagrange multiplier. The above variational formulation follows through for this case also. After similar intermediate steps, exactly the same equations given by the formulae from (2.9a) to (2.13) are obtained. The only difference is that η does not appear in the right hand side of the eq. (2.14), and thus we may replace eq. (2.14) with the following more general form:

$$O(\mathbf{q}(T), \mathbf{p}(T)) = \tilde{O} + \alpha\eta\,, \tag{2.16}$$

where the new parameter α is defined below:

$$\alpha = \begin{cases} 1 & \text{if } \mathcal{J}_o \text{ in eq. (2.3) is used (flexible case)}, \\ 0 & \text{if } \mathcal{J}_{c,o} \text{ in eq. (2.15) is used (constrained case)}\ . \end{cases} \tag{2.17}$$

In the case involving $\mathcal{J}_o$ the coefficient η just measures the deviation of the objective from its target value. In section 4, the coefficient η will play an important role in establishing the existence of multiple solutions to the optimal control problem. The cost functional prescribed above is physically reasonable, although other forms could be chosen. The purpose of this paper is to explore the existence of multiple solutions for eqs. (2.9)–(2.14), and the form of these equations directly depends on the form of $\mathcal{J}$ and also the potential and dipole functions.

The evolution of the costate functions is backwards in time due to the final condition in eqs. (2.11b), (2.12b) while the molecular dynamics alone is an initial value problem. Thus the overall variational equations to be solved form a boundary value problem in time. It is this nature of optimal control theory that will lead to the possibility of there existing multiple solutions to these equations.

3. Linearization of the variational equations

The equations to be solved in (2.9)–(2.14) to achieve an optimal control solution are coupled and nonlinear. Furthermore, the equations for the coordinates and momenta in (2.9) and (2.10) are initial value problems which may be integrated forward in time with an initial guess for the control field, $\mathcal{E}(T)$. In contrast the equations for the costate function in (2.11) and (2.12) must be integrated backwards in time also with a trial guess for the input field, $\mathcal{E}(t)$. Here we are primarily not concerned with the computational aspects of such problems, and we shall employ a perturbation expansion in increasing powers of $\mathcal{E}(t)$. Although such an expansion could be practically employed for sufficiently weak fields, our purpose in this paper is to gain analytical insight into the multiplicity of solutions of the control equations and the perturbation expansion facilitates this analysis without actually requiring numerical implementation. In particular the expansion allows for an effective decoupling of the forward and backward evolutions in eqs. (2.9) and (2.14).

We introduce a dummy perturbation parameter, ν, (which is ultimately set to one) to enable the further analysis. By multiplying $\mathcal{E}(t)$ in eqs. (2.9a), (2.10a), and (2.11a) with ν and explicitly denoting the dependence of the dynamical variables on t and ν we can write the following generalized equations for the dynamical variables:

$$\dot{q}_j(t,\nu) = \sum_{k=1}^{N} P_{jk} p_k(t,\nu), \quad q_j(0,\nu) = \tilde{q}_j, \quad 1 \leqslant j \leqslant N, \tag{3.1a, b}$$

$$\dot{p}_j(t,\nu) = -\frac{\partial V(\mathbf{q}(t,\nu))}{\partial q_j(t,\nu)} - \nu \mathcal{E}(t) \frac{\partial \mu(\mathbf{q}(t,\nu))}{\partial q_j(t,\nu)}, \quad p_j(0,\nu) = \tilde{p}_j, \quad 1 \leqslant j \leqslant N, \tag{3.2a, b}$$

$$\dot{\lambda}_j^{(q)}(t,\nu) = \sum_{k=1}^{N} \frac{\partial^2 V(\mathbf{q}(t,\nu))}{\partial q_j(t,\nu) \partial q_k(t,\nu)} \lambda_k^{(p)}(t,\nu) + \nu \mathcal{E}(t) \sum_{k=1}^{N} \frac{\partial^2 \mu(\mathbf{q}(t,\nu))}{\partial q_j(t,\nu) \partial q_k(t,\nu)} \lambda_k^{(p)}(t,\nu) + W_p(t) O'(\mathbf{q}(t,\nu), \mathbf{p}(t,\nu)) \frac{\partial O'(\mathbf{q}(t,\nu), \mathbf{p}(t,\nu))}{\partial q_j(t,\nu)}, \quad 1 \leqslant j \leqslant N, \tag{3.3a}$$

$$\lambda_j^{(q)}(T,\nu) = -\eta \frac{\partial O(\mathbf{q}(T,\nu), \mathbf{p}(T,\nu))}{\partial q_j(T,\nu)}, \quad 1 \leqslant j \leqslant N, \tag{3.3b}$$

$$\dot{\lambda}_j^{(p)}(t,\nu) = W_p(t) O'(\mathbf{q}(t,\nu), \mathbf{p}(t,\nu)) \frac{\partial O'(\mathbf{q}(t,\nu), \mathbf{p}(t,\nu))}{\partial p_j(t,\nu)} - \sum_{k=1}^{N} P_{jk} \lambda_k^{(q)}(t,\nu), \quad 1 \leqslant j \leqslant N, \tag{3.4a}$$

$$\lambda_j^{(p)}(T,\nu) = -\eta \frac{\partial O(\mathbf{q}(T,\nu), \mathbf{p}(T,\nu))}{\partial p_j(T,\nu)}, \quad 1 \leqslant j \leqslant N, \tag{3.4b}$$

where $\mathcal{E}(t)$ and η are assumed to be independent of ν. We expand all the dynamical variables in a perturbation series as follows:

$$q_j(t,\nu) = \sum_{k=0}^{\infty} q_{j,k}(t) \nu^k, \quad q_{j,l}(0) = \delta_{l,0} \tilde{q}_j, \quad 1 \leqslant j \leqslant N, \quad l = 0, 1, \ldots, \tag{3.5a, b}$$

$$p_j(t,\nu) = \sum_{k=0}^{\infty} p_{j,k}(t) \nu^k, \quad p_{j,l}(0) = \delta_{l,0} \tilde{p}_j, \quad 1 \leqslant j \leqslant N, \quad l = 0, 1, \ldots, \tag{3.6a, b}$$

$$\lambda_j^{(q)}(t,\nu) = \sum_{k=0}^{\infty} \lambda_{j,k}^{(q)}(t) \nu^k, \quad \lambda_{j,l}^{(q)}(T) = -\eta O_l^{(q)}, \quad 1 \leqslant j \leqslant N, \quad l = 0, 1, \ldots, \tag{3.7a, b}$$

$$\lambda_j^{(p)}(t,\nu) = \sum_{k=0}^{\infty} \lambda_{j,k}^{(p)}(t) \nu^k, \quad \lambda_{j,l}^{(p)}(T) = -\eta O_l^{(p)}, \quad 1 \leqslant j \leqslant N, \quad l = 0, 1, \ldots, \tag{3.8a, b}$$

where $O_k^{(q)}$ and $O_k^{(p)}$ depend on the space, $q_{j,k}(t)$, and momentum, $p_{j,k}(t)$, variables at $t = T$ up to orders less than $(k+1)$. These coefficients are defined through the following expansions:

$$\frac{\partial O(\mathbf{q}(T,\nu),\mathbf{p}(T,\nu))}{\partial q_j(T,\nu)} = \sum_{k=0}^{\infty} O_k^{(q)} \nu^k ,$$

$$\frac{\partial O(\mathbf{q}(T,\nu),\mathbf{p}(T,\nu))}{\partial p_j(T,\nu)} = \sum_{k=0}^{\infty} O_k^{(p)} \nu^k , \quad 1 \leqslant j \leqslant N . \tag{3.9a, b}$$

The unknown coefficients of the expansions given in eqs. (3.5)–(3.8) can be evaluated through eqs. (3.1)–(3.4). If we consecutively differentiate both sides of eqs. (3.1a) and (3.2a) with respect to ν and set $\nu = 0$, we can obtain recursive differential equations for the perturbation coefficients of the space and momentum variables. Equations (3.5b) and (3.6b) serve as the initial temporal conditions for these equations. The same operations can be performed for the perturbation expansion of the λ-variables in eqs. (3.7) and (3.8) by use of eqs. (3.3) and (3.4). The differential equations for the λ-variables are accompanied by the final temporal conditions given in eqs. (3.7b) and (3.9b). A careful analysis shows that all perturbation coefficients except the zeroth order ones, satisfy inhomogeneous linear ordinary differential equations. Hence, their solution can be expressed, at least formally, in explicit form. Our main goal is to explore the *number* of solutions permitted by these equations, and the essential features of this issue are revealed by the zeroth and first order perturbation expansion coefficients. In this context the role of the higher order terms enters in the global analysis given in section 5 where attention is on the convergence of the perturbation expansions.

The zeroth order terms for dynamical variables satisfy the following equations obtained from eqs. (3.1a)–(3.4b) by setting $\nu = 0$:

$$\dot{q}_{j,0}(t) = \sum_{k=1}^{N} P_{jk} p_{k,0}(t) , \quad q_{j,0}(0) = \tilde{q}_j , \quad 1 \leqslant j \leqslant N , \tag{3.10a, b}$$

$$\dot{p}_{j,0}(t) = -\frac{\partial V(\mathbf{q}_0(t))}{\partial q_{j,0}(t)} , \quad p_{j,0}(0) = \tilde{p}_j , \quad 1 \leqslant j \leqslant N , \tag{3.11a, b}$$

$$\dot{\lambda}_{j,0}^{(q)}(t) = \sum_{k=1}^{N} \frac{\partial^2 V(\mathbf{q}_0(t))}{\partial q_{j,0}(t) \partial q_{k,0}(t)} \lambda_{k,0}^{(p)}(t) + W_p(t) O'(\mathbf{q}_0(t), \mathbf{p}_0(t)) \times \frac{\partial O'(\mathbf{q}_0(t), \mathbf{p}_0(t))}{\partial q_{j,0}(t)} , \quad 1 \leqslant j \leqslant N ,$$

$$\lambda_{j,0}^{(q)}(T) = -\eta \frac{\partial O(\mathbf{q}_0(T), \mathbf{p}_0(T))}{\partial q_{j,0}(T)} , \quad 1 \leqslant j \leqslant N , \tag{3.12a, b}$$

$$\dot{\lambda}_{j,0}^{(p)}(t) = -\sum_{k=1}^{N} P_{jk}\lambda_{k,0}^{(q)}(t) + W_p(t)O'(\mathbf{q}_0(t),\mathbf{p}_0(t)) \times \frac{\partial O'(\mathbf{q}_0(t),\mathbf{p}_0(t))}{\partial p_{j,0}(t)}, \quad 1\leqslant j\leqslant N, \tag{3.13a}$$

$$\lambda_{j,0}^{(p)}(T) = -\eta\frac{\partial O(\mathbf{q}_0(T),\mathbf{p}_0(T))}{\partial p_{j,0}(T)}, \quad 1\leqslant j\leqslant N, \tag{3.13b}$$

where

$$\mathbf{p}_0^{\mathrm{T}}(t) = [p_{1,0}(t),p_{2,0}(t),\ldots,p_{N,0}(t)], \quad \mathbf{q}_0^{\mathrm{T}}(t) = [q_{1,0}(t),q_{2,0}(t),\ldots,q_{N,0}(t)]. \tag{3.14a, b}$$

These equations determine the forward free motion of the molecule and the backward evolution of the Lagrange multiplier functions. Since there is no coupling between forward and backward evolutions (the equations are successively uncoupled in the sense that the $\mathbf{p}_0(t), \mathbf{q}_0(t)$ equations are self contained, but the $\lambda_0(t)$ equations also depend on $\mathbf{p}_0(t)$, $\mathbf{q}_0(t)$), these equations can be solved with standard techniques for treating initial value problems of ordinary differential equations. Henceforth we assume that the zeroth order dynamical variables are known.

The first order perturbation corrections for the dynamical variables can be evaluated through the following equations obtained from eqs. (3.1a)–(3.4b) by setting $\nu = 0$ after differentiation with respect to ν:

$$\dot{q}_{j,1}(t) = \sum_{k=1}^{N} P_{jk}p_{k,1}(t), \quad q_{j,1}(0) = 0, \quad 1\leqslant j\leqslant N, \tag{3.15a, b}$$

$$\dot{p}_{j,1}(t) = -\sum_{k=1}^{N}\frac{\partial^2 V(\mathbf{q}_0(t))}{\partial q_{j,0}(t)\partial q_{k,0}(t)}q_{k,1}(t) - \mathcal{E}(t)\frac{\partial\mu(\mathbf{q}_0(t))}{\partial q_{j,0}(t)}, \quad p_{j,1}(0) = 0, \tag{3.16a, b}$$

$$\dot{\lambda}_{j,1}^{(q)}(t) = \sum_{k=1}^{N}\frac{\partial^2 V(\mathbf{q}_0(t))}{\partial q_{j,0}(t)\partial q_{k,0}(t)}\lambda_{k,1}^{(p)}(t) + \sum_{k=1}^{N}\Lambda_{j,k}^{(q,q)}(t)q_{k,1}(t) + \sum_{k=1}^{N}\Lambda_{j,k}^{(q,p)}(t)p_{k,1}(t) + \mathcal{E}(t)\sum_{k=1}^{N}\frac{\partial^2\mu(\mathbf{q}_0(t))}{\partial q_{j,0}(t)\partial q_{k,0}(t)}\lambda_{k,0}^{(p)}(t), \quad 1\leqslant j\leqslant N, \tag{3.17a}$$

$$\Lambda_{j,k}^{(q,q)}(t) = \left\{\frac{\partial O'(\mathbf{q}_0(t),\mathbf{p}_0(t))}{\partial q_{j,0}(t)}\frac{\partial O'(\mathbf{q}_0(t),\mathbf{p}_0(t))}{\partial q_{k,0}(t)} + O'(\mathbf{q}_0(t),\mathbf{p}_0(t))\frac{\partial^2 O'(\mathbf{q}_0(t),\mathbf{p}_0(t))}{\partial q_{j,0}(t)\partial q_{k,0}(t)}\right\} \times W_p(t) + \sum_{l=1}^{N}\frac{\partial^3 V(\mathbf{q}_0(t))}{\partial q_{j,0}(t)\partial q_{k,0}(t)\partial q_{l,0}(t)}\lambda_{l,0}^{(p)}(t), \quad 1\leqslant j\leqslant N, \tag{3.17b}$$

$$\Lambda_{j,k}^{(q,p)}(t)=\left\{\frac{\partial O'(\mathbf{q}_0(t),\mathbf{p}_0(t))}{\partial q_{j,0}(t)}\frac{\partial O'(\mathbf{q}_0(t),\mathbf{p}_0(t))}{\partial q_{k,0}(t)}+O'(\mathbf{q}_0(t),\mathbf{p}_0(t))\frac{\partial^2 O'(\mathbf{q}_0(t),\mathbf{p}_0(t))}{\partial q_{j,0}(t)\partial q_{k,0}(t)}\right\}$$

$$\times W_p(t)\,,\quad 1\leqslant j\leqslant N\,, \tag{3.17c}$$

$$\lambda_{j,1}^{(q)}(T)=-\eta\sum_{k=1}^{N}\left\{\frac{\partial^2 O(\mathbf{q}_0(T),\mathbf{p}_0(T))}{\partial q_{j,0}(T)\partial q_{k,0}(T)}q_{k,1}(T)+\frac{\partial^2 O(\mathbf{q}_0(T),\mathbf{p}_0(T))}{\partial q_{j,0}(T)\partial p_{k,0}(T)}p_{k,1}(T)\right\}, \tag{3.17d}$$

$$\dot{\lambda}_{j,1}^{(p)}(t)=-\sum_{k=1}^{N}P_{j,k}\lambda_{k,1}^{(q)}(t)+\sum_{k=1}^{N}\Lambda_{j,k}^{(p,q)}(t)q_{k,1}(t)+\sum_{k=1}^{N}\Lambda_{j,k}^{(p,p)}(t)p_{k,1}(t)\,, \tag{3.18a}$$

$$\Lambda_{j,k}^{(p,q)}(t)=\left\{\frac{\partial O'(\mathbf{q}_0(t),\mathbf{p}_0(t))}{\partial p_{j,0}(t)}\frac{\partial O'(\mathbf{q}_0(t),\mathbf{p}_0(t))}{\partial q_{k,0}(t)}+O'(\mathbf{q}_0(t),\mathbf{p}_0(t))\frac{\partial O'(\mathbf{q}_0(t),\mathbf{p}_0(t))}{\partial p_{j,0}(t)\partial q_{k,0}(t)}\right\}$$

$$\times W_p(t)\,,\quad 1\leqslant j\leqslant N\,, \tag{3.18b}$$

$$\Lambda_{j,k}^{(p,p)}(t)=\left\{\frac{\partial O'(\mathbf{q}_0(t),\mathbf{p}_0(t))}{\partial p_{j,0}(t)}\frac{\partial O'(\mathbf{q}_0(t),\mathbf{p}_0(t))}{\partial p_{k,0}(t)}+O'(\mathbf{q}_0(t),\mathbf{p}_0(t))\frac{\partial^2 O'(\mathbf{q}_0(t),\mathbf{p}_0(t))}{\partial p_{j,0}(t)\partial p_{k,0}(t)}\right\}$$

$$\times W_p(t)\,,\quad 1\leqslant j\leqslant N\,, \tag{3.18c}$$

$$\lambda_{j,1}^{(p)}(T)=-\eta\sum_{k=1}^{N}\left\{\frac{\partial^2 O(\mathbf{q}_0(T),\mathbf{p}_0(T))}{\partial p_{j,0}(T)\partial q_{k,0}(T)}q_{k,1}(T)+\frac{\partial^2 O(\mathbf{q}_0(T),\mathbf{p}_0(T))}{\partial p_{j,0}(T)\partial p_{k,0}(T)}p_{k,1}(T)\right\}. \tag{3.18d}$$

We can define the following entities to facilitate the analysis:

$$\mathbf{A}(t)=\begin{pmatrix}0 & \mathbf{P}\\ \mathbf{A}_{21}(t) & 0\end{pmatrix},\quad \{\mathbf{A}_{21}(t)\}_{jk}=-\frac{\partial^2 V(\mathbf{q}_0(t))}{\partial q_{j,0}(t)\partial q_{k,0}(t)}\,,\quad 1\leqslant j,k\leqslant N\,, \tag{3.19a, b}$$

$$\mathbf{q}_1^{\mathrm{T}}(t)=[q_{1,1}(t),\ldots,q_{1,N}]\,,\quad \mathbf{p}_1^{\mathrm{T}}(t)=[p_{1,1}(t),\ldots,p_{1,N}]\,,\quad \mathbf{x}_1^{\mathrm{T}}(t)=[\mathbf{q}_1^{\mathrm{T}}(t),\mathbf{p}_1^{\mathrm{T}}(t)] \tag{3.20a, b, c}$$

$$a_j(t)=\begin{cases}0\,, & 1\leqslant j\leqslant N\,,\\ \dfrac{\partial\mu(\mathbf{q}_0(t))}{\partial q_{j-N,0}(t)}\,, & N+1\leqslant j\leqslant 2N\,.\end{cases} \tag{3.21}$$

Equations (3.15a,b) and (3.16a,b) can be written in the following matrix form via these new terms:

$$\dot{\mathbf{x}}_1(t) = \mathbf{A}(t)\mathbf{x}_1(t) - \mathcal{E}(t)\mathbf{a}(t), \quad \mathbf{x}_1(0) = \mathbf{0}. \tag{3.22a, b}$$

To solve this equation we introduce the matrix differential equations,

$$\dot{\mathbf{Q}}_R(t) = \mathbf{A}(t)\mathbf{Q}_R(t), \quad \mathbf{Q}_R(0) = \mathbf{I}, \tag{3.23a, b}$$

$$\dot{\mathbf{Q}}_L(t) = -\mathbf{Q}_L(t)\mathbf{A}(t), \quad \mathbf{Q}_L(0) = \mathbf{I}, \tag{3.23a, b}$$

where $\mathbf{I}$ is a $2n$-dimensional unit matrix. As can easily be shown, $\mathbf{Q}_L(t)$ is the inverse of $\mathbf{Q}_R(t)$. Therefore we have the following solution for the first order space and momentum variables:

$$\mathbf{x}_1(t) = -\int_0^t \mathrm{d}\tau\, \mathcal{E}(\tau)\mathbf{Q}_R(t)\mathbf{Q}_L(\tau)\mathbf{a}(\tau). \tag{3.24}$$

The first order terms for λ can be evaluated with the aid of the following entities:

$$y_{1j}(t) = \begin{cases} \lambda^{(q)}_{j,1}(t), & 1 \leqslant j \leqslant N, \\ \lambda^{(p)}_{j-N,1}(t), & N+1 \leqslant j \leqslant 2N, \end{cases} \tag{3.25}$$

$$\Lambda_{jk}(t) = \begin{cases} \Lambda^{(q,q)}_{j,k}, & 1 \leqslant j \leqslant N, \quad 1 \leqslant k \leqslant N, \\ \Lambda^{(q,p)}_{j,k-N}, & 1 \leqslant j \leqslant N, \quad N+1 \leqslant k \leqslant 2N, \\ \Lambda^{(p,q)}_{j-N,k}, & N+1 \leqslant j \leqslant 2N, \quad 1 \leqslant k \leqslant N, \\ \Lambda^{(p,p)}_{j-N,k-N}, & N+1 \leqslant j \leqslant 2N, \quad N+1 \leqslant k \leqslant 2N, \end{cases} \tag{3.26}$$

$$\mathcal{O}_{jk} = \begin{cases} \dfrac{\partial^2 O(\mathbf{q}_0(T), \mathbf{p}_0(T))}{\partial q_{j,0}(T)\partial q_{k,0}(T)}, & 1 \leqslant j \leqslant N, \quad 1 \leqslant k \leqslant N, \\ \dfrac{\partial^2 O(\mathbf{q}_0(T), \mathbf{p}_0(T))}{\partial q_{j,0}(T)\partial p_{k-N,0}(T)}, & 1 \leqslant j \leqslant N, \quad N+1 \leqslant k \leqslant 2N, \\ \dfrac{\partial^2 O(\mathbf{q}_0(T), \mathbf{p}_0(T))}{\partial p_{j-N,0}(T)\partial q_{k,0}(T)}, & N+1 \leqslant j \leqslant 2N, \quad 1 \leqslant k \leqslant N, \\ \dfrac{\partial^2 O(\mathbf{q}_0(T), \mathbf{p}_0(T))}{\partial p_{j-N,0}(T)\partial p_{k-N,0}(T)}, & N+1 \leqslant j \leqslant 2N, \quad N+1 \leqslant k \leqslant 2N, \end{cases} \tag{3.27}$$

$$b_j(t) = \begin{cases} \sum_{k=1}^{N} \dfrac{\partial^2 \mu(\mathbf{q}_0(t))}{\partial q_{j,0}(t) \partial q_{k,0}(t)} \lambda_{k,0}^{(p)}, & 1 \leqslant j \leqslant N, \\ 0, & N+1 \leqslant j \leqslant 2N. \end{cases} \tag{3.28}$$

With these definitions we can obtain an equation for $y_1(t)$:

$$\dot{\mathbf{y}}_1(t) = -\mathbf{A}^{\mathrm{T}}(t)\mathbf{y}_1(t) + \mathbf{\Lambda}(t)\mathbf{x}_1(t) + \mathcal{E}(t)\mathbf{b}(t), \quad \mathbf{y}_1(T) = -\eta \mathcal{O}\mathbf{x}_1(T), \tag{3.29a, b}$$

which may be explicitly solved,

$$\mathbf{y}_1(t) = \eta \mathbf{Q}_L^{\mathrm{T}}(t)\mathbf{Q}_R^{\mathrm{T}}(T)\mathcal{O} \int_0^T \mathrm{d}\tau\, \mathcal{E}(\tau)\mathbf{Q}_R(T)\mathbf{Q}_L(\tau)\mathbf{a}(\tau) + \int_t^T \mathrm{d}\tau\, \mathbf{Q}_L^{\mathrm{T}}(t)\mathbf{Q}_R^{\mathrm{T}}(\tau)\mathbf{\Lambda}(\tau)$$
$$\times \int_0^\tau \mathrm{d}\tau_1\, \mathcal{E}(\tau_1)\mathbf{Q}_R(\tau)\mathbf{Q}_L(\tau_1)\mathbf{a}(\tau_1) - \int_t^T \mathrm{d}\tau\, \mathcal{E}(\tau)\mathbf{Q}_L^{\mathrm{T}}(t)\mathbf{Q}_R^{\mathrm{T}}(\tau)\mathbf{b}(\tau). \tag{3.30}$$

Armed with $\mathbf{x}_1(t)$ and $\mathbf{y}_1(t)$ we may now proceed to consider the issue of field multiplicity. To enable this analysis of the field solution multiplicity consider the re-expression of eq. (2.13):

$$\Phi(t, \nu) \equiv -\frac{1}{W_{\mathcal{E}}(t)} \sum_{k=1}^{N} \lambda_k^{(p)}(t, \nu) \frac{\partial \mu(\mathbf{q}(t, \nu))}{\partial q_k(t, \nu)} \tag{3.31}$$

and the objective

$$\Omega(\nu) \equiv O(\mathbf{q}(T, \nu), \mathbf{p}(T, \nu)). \tag{3.32}$$

Thus, we may now respectively define the *field* and *spectral* equations as follows:

$$\mathcal{E}(t) = \Phi(t, 1), \tag{3.33}$$

$$\alpha\eta = \Omega(1) - \tilde{O}, \tag{3.34}$$

Equation (3.34) is referred to as the spectral equation as it explicitly contains the generalized eigenvalue η whose admissible values will determine the fields and the quality of the corresponding control solutions. If we expand $\Phi(t, \nu)$ and $\Omega(t, \nu)$ in powers of ν,

$$\Phi(t, \nu) = \sum_{j=0}^{\infty} \Phi_j(t)\nu^j, \tag{3.35}$$

$$\Omega(\nu) = \sum_{j=0}^{\infty} \Omega_j \nu^j, \tag{3.36}$$

then we can express the zeroth and first order coefficients as below:

$$\Phi_0(t) = -\frac{1}{W_{\mathcal{E}}(t)} \sum_{k=1}^{N} \lambda_{k,0}^{(p)}(t) \frac{\partial \mu(\mathbf{q}_0(t))}{\partial q_{k,0}(t)} = -\frac{1}{W_{\mathcal{E}}(t)} \mathbf{a}^{\mathrm{T}}(t) \mathbf{y}_0(t) , \tag{3.37a}$$

$$\Phi_1(t) = -\frac{1}{W_{\mathcal{E}}(t)} \sum_{j=1}^{N} \lambda_{j,1}^{(p)}(t) \frac{\partial \mu(\mathbf{q}_0(t))}{\partial q_{j,0}(t)} - \frac{1}{W_{\mathcal{E}}(t)} \sum_{j=1}^{N} \sum_{k=1}^{N} \lambda_{j,0}^{(p)}(t) \frac{\partial^2 \mu(\mathbf{q}_0(t))}{\partial q_{j,0}(t) \partial q_{k,0}(t)}$$

$$\times q_{k,1}(t) = -\frac{1}{W_{\mathcal{E}}(t)} (\mathbf{a}^{\mathrm{T}}(t) \mathbf{y}_1(t) + \mathbf{b}^{\mathrm{T}}(t) \mathbf{x}_1(t)) , \tag{3.37b}$$

$$\Omega_0 = O(\mathbf{q}_0(T), \mathbf{p}_0(T)) , \tag{3.38a}$$

$$\Omega_1 = \sum_{j=1}^{N} \frac{\partial O(\mathbf{q}_0(T), \mathbf{p}_0(T))}{\partial q_{j,0}(T)} q_{j,1}(T) + \sum_{j=1}^{N} \frac{\partial O(\mathbf{q}_0(T), \mathbf{p}_0(T))}{\partial p_{j,0}(T)}$$

$$\times p_{j,1}(T) = \mathbf{o}^{\mathrm{T}} \mathbf{x}_1(T) , \tag{3.38b}$$

where

$$y_{0,j} = \begin{cases} \lambda_{j,0}^{(q)}(t) & 1 \leqslant j \leqslant N , \\ \lambda_{j-N,0}^{(p)}(t), & N+1 \leqslant j \leqslant 2N , \end{cases} \tag{3.39}$$

and

$$o_j = \begin{cases} \dfrac{\partial O(\mathbf{q}_0(T), \mathbf{p}_0(T))}{\partial q_{j,0}(T)} , & 1 \leqslant j \leqslant N , \\ \dfrac{\partial O(\mathbf{q}_0(T), \mathbf{p}_0(T))}{\partial p_{j-N,0}(T)} , & N+1 \leqslant j \leqslant 2N , \end{cases} \tag{3.40}$$

The explicit structure of $\mathbf{y}_0(t)$ can be determined after some intermediate algebra,

$$\mathbf{y}_0(t) = -\eta \mathbf{Q}_L^{\mathrm{T}}(t) \mathbf{Q}_R^{\mathrm{T}}(T) \mathbf{o} - \int_t^T \mathrm{d}\tau \, \mathbf{Q}_L^{\mathrm{T}}(t) \mathbf{Q}_R^{\mathrm{T}}(\tau) \mathbf{c}(\tau) , \tag{3.41}$$

where

$$c_j(t) = \begin{cases} W_p(t) O'(\mathbf{q}_0(t), \mathbf{p}_0(t)) \dfrac{\partial O'(\mathbf{q}_0(t), \mathbf{p}_0(t))}{\partial q_{j,0}(t)} , & 1 \leqslant j \leqslant N , \\ W_p(t) O'(\mathbf{q}_0(t), \mathbf{p}_0(t)) \dfrac{\partial O'(\mathbf{q}_0(t), \mathbf{p}_0(t))}{\partial p_{j,0}(t)} , & N+1 \leqslant j \leqslant 2N . \end{cases} \tag{3.42}$$

This enables us to write $\mathbf{b}$ in eq. (3.28) as

$$\mathbf{b} = \mathbf{D}(t) \mathbf{y}_0(t) = -\eta \mathbf{D}(t) \mathbf{Q}_L^{\mathrm{T}}(t) \mathbf{Q}_R^{\mathrm{T}}(T) \mathbf{o} - \int_t^T \mathrm{d}\tau \, \mathbf{D}(t) \mathbf{Q}_L^{\mathrm{T}} \mathbf{Q}_R^{\mathrm{T}}(\tau) \mathbf{c}(\tau) , \tag{3.43}$$

where

$$\mathbf{D}(t) = \begin{pmatrix} 0 & \mathbf{D}_{12}(t) \\ 0 & 0 \end{pmatrix}, \quad \{\mathbf{D}_{12}(t)\}_{jk} = \frac{\partial^2 \mu(\mathbf{q}_0(t))}{\partial q_{j,0}(t) \partial q_{k,0}(t)}, \quad 1 \leqslant j,k \leqslant N. \tag{3.44a, b}$$

The above equations provide working solutions for the control equations up to first order in the field strength. Now, we can linearize the field and spectral equations (3.33) and (3.34), respectively, as follows:

$$\mathcal{E}_L(t) = \Phi_0^{(L)}(t) + \Phi_1^{(L)}(t), \tag{3.45}$$

$$\alpha \eta_L = \Omega_0 - \tilde{O} + \Omega_1^{(L)}, \tag{3.46}$$

where L denotes that up to linear terms are retained.

Since $\Phi_1^{(L)}(t)$ is a linear functional of $\mathcal{E}(t)$, then eq. (3.45) is a linear integral equation for $\mathcal{E}(t)$. Furthermore $\Phi_0^{(L)}(t)$ and $\Phi_1^{(L)}(t)$ depend on η_L, thus making eq. (3.46) a nonlinear algebraic equation for η_L. Since $\mathcal{E}_L(t)$ from (3.45) depends on η_L and there may be multiple values of η_L satisfying the non-linear equation (3.46), then the prospect opens up for the existence of multiple field solutions to the optimal control problem. The detailed structure of these equations and their solutions are treated in the next section.

4. Multiple solutions in the linearized case

The structure of the linearized field and spectral equations given in eqs. (3.45) and (3.46) need further elaboration as explicit forms of the operators involved are important to reveal the behavior of their solutions. The kernels of the integral operators and some necessary additional entities are reported below without the intermediate algebraic steps. First we shall treat the field equation (3.45) through elaboration of the structures of $\Phi_0^{(L)}(t)$ and $\Phi_1^{(L)}(t)$. We have $\Phi_0^{(L)}(t)$ taking on the form

$$\Phi_0^{(L)}(t) = u_1(t) + \eta_L u_2(t), \tag{4.1}$$

where

$$u_1(t) = \frac{1}{W_{\mathcal{E}}(t)} \int_t^T \mathrm{d}\tau \, \mathbf{a}^{\mathrm{T}}(t) \mathbf{Q}_L^{\mathrm{T}}(t) \mathbf{Q}_R^{\mathrm{T}}(\tau) \mathbf{c}(\tau), \tag{4.2}$$

$$u_2(t) = \frac{1}{W(t)} \mathbf{a}^{\mathrm{T}}(t) \mathbf{Q}_L^{\mathrm{T}}(t) \mathbf{Q}_R^{\mathrm{T}}(T) \mathbf{o}. \tag{4.3}$$

Similarly the function $\Phi_1^{(L)}(t)$ can be expressed as

$$\Phi_1^{(L)}(t) = \frac{1}{W_\mathcal{E}(t)} \int_0^t \mathrm{d}\tau\, u_3(t,\tau)\mathcal{E}_L(\tau) + \frac{1}{W_\mathcal{E}(t)} \int_t^T \mathrm{d}\tau\, u_4(t,\tau)\mathcal{E}_L(\tau)$$

$$- \eta_L \frac{1}{W_\mathcal{E}(t)} \int_0^t \mathrm{d}\tau\, u_5(t,\tau)\mathcal{E}_L(\tau) - \eta_L \frac{1}{W_\mathcal{E}(t)} \int_t^T \mathrm{d}\tau\, u_6(t,\tau)\mathcal{E}_L(\tau)\,, \tag{4.4}$$

where

$$v_1(t,\tau) = \mathbf{a}^{\mathrm{T}}(t)\mathbf{Q}_L^{\mathrm{T}}(t)\mathbf{Q}_R^{\mathrm{T}}(T)\mathbb{O}\mathbf{Q}_R(T)\mathbf{Q}_L(\tau)\mathbf{a}(\tau)\,, \tag{4.5}$$

$$v_2(t,\tau,\tau_1) = -\mathbf{a}^{\mathrm{T}}(t)\mathbf{Q}_L^{\mathrm{T}}(t)\mathbf{Q}_R^{\mathrm{T}}(\tau)\mathbf{\Lambda}(\tau)\mathbf{Q}_R(\tau)\mathbf{Q}_L(\tau_1)\mathbf{a}(\tau_1)\,, \tag{4.6}$$

$$v_3(t,\tau) = \mathbf{a}^{\mathrm{T}}(t)\mathbf{Q}_L^{\mathrm{T}}(t)\mathbf{Q}_R^{\mathrm{T}}(\tau)\mathbf{D}(\tau)\mathbf{Q}_L(\tau)\mathbf{Q}_R(T)\mathbf{o}\,, \tag{4.7}$$

$$v_4(t,\tau,\tau_1) = -\mathbf{a}^{\mathrm{T}}(t)\mathbf{Q}_L^{\mathrm{T}}(t)\mathbf{Q}_R^{\mathrm{T}}(\tau)\mathbf{D}(\tau)\mathbf{Q}_L(\tau)\mathbf{Q}_R(\tau_1)\mathbf{c}(\tau_1)\,, \tag{4.8}$$

$$u_3(t,\tau) = \int_t^T \mathrm{d}\tau_1\, v_2(t,\tau_1,\tau) + \int_t^T \mathrm{d}\tau_1\, v_4(\tau,t,\tau_1)\,, \tag{4.9}$$

$$u_4(t,\tau) = \int_\tau^T \mathrm{d}\tau_1\, v_2(t,\tau_1,\tau) + \int_\tau^T \mathrm{d}\tau_1\, v_4(t,\tau,\tau_1)\,, \tag{4.10}$$

$$u_5(t,\tau) = v_1(t,\tau) + v_3(\tau,t)\,, \tag{4.11}$$

$$u_6(t,\tau) = v_1(t,\tau) + v_3(t,\tau)\,. \tag{4.12}$$

By using these results in eqs. (4.1) and (4.4) we can arrive at the following integral equation for the field amplitude:

$$\mathcal{M}\mathcal{E}_L(t) - \eta_L \mathcal{N}\mathcal{E}_L(t) = u_1(t) + \eta_L u_2(t)\,, \tag{4.13}$$

where $\mathcal{M}$ and $\mathcal{N}$ are defined, through their actions on a square integrable function, $f(t)$, over $[0, T]$ under the weight $W_\mathcal{E}(t)$, as follows:

$$\mathcal{M}f(t) \equiv \frac{1}{W_\mathcal{E}(t)} \int_0^t \mathrm{d}\tau\, u_3(t,\tau)f(\tau) + \frac{1}{W_\mathcal{E}(t)} \int_t^T \mathrm{d}\tau\, u_4(t,\tau)f(\tau) - f(t)\,, \tag{4.14}$$

$$\mathcal{N}f(t) \equiv \frac{1}{W_\mathcal{E}(t)} \int_0^t \mathrm{d}\tau\, u_5(t,\tau)f(\tau) + \frac{1}{W_\mathcal{E}(t)} \int_t^T \mathrm{d}\tau\, u_6(t,\tau)f(\tau)\,. \tag{4.15}$$

By using the triangular identity for two-dimensional integration, we may show that the kernels of these operators are symmetric:

$$(f(t), \mathcal{M}g(t)) = (g(t), \mathcal{M}f(t))\,, \tag{4.16}$$

$$(f(t), \mathcal{N}g(t)) = (g(t), \mathcal{N}f(t)), \tag{4.17}$$

where $f(t)$ and $g(t)$ are square integrable under the weight function, $W_\varepsilon(t)$, over the time interval, $[0, T]$. Here the new scalar product is defined as

$$(f(t), g(t)) \equiv \int_0^T \mathrm{d}t\, W_\varepsilon(t) f(t) g(t). \tag{4.18}$$

The definiteness of $\mathcal{N}$ is important for establishing the solutions to eq. (4.13). We can proceed for this purpose by evaluating the diagonal matrix elements of $\mathcal{N}$ for any $f(t)$,

$$(f(t), \mathcal{N}f(t)) = \mathcal{I}_1 + 2\mathcal{I}_2, \tag{4.19}$$

where

$$\mathcal{I}_1 = \int_0^T \mathrm{d}t \int_0^T \mathrm{d}\tau\, f(t) f(\tau) \mathbf{a}^{\mathrm{T}}(t) \mathbf{Q}_L^{\mathrm{T}}(t) \mathbf{Q}_R^{\mathrm{T}}(T) \mathcal{O} \mathbf{Q}_R(T) \mathbf{Q}_L(\tau) \mathbf{a}(\tau), \tag{4.20}$$

$$\mathcal{I}_2 = \int_0^T \mathrm{d}t \int_0^t f(t) f(\tau) \mathbf{a}^{\mathrm{T}}(\tau) \mathbf{Q}_L^{\mathrm{T}}(\tau) \mathbf{Q}_R^{\mathrm{T}}(t) \mathbf{D}(t) \mathbf{Q}_L(t) \mathbf{Q}_R(T) \mathbf{o}. \tag{4.21}$$

If we denote the lowest eigenvalue of $\mathcal{O}$ by σ and observe the fact that the spectral norm of $\mathbf{Q}_R^{\mathrm{T}}(T)\mathbf{Q}_R(T)$ is greater than $\|\mathbf{Q}_L(T)\|^{-2}$, then we can write the following inequality for $\mathcal{I}_1$:

$$\mathcal{I}_1 > \sigma \|\mathbf{Q}_L(T)\|^{-2} \mathcal{I}_3, \tag{4.22}$$

where

$$\mathcal{I}_3 = \int_0^T \mathrm{d}t \int_0^T \mathrm{d}\tau\, f(t) f(\tau) \mathbf{a}^{\mathrm{T}}(t) \mathbf{Q}_L^{\mathrm{T}}(t) \mathbf{Q}_L(\tau) \mathbf{a}(\tau). \tag{4.23}$$

A norm analysis through the Schwartz inequality for scalar products enables us to write

$$\mathcal{I}_2 > -T\mathcal{I}_3^{\frac{1}{2}} \Bigg[\int_0^T \mathrm{d}t \int_0^T \mathrm{d}\tau\, f(t) f(\tau) \|\mathbf{Q}_R(t)\| \|\mathbf{Q}_R(\tau)\| \|\mathbf{Q}_R(T)\|^2 \|\mathbf{Q}_L(t)\| \times \|\mathbf{Q}_L(\tau)\| \|\mathbf{D}(t)\| \|\mathbf{D}(\tau)\| \|\mathbf{o}\|^2 \Bigg]^{1/2}. \tag{4.24}$$

Equations (4.22) and (4.24) produce a lower bound for the diagonal matrix elements of $\mathcal{N}$. If this bound is positive for arbitrary $f(t)$, then $\mathcal{N}$ is positive definite. Therefore using eq. (4.19) we can write the following sufficient condition for the positive definiteness of $\mathcal{N}$:

$$\frac{\sigma^2}{4T\|\mathbf{Q}_L(T)\|^4} \mathbf{a}^{\mathrm{T}}(t) \mathbf{Q}_L^{\mathrm{T}}(t) \mathbf{Q}_L(\tau) \mathbf{a}(\tau) > \|\mathbf{Q}_R(t)\| \|\mathbf{Q}_R(\tau)\| \times \|\mathbf{Q}_R(T)\|^2 \|\mathbf{Q}_L(t)\| \|\mathbf{Q}_L(\tau)\| \|\mathbf{D}(t)\| \|\mathbf{D}(\tau)\| \|\mathbf{o}\|^2, \tag{4.25}$$

where t and τ lie in the time interval, $[0, T]$. (Here, σ is assumed to be positive. Otherwise the bound analysis above can not guarantee the positive definiteness of $\mathcal{N}$. In such cases operators in the objective term can be re-defined to produce positive σ values.) According to this condition, the objective term, as reflected here in the lowest eigenvalue σ of $\mathcal{O}$, must have a special functional structure in terms of its dependence on the momentum and space variables. Since an appropriately chosen function of the objective term can be used instead of itself without any substantial loss of generality, the criterion in eq. (4.25) can be taken as valid by a suitable redefinition of the control problem. It is also possible to obtain milder conditions than (4.25) through more complex analysis. Henceforth, we assume that the optimally controlled molecular design problem is given in a way such that $\mathcal{N}$ is positive definite.

Now we can explore the solution to eq. (4.13) by considering the following generalized eigenvalue problem:

$$\mathcal{M}e_k = \eta_k \mathcal{N} e_k \,, \quad k \geqslant 1 \,, \tag{4.26}$$

$$(e_j, \mathcal{N} e_k) = \delta_{j,k} \,, \quad j, k \geqslant 1 \,, \tag{4.27}$$

with eigenfunctions e_k and eigenvalues η_k. The above eigenfunctions form a complete basis set for functions which are square integrable with respect to $W_{\mathcal{E}}(t)$ over the interval $[0, T]$. The existence and the discreteness of the relevant spectrum can be shown via the theory of linear integral operators [30]. Usually one considers unit operator weighted eigenvalue problems, and we can transform the eigenvalue problem in eq. (4.26) to this type through a transformation with $\mathcal{N}^{1/2}$ since $\mathcal{N}$ is positive definite. The existence of a symmetric and nonsingular kernel (i.e., Hilbert–Schmidt kernel) in $\mathcal{M}$ from eq. (4.14) enables us to prove the discreteness of the spectrum given in eq. (4.26). Any function in the $W_{\mathcal{E}}(t)$ weighted Hilbert space can be uniquely expanded in a linear combination of the eigenfunction e_k. This result can be employed to expand the solution of the linearized field equation, for the case where η_L is outside the above spectrum,

$$\mathcal{E}_L(t) = \sum_{k=1}^{\infty} \frac{(e_k, u_1 + \eta_L u_2)}{\eta_k - \eta_L} e_k(t) \,. \tag{4.28}$$

As long as u_1 and u_2 do not become orthogonal to any $e_k(t)$ and η_L is outside the spectrum, $\{\eta_k, k = 1, 2, \ldots\}$, then $\mathcal{E}_L(t)$ depends on only a single, as yet undetermined parameter, η_L. However if the following equations hold:

$$(e_K, u_1) = 0 \,, \quad (e_K, u_2) = 0 \,, \quad K = k_1, k_2, \ldots \geqslant 1 \,, \tag{4.29}$$

then the associated coefficients of the eq. (4.28) becomes arbitrary and η_L can be equal to the corresponding eigenvalues. Hence, the solution of the linearized field equation contains additional undetermined arbitrary parameters in this case. Specification of η_L is achieved by finding those values that satisfy the linearized spectral equation (3.46).

The linearized spectral equation (3.46) can be rewritten in the following manner after the elimination of the field amplitude:

$$\Omega_0 + \Omega_1 = \tilde{O} + \alpha\eta\,, \tag{4.30a}$$

$$\mathbf{o}^{\mathrm{T}}\mathbf{x}_1(T) + O(\mathbf{q}_0(T), \mathbf{p}_0(T)) = \tilde{O} + \alpha\eta\,, \tag{4.30b}$$

where eqs. (3.38a) and (3.38b) were used. Now employing eq. (5.24) we have

$$O(\mathbf{q}_0(T), \mathbf{p}_0(T)) - \tilde{O} - \alpha\eta = \int_0^T \mathrm{d}\tau\, \mathcal{E}(\tau)\mathbf{o}^{\mathrm{T}}\mathbf{x}_1^{\mathrm{T}}(T)\mathbf{Q}_R(T)\mathbf{Q}_L(\tau)\mathbf{a}(\tau)\,. \tag{4.30c}$$

Utilizing eq. (4.3) we have

$$O(\mathbf{q}_0(T), \mathbf{p}_0(T)) - \tilde{O} - \alpha\eta = (\mathcal{E}_L, u_2) \tag{4.30d}$$

and substituting in $\mathcal{E}_L$ from eq. (4.28) gives

$$\sum_{k=1}^{\infty} \frac{(e_k, u_2)^2\eta_L + (e_k, u_1)(e_k, u_2)}{\eta_k - \eta_L} = O(\mathbf{q}_0(t), \mathbf{p}_0(t)) - \tilde{O} - \alpha\eta_L\,. \tag{4.30}$$

The left hand side of this equation is a meromorphic function with an infinite number of simple poles located at the generalized eigenvalues of $\mathcal{M}$ under the weight operator $\mathcal{N}$. The residues at the poles are not guaranteed to be positive unless u_1 vanishes. When u_1 vanishes the linear structure of the right side creates exactly one single intersection, therefore a solution for η_L, between two consecutive vertical asymptotes. The possible survival of u_1 in eq. (4.30e) complicates the situation, since depending on the structure of u_1, the residues may change sign from pole to pole. This can produce a minimum or maximum between two consecutive vertical asymptotes in the meromorphic function on the left hand side of eq. (4.30e). In this case we may have either two or no of intersection points with the right side of eq. (4.30e). The function u_1 depends on the structure of O' and the free motion Hamiltonian of the system under consideration. By appropriately changing the structure of the free motion Hamiltonian of the system, or the functional structure of O' one can, in principle, annihilate u_1. Therefore, we may assume that u_1 vanishes. Then a denumerably infinite number of solutions for the control field $\mathcal{E}(t)$ can be produced when $u_1 = 0$, while the case of nonvanishing u_1 may reduce the number of solutions to a finite value, even to zero.

5. Effect of the nonlinear terms on control field multiplicity

Our concern here is with regard to the non-linear terms entering the field and spectral equations (3.33) and (3.34). These equations depend on all of the dynamical variables which in turn have been expanded in eqs. (3.5)–(3.8). We desire to seek bounds for these variables regardless of the value of ν on the interval $0 \leqslant \nu \leqslant 1$ and thus to argue their impact on the multiplicity of solutions to (3.33) and (3.34).

For the purpose stated above, we can usefully employ the following inequality for a multivariable complex function.

$$|f(\mathbf{z})| < \frac{A_f(\bar{\mathbf{z}})}{\prod_{j=1}^{N}\left(1 - \frac{|z_j - \bar{z}_j|}{\rho_j^{(f)}(\bar{\mathbf{z}})}\right)}, \tag{5.1}$$

where $\mathbf{z}$ denotes the set of z-variables and $\bar{\mathbf{z}}$ denotes the Taylor series expansion point [31]. The constant, $A_f(\bar{\mathbf{z}})$ and the convergence radii, $\rho_j^{(f)}(\bar{\mathbf{z}})$, $1 \leqslant j \leqslant N$, depend on the location of the expansion point and the structure of the function, $f(\mathbf{z})$. The convergence domain of $f(\mathbf{z})$ is a hyperellipsoid in the N-tuple complex space of the z-variables. The actual convergence domain of $f(\mathbf{z})$ may be larger than this hyperellipsoid, however, we can always locate a hyperellipsoid inside the actual convergence volume.

The potential and dipole functions critically control the dynamics and their analysis is useful here. We assume that the location of the Taylor series expansion point of $\mathbf{q}(t, \nu)$ changes in time and is characterized by $\mathbf{q}(t, 0)$; using eq. (5.1) we can write the following bounds:

$$|V(\mathbf{q}_0(T), \mathbf{p}_0(T))| < \frac{A_V(\mathbf{q}(t,0))}{\prod_{j=1}^{N}\left(1 - \frac{|q_j(t,\nu) - q_j(t,0)|}{\rho_j^{(V)}(\mathbf{q}(t,0))}\right)}, \tag{5.2}$$

$$|\mu(\mathbf{q}_0(T), \mathbf{p}_0(T))| < \frac{A_\mu(\mathbf{q}(t,0))}{\prod_{j=1}^{N}\left(1 - \frac{|q_j(t,\nu) - q_j(t,0)|}{\rho_j^{(\mu)}(\mathbf{q}(t,0))}\right)}. \tag{5.3}$$

These bounds can be simplified by diminishing the convergence volume to facilitate the further analysis as follows:

$$|V(\mathbf{q}_0(T), \mathbf{p}_0(T))| < \frac{A_V(\mathbf{q}(t,0))}{\left(1 - \frac{B_q(\nu)}{\rho}\right)^N}, \tag{5.4}$$

$$|\mu(\mathbf{q}_0(T), \mathbf{p}_0(T))| < \frac{A_\mu(\mathbf{q}(t,0))}{\left(1 - \frac{B_q(\nu)}{\rho}\right)^N}, \tag{5.5}$$

where ρ denotes the minimum of the convergence radius values for $V(\mathbf{q}_0(T), \mathbf{p}_0(T))$ and $\mu(\mathbf{q}_0(T), \mathbf{p}_0(T))$ with respect to their arguments over the time interval $[0, T]$.

$$\rho = \min_{\substack{t\in[0,T]\\ 1\leqslant j\leqslant N}} \left\{ \rho_j^{(V)}(\mathbf{q}(t)), \rho_j^{(\mu)}(\mathbf{q}(t)) \right\} . \tag{5.6}$$

The constant, $B_q(\nu)$ is the maximum deviation in the q-variables due to the field perturbation.

$$|q_j(t,\nu) - q_j(t,0)| < B_q , \quad 1\leqslant j\leqslant N , \quad t\in[0,T] . \tag{5.7}$$

The integration of the eq. (3.2a, b) gives the following inequality for the momentum by making use of the above inequalities and some properties of the maximum value norm:

$$|p_j(t,\nu)| < \tilde{B}_p + \frac{T(\alpha_V + |\nu|\alpha_\varepsilon\alpha_\mu)}{\rho\left(1 - \dfrac{B_q(\nu)}{\rho}\right)^{N+1}} , \quad 1\leqslant j\leqslant N , \tag{5.8}$$

where

$$|\tilde{p}_j| < \tilde{B}_p , \quad 1\leqslant j\leqslant N , \tag{5.9}$$

$$\alpha_V = T^{-1/2}\left\{ \int_0^T \mathrm{d}t\, A_V^2(\mathbf{q}(t,\nu)) \right\}^{1/2} , \quad \alpha_\mu = T^{-1/2}\left\{ \int_0^T \mathrm{d}t\, A_\mu^2(\mathbf{q}(t,\nu)) \right\}^{1/2} ,$$

$$\alpha_\varepsilon = T^{-1/2}\left\{ \int_0^T \mathrm{d}t\, \mathcal{E}^2(t) \right\}^{1/2} . \tag{5.10a, b, c}$$

These equations also made use of the following inequalities for the first order partial derivatives of the potential and dipole function:

$$\left| \frac{\partial V(\mathbf{q}(t,\nu))}{\partial q_j(t,\nu)} \right| < \frac{A_V(\mathbf{q}(t))}{\rho\left(1 - \dfrac{B_q(\nu)}{\rho}\right)^{N+1}} , \tag{5.11}$$

$$\left| \frac{\partial \mu(\mathbf{q}(t,\nu))}{\partial q_j(t,\nu)} \right| < \frac{A_\mu(\mathbf{q}(t))}{\rho\left(1 - \dfrac{B_q(\nu)}{\rho}\right)^{N+1}} . \tag{5.12}$$

A similar treatment applied to eq. (3.1a,b) and the use of the eq. (5.8) permits us to bound the displacement due to the field perturbation,

$$|q_j(t,\nu) - q_j(t,0)| < \tilde{B}_q + |P|\tilde{B}_p T + \frac{T^2(\alpha_V + |\nu|\alpha_\varepsilon\alpha_\mu)}{\rho\left(1 - \dfrac{B_q(\nu)}{\rho}\right)^{N+2}} , \quad 1\leqslant j\leqslant N , \tag{5.13}$$

where

$$|P| = \max_{1 \leqslant j \leqslant N} \{|P_{jk}|\}, \quad |q_j(t,0) - \tilde{q}| < \tilde{B}_q \tag{5.14a,b}$$

and without changing the direction of the inequality we have increased the power in the denominator of the rightmost term to simplify the bound analysis for the remaining unknowns.

We desire to obtain the explicit structure of $B_q(\nu)$ in eq. (5.7), and to this end it is preferable to write an equation instead of the inequality given in eq. (5.13). If we increase the left hand side of eq. (5.13), we can change the inequality to an equality. This could be done by simply writing $B_q(\nu)$ in place of the left hand side. However, the resulting polynomial equation in $B_q(\nu)$ cannot be easily handled. Hence we increase the left hand side to ρ which is greater than $B_q(\nu)$ by assumption and determine the value of $B_q(\nu)$ making the resultant equation valid:

$$\rho = \tilde{B}_q + |P|\tilde{B}_p T + \frac{T^2(\alpha_V + |\nu|\alpha_\varepsilon\alpha_\mu)}{\rho\left(1 - \dfrac{B_q(\nu)}{\rho}\right)^{N+2}}, \quad 1 \leqslant j \leqslant N, \tag{5.15}$$

$$B_q(\nu) = \rho\left\{1 - C_1(T)\left(1 + |\nu|\frac{\alpha_\varepsilon\alpha_\mu}{\alpha_V}\right)^{\frac{1}{N+2}}\right\}, \tag{5.16}$$

where

$$C_1(T) = \left(\frac{T^2\alpha_V}{\rho[\rho - \tilde{B}_q - |P|\tilde{B}_p T]}\right)^{\frac{1}{N+2}}. \tag{5.17}$$

The above value of $B_q(\nu)$ leads to the following ν-independent bound for the momentum variables

$$|p_j(t,\nu)| < B_p = \frac{\rho - \tilde{B}_q}{T} - |P|\tilde{B}_p. \tag{5.18}$$

Equation (5.16) remains valid unless the braced entity becomes negative. Since our system corresponds to the case where $\nu = 1$, we can easily show that the following condition suffices for the convergence of the dynamical variable perturbation expansion in powers of ν:

$$\tilde{B}_q + |P|\tilde{B}_p T + \frac{T^2(\alpha_V + \alpha_\varepsilon\alpha_\mu)}{\rho} < \rho. \tag{5.19}$$

Equation (5.19) dictates that the aforementioned perturbation expansion converges as long as the system remains in the convergence volume which is a hypersphere around the point, $\mathbf{q}(t,0)$, with a radius, ρ. Since everything except α_ε is known, then eq. (5.19) can be considered as a restriction on the field amplitude. Conversely, if the field is known then eq. (5.19) can be interpreted as a constraint on the interaction time, T. If we desire to find a bound on the field amplitude, then,

we must deal with these limitations in a more detailed manner. However, here, we shall only utilize the convergence condition in eq. (5.19) as being a sufficient criterion, and very probably a highly conservative one. Less conservative bounds can also be obtained, but they will not alter the basic conclusion to follow.

Similar procedures can be constructed to develop bounds for the remaining unknowns λ_q and λ_p. Without giving the intermediate steps, we report them below.

$$B_{\lambda,q}(\nu) = \frac{T(\rho - B_q(\nu)) + (\rho - \tilde{B}_q - |P|\tilde{B}_p T)}{T(\rho - B_q(\nu)) - |P|(\rho - \tilde{B}_q - |P|\tilde{B}_p T)} \{B_\eta B_0(\nu) + TB_c(\nu)\}, \quad (5.20)$$

$$B_{\lambda,p}(\nu) = \frac{(1 + |P|)\rho T}{T(\rho - B_q(\nu)) - |P|(\rho - \tilde{B}_q - |P|\tilde{B}_p T)} \{B_\eta B_0(\nu) + TB_c(\nu)\}, \quad (5.21)$$

$$\alpha_\mu = \frac{N\alpha_\varepsilon \alpha_W}{T\alpha_V} B_{\lambda,p}(1)(\rho - \tilde{B}_q - |P|\tilde{B}_p T), \quad (5.22)$$

$$\alpha_W = T^{-1/2}\left[\int_0^T \mathrm{d}t\ W_\varepsilon^{-2}(t)\right]^{1/2}, \quad (5.23)$$

where $B_{\lambda,q}(\nu)$ and $B_{\lambda,p}(\nu)$ respectively are the bounds on $\lambda_j^{(q)}$ and $\lambda_j^{(p)}$ for $1 \leqslant j \leqslant N$ and $t \in [0, T]$ whereas $B_o(\nu)$ and $B_c(\nu)$ are the bounds for the elements of the previously defined $\mathbf{c}(t)$ and $\mathbf{o}(t)$ vectors. The quantity B_η bounds the η-parameter, and thus measures the deviation in the final value of the objective term from its target values. There is wide latitude in the choice of the objective functional and the penalty functional, and they often can be appropriately changed without altering the overall purpose of the control goals. Hence, we may consider $B_o(1)$, $B_c(1)$ and B_η as finite parameters (ultimately bounded by the dependence on $\mathbf{p}, \mathbf{q}$ and λ) whose values can be controlled by the designer via redefinition of them without any significant loss of generality. Then the control designer can assume the convergence of dynamical perturbation expansions via the definitions of $O(\mathbf{q}(t,\nu), \mathbf{p}(t,\nu))$ and $O'(\mathbf{q}(t,\nu), \mathbf{p}(t,\nu))$ through eq. (5.22). However, the duration of the field-molecule interaction, T, is bounded from *both* sides. Although its upper bound can be affected by redefining $O(\mathbf{q}(t,\nu), \mathbf{p}(t,\nu))$ and $O'(\mathbf{q}(t,\nu), \mathbf{p}(t,\nu))$ the demand for a finite value of T can not be removed. This situation causes no problem since the duration of the quantum control must be finite due to practical reasons.

Now, we have proved that the solutions for $\mathbf{p}, \mathbf{q}, \lambda$ are all bounded as long as their perturbation expansion converges when $\nu = 1$. This means that the nonlinear contributions to the field and spectral equations (3.33) and (3.34) are also bounded for the actual field amplitude and spectral parameter values. The boundedness of the nonlinear terms means that there is no new poles introduced in the meromorphic function constructed to η-values and the solutions remain around the linearized solutions to η. It can be shown that the η-value can never get closer to the poles of the meromorphic function as proved by bounding all of the nonlinear contributions to

the field and spectral equations. The structure of the nonlinear spectral equation dictates that there is, at least, one solution for η between two consecutive poles of the meromorphic function. Finally, it is worth commenting that, in special cases and under particular approximations, the multiplicity of control solutions is evident [32,33]. The work in the present paper rigorously establishes the existence of multiple solutions under general conditions.

6. Concluding remarks

The primary goal of this work is to prove the existence of multiple solutions to the problem of optimally controlling molecular motion described by classical mechanics. The analysis for this purpose was carried out by starting with a rather general optimizing cost functional and proceeding with a perturbation expansion of the resultant Euler equations. The perturbation expansion for the position, momentum and corresponding Lagrange multiplier functions lead to the field and spectral equations. These equations were then linearized with respect to the field. Under rather flexible conditions and assumptions, it was concluded that an infinite number of solutions to the classical mechanical optimal control problem will generally exist. The structure of the integral operator to determine the field amplitude has the same general form as the one for the analogous quantum mechanical case except that the explicit expressions for the kernels are different. Hence, the numerical algorithm to obtain the field amplitudes using perturbation theory is expected be same for both cases after construction of the kernels.

In practice, the existence of multiple solutions will give flexibility to the designer to introduce additional costs and constraints into the cost function, to ultimately further discriminate amongst the multiple solutions. Although the use of classical mechanics to describe the molecular motion is limited, the model should be useful for polyatomic molecules especially with heavier atoms. The essentially same conclusions on multiple solution structure of both classical and quantum implies that the multiplicity in the solutions is completely due to the optimal control phenomena and not form of the dynamics.

We proved that the nonlinear terms in the spectral equation can alter the locations of the solutions for η (and hence the form of the corresponding fields) but do not eliminate any of the linearized case solutions. However, this does not imply that new solutions may be added. Indeed, we have just considered the effect of the nonlinear terms on the already existing solutions in the linearized case. Although the location of the poles in the final spectral equation is not affected by the nonlinear terms, the functional structure of the non-meromorphic part may fluctuate finitely or even infinitely between two consecutive poles. This behavior may create a finite or infinite number of new additional members to the solution family. The nonlinear structure in the Euler equations may even result in bifurcations with regard to the perturbation parameter. The bifurcational structure, if it exists,

depends on the nature of the inputs of the control problem and necessitates a further analysis to reveal its nature.

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