Gauge-invariance aspects of the canonical perturbation theory

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It is shown that the time-dependent canonical perturbation theory in classical mechanics has unsatisfactory features when dealing with electromagnetic perturbed fields (the perturbed vector potential $\tilde{\mathbf{A}} \neq \mathbf{0}$). As a numerical apparatus, the theory relates to gauge-dependent errors larger than expected. As an analytic apparatus, the theory is involved in unphysical concepts and yields inherently non-gauge-invariant formalisms. By defining the root cause of the problem, an alternative approach is accordingly introduced.

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The time-dependent canonical perturbation theory is now considered as conventional wisdom; the theory has been accepted by classical books [1,2] and applied to many physical fields, such as celestial mechanics, plasma physics, and astrophysics.

To invoke the theory, a canonical transformation

$$p, q \longrightarrow \alpha(p,q), \beta(p,q), \tag{1}$$

where the variables α, β are invariants in the unperturbed system, needs to be defined. Under perturbations the invariant variables evolve in time according to (we will use γ to stand for both α and β throughout the paper)

$$\dot{\gamma} = [\gamma, \tilde{H}] \approx [\gamma, \tilde{H}]_{\gamma=\gamma_c}, \tag{2}$$

where γ_c represents the unperturbed constant value ot γ. With Eq. (2), the system's behavior can be readily investigated in a numerical or analytic way.

In usual situations the perturbation theory possesses many nice features and works very well. The defined variables form a new phase space and the trajectory of the perturbed system in the space is just a nearby orbit around the fixed point describing the unperturbed system. Based on this picture, not only the system becomes approximately solvable but, more importantly, those variables, very often defined as meaningful fundamental quantities, such as energy, momentum, angular momentum, magnetic moment, and so on, provide a conceptually convenient frame to observe the system's dynamics and the variables' evolution equation (2) provides a universally applicable means to describe the dynamics. Those features together with other things, such as Darboux's theorem to guarantee the existence of the phase space [2] and the invariance of the phase-space volume with canonical transformations, all make the theory more applicable.

While the theory seemed flawless, there were some discussions revealing the necessity to think of the problem differently. Littlejohn, in his paper [3,4] mainly related to particle motion in a magnetic field, pointed out that with the use of the vector potential $\tilde{\mathbf{A}}$ the standard theory mixed ordering and proposed to use an elegant Lie-transformation approach [5–7] to formulate the problem. In one of our earlier papers [8] we expressed that the standard theory had certain technical drawbacks.

Despite these efforts to somewhat discredit the standard theory, the theory is not seriously challenged in the sense that it is almost uniformly believed that as long as the ordering of the perturbed Hamiltonian $\tilde{H}$ is in line the theory holds. Many papers regularly using the theory keep appearing in the literature and, in particular, there is no direct and relevant analysis (as we know) to pinpoint and investigate the important gauge-invariance problem of the theory.

It is quite obvious that in the standard theory the perturbed Hamiltonian $\tilde{H}$, written for a charged particle in electromagnetic fields as ($m = c = e = 1$ in this paper)

$$\tilde{H} = -(\mathbf{p} - \mathbf{A}_0) \cdot \tilde{\mathbf{A}} + \frac{\tilde{\mathbf{A}}^2}{2} + \tilde{\Phi}, \tag{3}$$

is not uniquely defined since the gauge potential fields $\tilde{\mathbf{A}}, \tilde{\Phi}$ may be transformed into a different form,

$$\tilde{\mathbf{A}} \to \tilde{\mathbf{A}} + \nabla f, \qquad \tilde{\Phi} \to \tilde{\Phi} - \partial_t f, \tag{4}$$

where f represents any differentiable function. In this context, Eq. (2) yields different equations, at least formally, when different gauge choices are adopted. A fundamental notion in physics is that a generally correct theory must be gauge invariant in regard to its results. Thus questions arise: Is the standard perturbation theory gauge invariant? Or, if it is not stringently gauge invariant, can one define some conditions under which the theory may still be accepted as a gauge-invariant one?

In this paper, we will show that as a numerical apparatus the theory yields gauge-invariant results only in a quite limited sense and that as an analytic apparatus the theory relating to unphysical quantities is inherently non-gauge-invariant. After defining the root cause of the problem we propose an almost-canonical approach which is formulated in terms of $\tilde{\Phi}, \tilde{\mathbf{A}}$ and still gauge invariant.

We proceed in the following way. We examine the theory in illustrating examples, and then analyze emerging difficulties in light of the related mathematical and physical arguments. To put the problem in clearer perspective, we only discuss the situations in which the perturbed Hamiltonian $\tilde{H}$ is relatively small.

For simplicity, a one-dimensional harmonic oscillator, whose Hamiltonian reads

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$$H_0 = \frac{p_x^2}{2} + \frac{\omega_c^2 q_x^2}{2}, \tag{5}$$

is chosen as the example of the unperturbed system; the expression

$$p_x = \sqrt{2\alpha\omega_c}\cos(\beta + \omega_c t), \quad q_x = \sqrt{2\alpha/\omega_c}\sin(\beta + \omega_c t) \tag{6}$$

virtually defines the new variables α, β, which take the constant values α_c, β_c in the unperturbed system.

We note that with the transformation

$$\tilde{\mathbf{A}} \to \tilde{\mathbf{A}} + \mathbf{a}, \tag{7}$$

where $\mathbf{a}$ is a constant vector comparable to $\tilde{\mathbf{A}}$ in magnitude the perturbed Hamiltonian of Eq. (3) remains to be of the same smallness, but the outcome of the theory changes significantly. In particular, if the zero perturbation field $\{\tilde{A}_x = \epsilon, \tilde{\Phi} = 0\}$ is applied, the oscillator will be perturbed substantially according to the theory. To avoid such irrational results, we propose, only for the sake of discussing the standard theory, that the initial condition

$$\tilde{\mathbf{A}}(t_0, \mathbf{q}(t_0)) = 0 \tag{8}$$

should be imposed upon the standard theory, although the condition literally means some novel constraints, such as that some usual forms for perturbed fields, like $\tilde{A}_x = \epsilon \exp(-i\omega t + ikq_x)$, cannot be used and that when dealing with a multiparticle system one generally needs to use different perturbed vector potentials for different particles.

We now assume that the oscillator is perturbed by $\tilde{E} = \epsilon_0 \sin(\omega t - kq_x)$, for which the two types of perturbed gauge fields $\{\tilde{\Phi} = -\epsilon_0 \cos(\omega t - kq_x)/k, \tilde{A}_x = 0\}$ and $\{\tilde{\Phi} = 0, \tilde{A}_x = \epsilon_0[\cos(\omega t - kq_x) - 1]/\omega\}$ are supposed to be usable. By setting $\beta_c = 0$ and $t_0 = 0$, the condition Eq. (8) is satisfied here. Then, trajectory solutions $q_x(t) = q_x(\alpha(t), \beta(t))$ can be obtained by integrating Eq. (2) and applying Eq. (6). Figures 1 and 2, with parameters given in the captions, illustrate the numerical results [for clearness the figures actually show $q_x(t) - q_x^0(t)$, where $q_x^0(t)$ describes the unperturbed trajectory]. In the figures, the trajectories with the two different gauge choices stick to each other at the beginning, and after a relatively short time they diverge significantly. With the help of other numerical algorithms, such as the Runge-Kutta method, we find that the result with $\tilde{\mathbf{A}} = \mathbf{0}$ is very accurate while the result with $\tilde{\mathbf{A}} \neq \mathbf{0}$ is not.

Before analyzing the problem, we recall a similar perturbation method in mathematics which can be symbolicly expressed in the following way. A dynamic system described by a set of $2i$ equations

$$\dot{g}_j = \epsilon f_j(t, q_i, \dot{q}_i) \quad (j = 1, \ldots, 2i) \tag{9}$$

can be solved approximately by carrying out the integral

$$g_j(t) \approx g_j(t_0) + \int \epsilon f_j(t, q_i, \dot{q}_i)|_{q_i = q_i^0(t), \dot{q}_i = \dot{q}_i^0(t)} dt, \tag{10}$$

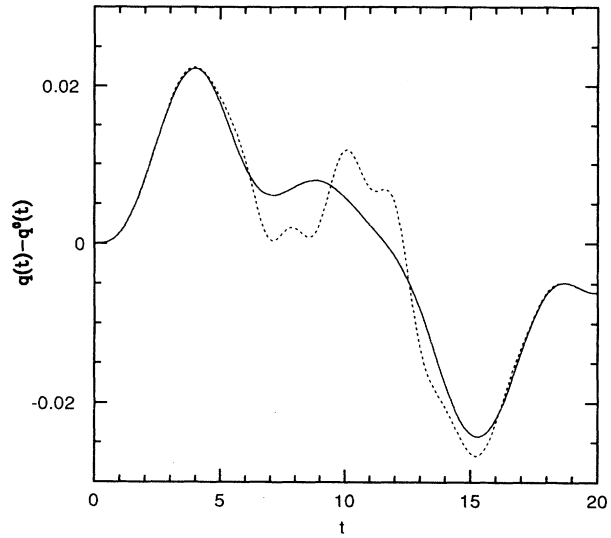

FIG. 1. Trajectory difference $q_x(t) - q_x^0(t)$ by the two gauge choices. Parameters with the perturbed field are $\epsilon_0 = 0.015$, $\omega = 0.3$, $k = -0.3$. Parameters with the oscillator are $\omega_c = 1.0, \alpha_c = 0.5$, and $\beta_c = 0$. The solid line and the dotted line illustrate the results with the first and second gauge choice, respectively.

where the set of $q_i^0(t), \dot{q}_i^0(t)$ is the solution of the equations $\dot{g}_j = 0$, which essentially describes the unperturbed orbit of the system. Exactly speaking, the integral should be taken along the true orbit of the perturbed system; however, integrating along the unperturbed orbit yields a rather small error, since the system only slightly and slowly leaves its unperturbed state (which reflects a physical fact that a dynamic system must have inertia).

The standard theory is supposed to be nothing but the aforementioned method in the Hamiltonian language.

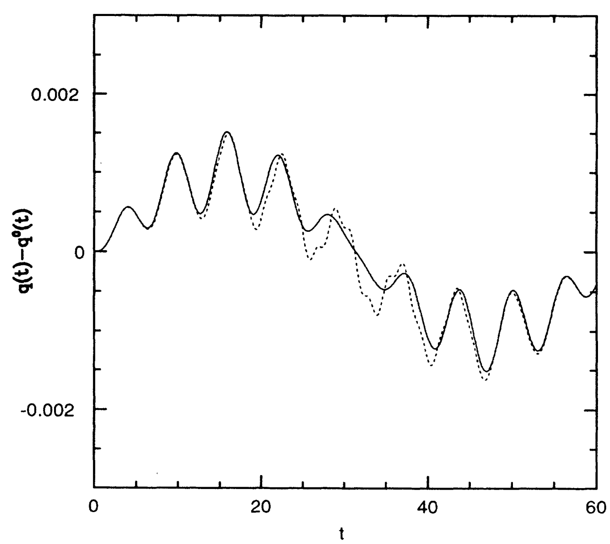

FIG. 2. Trajectory difference $q_x(t) - q_x^0(t)$ by the two gauge choices. Parameters with the perturbed field are $\epsilon_0 = 0.001$, $\omega_c = 0.1$, $k = -0.1$. Other parameters and the meaning of the lines are the same as in Fig. 1.

Indeed, when $\tilde{\mathbf{A}} = \mathbf{0}$ the equation set of $\gamma = \gamma_c$ describes an unperturbed orbit. However, when $\tilde{\mathbf{A}}$ is nonzero, there is a subtle change in the definition system. The variable γ becomes

$$\gamma(\mathbf{p}, \mathbf{q}) = \gamma(\dot{\mathbf{q}} + \mathbf{A}_0 + \tilde{\mathbf{A}}, \mathbf{q}), \tag{11}$$

so that the orbit of $\gamma = \gamma_c$, being deformed by the involvement of $\tilde{\mathbf{A}}$, is no longer the unperturbed one and an extra error (using the unperturbed orbit has brought in an error already) is introduced. By noting $\gamma \approx \gamma_c + (\partial_{\mathbf{p}}\gamma) \cdot \tilde{\mathbf{A}}$ here, we can use the following expression to characterize the extra error with integrating Eq. (2)

$$\int \{\partial_{\mathbf{p}}[\gamma, \tilde{H}]\}_{\gamma_c} \cdot \tilde{\mathbf{A}}\, dt. \tag{12}$$

In some situations, the gauge-dependent error may grow almost linearly with respect to time (Figs. 1 and 2 manifestingly show the growth pattern in our exemplary cases), and imposing the additional condition Eq. (8) can only ensure the gauge invariance at the initial stage $[\tilde{A}(t - t_0) \sim \epsilon]$.

As an analytic apparatus, the theory has more serious difficulties in the sense that it directly relates to unphysical concepts and misleading formalisms. For instance, the invariant $\alpha = (p_x^2 + \omega_c^2 q_x^2)/2$ defined in Eq. (6) can be easily interpreted as energy of the oscillator, and the concept works smoothly if $\tilde{\mathbf{A}} = \mathbf{0}$. However, the interpretation runs into trouble if we allow the vector potential $\tilde{\mathbf{A}}$ to be nonzero. Assuming there is a perturbative electric field $\tilde{E}_x = \epsilon$, we have under the gauge choice $\tilde{\Phi} = -\epsilon q_x, \tilde{A}_x = 0$

$$\dot{\alpha} = [\alpha, \tilde{H}] = \epsilon p_x, \tag{13}$$

or under the gauge choice $\tilde{\Phi} = 0, \tilde{A}_x = -\epsilon t$

$$\dot{\alpha} = [\alpha, \tilde{H}] = \epsilon t \omega_c^2 q_x. \tag{14}$$

The two results are very different and sometimes get different signs (q_x, p_x are sometimes opposite in sign during the oscillation). If α is interpreted as "energy," the energy may decrease while the system actually obtains energy from the perturbed force. Knowing the basic physical fact that a time derivative of energy should be expressed as $\tilde{\mathbf{E}} \cdot \mathbf{v} = -(\partial_t \tilde{\mathbf{A}} + \partial_{\mathbf{q}} \tilde{\Phi}) \cdot \mathbf{v}$, we find that Eq. (13) gives a correct result while Eq. (14) does not. More generally, when defining various energy forms, such as $\mathbf{p}^2/2$, $(\mathbf{p}^2 + \omega^2 \mathbf{q}^2)/2$, and $(\mathbf{p} - \mathbf{A}_0)^2/2$, for various systems and writing their evolution equations with Eq. (2), one should be able to find that the perturbed electric force $-\partial_t \tilde{\mathbf{A}}$ fails to appear expectantly in all the situations. There exist similar conceptual problems when dealing with other kinds of quantities defined by the theory.

We go back to the crucial definition Eq. (1) to see why such things happen. Due to the physicists' interest, quantities defined by Eq. (1) are basicly physical and observable quantities in an unperturbed system, which means that a canonical variable, appearing to be defined by $(\mathbf{A}_0, \Phi_0)$, is essentially a gauge-invariant quantity expressed by

$$\gamma = \gamma(\mathbf{q}, \dot{\mathbf{q}}, \mathbf{E}_0(\mathbf{q}), \mathbf{B}_0(\mathbf{q})) + C, \tag{15}$$

where C is an unimportant constant. However, when the perturbed system is perturbed the variable becomes

$$\gamma = \gamma(\mathbf{p}, \mathbf{q}) = \gamma(\dot{\mathbf{q}} + \mathbf{A}_0 + \tilde{\mathbf{A}}, \mathbf{q}), \tag{16}$$

which can be expressed neither by Eq. (15) nor by

$$\gamma(\mathbf{q}, \dot{\mathbf{q}}, \mathbf{E}_0(\mathbf{q}) + \tilde{\mathbf{E}}(\mathbf{q}), \mathbf{B}_0(\mathbf{q}) + \tilde{\mathbf{B}}(\mathbf{q})) + C. \tag{17}$$

This simple fact shows that mixing up physical and unphysical quantities is the reason why the conceptual difficulties exist. With such ill-defined variables, either Eq. (13) or (14), being equivalent to the exact Hamiltonian formula

$$\dot{\gamma} = \left.\frac{\partial \gamma}{\partial t}\right|_{\mathbf{p},\mathbf{q}} + [\gamma, H]_{\mathbf{p},\mathbf{q}} \tag{18}$$

in the circumstances, is capable of yielding any value from negative to positive according to gauge choices (we say that those variables have no physical inertia).

It may now be clear that the standard theory cannot be invoked to investigate the evolution of physical quantities when $\tilde{\mathbf{A}} \neq \mathbf{0}$. However, there may be one remaining question: does it make sense to use the theory to define variables without associating them with physical quantities and, then, to formally formulate a perturbed system even when $\tilde{\mathbf{A}} \neq \mathbf{0}$? The answer to the question is basicly negative. In such methodology, both the phase space and the trajectory of the system in the space possess a conceptually misguiding nature and one obtains, very often without consciousness, an inherently non-gauge-invariant formalism.

To avoid the difficulties in both numerical and analytic regimes the two following requirements for defining a new variable should be adopted. (1) When disregarding perturbations the variable can be reduced to a corresponding quantity in the unperturbed system. (2) Apart from an unimportant constant, the variable is an observable physical quantity with or without perturbations involved.

These two requirements limit the way to set up a perturbation theory. In the standard approach, the canonical variable system defined by Eq. (1) fulfills the first requirement, but not the second one. Here, we very briefly propose (see more details in Ref. [8]) an alternative approach to complete this paper and to show the significance of the two requirements.

The basic variables in the new approach, other than the usual canonical variables $\mathbf{q}$ and $\mathbf{p}$, are

$$\mathbf{q}_0 = \mathbf{q}, \qquad \mathbf{p}_0 = \mathbf{v} + \mathbf{A}_0. \tag{19}$$

A transformation, formally canonical,

$$\mathbf{q}_0, \mathbf{p}_0 \rightarrow \alpha_0, \beta_0 \tag{20}$$

defines new variables α_0, β_0 which take constant values in the unperturbed system. It is easy to see that since the definition process has nothing to do with $\tilde{\mathbf{A}}$ the two requirements mentioned above are virtually satisfied.

An immediate consequence of the new variable system is new forms for both the unperturbed and perturbed

Hamiltonians. The Hamiltonian $H = \frac{1}{2}(\mathbf{p} - \mathbf{A})^2 + \Phi$ is now divided into

$$H_0 = \tfrac{1}{2}(\mathbf{p}_0 - \mathbf{A}_0)^2 + \Phi_0, \qquad \tilde{H} = \tilde{\Phi}. \tag{21}$$

It is important to note that α_0, β_0 constitute a canonical set only in terms of $\mathbf{p}_0, \mathbf{q}_0$ (with this reason, one may name them neocanonical variables) but not in terms of $\mathbf{p}, \mathbf{q}$. This prohibits us from using Eq. (2) even after rewriting the unperturbed and perturbed Hamiltonians. Starting with Eq. (18) and noting $\mathbf{p} = \mathbf{p}_0 + \tilde{\mathbf{A}}$, we have

$$\dot{\gamma}_0 = [\gamma_0, \mathbf{q}_0] \cdot \partial_t \tilde{\mathbf{A}} + [\gamma_0, \tilde{\Phi}] + \{[\gamma_0, \mathbf{q}_0] \cdot [\tilde{\mathbf{A}}, H_0] - [\gamma_0, \tilde{\mathbf{A}}] \cdot [\mathbf{q}_0, H_0]\}, \tag{22}$$

where the Poisson brackets are given in terms of the variable system $(\mathbf{p}_0, \mathbf{q}_0)$ or (α_0, β_0). It is almost trivial to check that Eq. (22) is gauge invariant and all the difficulties are now resolved.

The present formalism is physically transparent. We can easily identify the terms representing the electric force and Lorentz force in Eq. (22). As an example of theoretical applications, we note that when energy is defined as $\varepsilon = \frac{1}{2}(\mathbf{p}_0 - \mathbf{A}_0)^2 + \Phi_0$ and its evolution is under investigation the last term in Eq. (22) simply disappears, which proves a physical fact that the Lorentz force does not affect energy of a system. By contrast, the proof is not possible with the standard theory.

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