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On generalizing the $K-\chi$ theorem

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ABSTRACT

The K- χ theorem, which states the proportionality between the linear polarizability of a plasma particle in a rapidly oscillating wave field and the adiabatic ponderomotive potential seen by this particle due to the wave, is generalized to arbitrary Hamiltonian dipole interactions.

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1. Introduction

Understanding of the classical particle adiabatic motion in a high-frequency wave packet is simplified within the oscillationcenter (OC) approach, as the latter maps out the quiver dynamics, thereby introducing OC as a quasiparticle undergoing motion slow compared to the oscillations [1–6]. Under the common assumption that the wave field is, in some sense, weak, its effect on the OC is then described in terms of an effective average potential, also known as the ponderomotive potential Φ , which is guadratic in the field amplitude [6–10]. For any given conditions, Φ can be deduced straightforwardly from scratch [6]. On the other hand, there also exists the so-called $K-\chi$ theorem, which yields a general expression for Φ in terms of the readily available *linear* susceptibility $\hat{\mathbf{x}}$ (per unit density) of the particles [11]. The theorem is usually derived by studying how the particle quiver dynamics is affected by the wave Lorentz force [2,4,12–16]. On the other hand, its final form suggests that the details of such interactions may be irrelevant; hence this Letter.

The purpose of the present work is to generalize the $K-\chi$ theorem. By extending the abstract dressed-particle approach, earlier proposed in our Ref. [10], to velocity-dependent ponderomotive potentials, we show that the $K-\chi$ theorem is not specific to motion of plasma particles, but rather represents a general property of Hamiltonian dynamics. As a spin-off, a nonconventional representation of the ponderomotive potential is also reported.

The Letter is organized as follows. In Section 2, we restate the general dressed-particle formalism of Ref. [10] with an emphasis on velocity-dependent average forces. In Section 3, we employ this formalism to deduce the ponderomotive potential in the dipole approximation. In Section 4, we use that to write down the ponderomotive Lagrangian and, in the weak-field approximation, the

* Corresponding author. *E-mail address:* idodin@princeton.edu (I.Y. Dodin). ponderomotive Hamiltonian. In Section 5, we discuss and summarize our main results.

2. Dressed-particle formalism

2.1. Particle-field system

Consider the dynamics of a classical particle traveling through an arbitrary oscillating field. Assume that the field envelope is sufficiently smooth, in both space and time, to allow for the adiabatic approximation [6,10]. Then, the particle can be described in terms of its OC coordinate **x** and the OC velocity **v**, whereas the particle polarization, understood here as the shift of the charge distribution from the OC trajectory, can be interpreted in terms of the OC having *internal modes* (such as due to the gyromotion in a background static magnetic field or, e.g., intra-molecular oscillations). The particle–field interaction can then be treated as coupling of these modes with those of the field; hence, the OC is understood as a "dressed" particle [10].

To describe driven oscillations of, say, free electrons, we will also allow for zero frequencies of the internal modes as a limiting case. In general, though, arbitrary nonlinear frequencies are assumed for the particle, $\dot{\varphi} = \Omega$, and the field, $\dot{\theta} = \omega$, where φ and θ are (sets of) canonical angles, with the corresponding canonical actions being **J** and **I**. At adiabatic interaction, both **J** and **I** are conserved; then, the Lagrangian of the particle–field system, *L*, can be put in the following form:

$$L = L(\dot{\boldsymbol{\varphi}}, \mathbf{J}; \boldsymbol{\theta}, \mathbf{I}; \mathbf{x}, \mathbf{v}; t), \tag{1}$$

where the dependence on **J** and **I** is parametric, and the slow dependence on **x** and *t* is henceforth omitted for brevity. Without the particle–field coupling, *L* equals the sum of $L_p(\dot{\boldsymbol{\varphi}}, \mathbf{J}, \mathbf{v})$ and $L_f(\dot{\boldsymbol{\theta}}, \mathbf{I})$ that describe the particle and the field separately¹; thus,

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 $^{^{1}\} L_{\rm p}$ may also account for interaction with additional slow large-scale background fields.

$$\mathbf{J} = \partial L_{\rm p} / \partial \dot{\boldsymbol{\varphi}}, \qquad \mathbf{I} = \partial L_{\rm f} / \partial \dot{\boldsymbol{\theta}}. \tag{2}$$

After integrating at constant J and I, one gets

$$L = \dot{\boldsymbol{\phi}} \cdot \mathbf{J} + \dot{\boldsymbol{\theta}} \cdot \mathbf{I} + \bar{L}_{p}(\mathbf{J}, \mathbf{v}) + \bar{L}_{f}(\mathbf{I}), \qquad (3)$$

where $\bar{L}_p(\mathbf{J}, \mathbf{v})$ and $\bar{L}_f(\mathbf{I})$ are some functions, which can be understood also as minus the Hamiltonians of the corresponding unperturbed oscillations (at fixed **v**). In the general case, the interaction energy *U* adds on:

$$L = \dot{\boldsymbol{\varphi}} \cdot \mathbf{J} + \dot{\boldsymbol{\theta}} \cdot \mathbf{I} + \bar{L}_{p}(\mathbf{J}, \mathbf{v}) + \bar{L}_{f}(\mathbf{I}) - U.$$
(4)

Yet, by definition, the canonical actions still satisfy

$$\mathbf{J} = \partial L / \partial \dot{\boldsymbol{\varphi}}, \qquad \mathbf{I} = \partial L / \partial \dot{\boldsymbol{\theta}}, \tag{5}$$

and, therefore, *U* is independent of $\dot{\phi}$ and $\dot{\theta}$.

2.2. Oscillation-center Lagrangian

Consider now the particle motion *alone*, that is, excluding the oscillation modes as independent degrees of freedom. Such dynamics is described by a different, particle OC Lagrangian (see Appendix A of Ref. [6])

$$\bar{\mathcal{L}} = L - \dot{\boldsymbol{\varphi}} \cdot \mathbf{J} - \dot{\boldsymbol{\theta}} \cdot \mathbf{I}, \tag{6}$$

where $\dot{\boldsymbol{\phi}} = \boldsymbol{\Omega}$ and $\dot{\boldsymbol{\theta}} = \boldsymbol{\omega}$ are treated as functions of (**J**, **I**, **v**), with the dependence on (**x**, *t*) also implied²; then,

$$\bar{\mathcal{L}} = \bar{L}_{p}(\mathbf{J}, \mathbf{v}) + \bar{L}_{f}(\mathbf{I}) - U(\mathbf{J}, \mathbf{I}, \mathbf{v}).$$
(7)

Using that $\bar{L}_{f}(\mathbf{I})$ is constant and thereby can be omitted, and introducing $\mathcal{L}_{0} \equiv \bar{L}_{p}$, an equivalent OC Lagrangian can be written as

$$\mathcal{L} = \mathcal{L}_0 - U. \tag{8}$$

Thus, \mathcal{L}_0 is the OC no-coupling Lagrangian, and U is the effective potential seen by the OC. Unlike for a true potential, though, U generally depends on **v**, so the translational canonical momentum **P** is now given by

$$\mathbf{P} = \frac{\partial \mathcal{L}_0}{\partial \mathbf{v}} - \frac{\partial U}{\partial \mathbf{v}}.$$
(9)

This means that the OC motion equations,

$$\frac{d\mathbf{P}}{dt} = \frac{\partial \mathcal{L}}{\partial \mathbf{x}},\tag{10}$$

can feature non-potential, albeit Hamiltonian, forces; cf. Ref. [17]. As shown in Refs. [6,18–20], those can be attributed to effective modification of the particle mass, yielding most dramatic effects at near-resonant interactions. (However, *too* close to resonances, nonadiabatic effects become essential; e.g., cf. Ref. [20] and Refs. [21–23]; also see Refs. [24–27].)

2.3. Frequency shifts

The translational canonical momentum in the particle–field system also equals **P**; hence the Hamiltonian

$$H = \mathbf{P} \cdot \mathbf{v} + \dot{\boldsymbol{\varphi}} \cdot \mathbf{J} + \dot{\boldsymbol{\theta}} \cdot \mathbf{I} - L.$$
(11)

From Eq. (6), one gets that

$$H = \mathbf{P} \cdot \mathbf{v} - \bar{\mathcal{L}}.\tag{12}$$

This yields an independent way of calculating the effective potential *U*, which is explained as follows.

Consider the canonical equations

$$\dot{\boldsymbol{p}} = \frac{\partial}{\partial \mathbf{J}} H(\mathbf{J}, \mathbf{I}, \mathbf{P}), \tag{13}$$

and similarly for $\dot{\theta}$. If we now treat the Hamiltonian as a function $H[\mathbf{J}, \mathbf{I}, \mathbf{v}(\mathbf{J}, \mathbf{I}, \mathbf{P})]$, Eqs. (13) rewrite as

$$\dot{\boldsymbol{\varphi}} = \left(\frac{\partial H}{\partial \mathbf{J}}\right)_{\mathbf{I},\mathbf{v}} + \left(\frac{\partial H}{\partial \nu_{\ell}}\right)_{\mathbf{J},\mathbf{I}} \left(\frac{\partial \nu_{\ell}}{\partial \mathbf{J}}\right)_{\mathbf{I},\mathbf{P}},\tag{14}$$

where summation over repeated indexes is implied, and the bold indexes show which variables are assumed fixed at differentiation. Then, using Eq. (12), one has

$$\left(\frac{\partial H}{\partial \mathbf{J}}\right)_{\mathbf{I},\mathbf{v}} = v_i \left(\frac{\partial P_i}{\partial \mathbf{J}}\right)_{\mathbf{I},\mathbf{v}} - \left(\frac{\partial \mathcal{L}_0}{\partial \mathbf{J}}\right)_{\mathbf{I},\mathbf{v}} + \left(\frac{\partial U}{\partial \mathbf{J}}\right)_{\mathbf{I},\mathbf{v}},\tag{15}$$

where $-\mathcal{L}_0$, for fixed **v**, is the Hamiltonian of the particle unperturbed oscillations (Section 2.1), so the second term equals $\boldsymbol{\Omega}_0$. Also, from the same equation (12), one has

$$\left(\frac{\partial H}{\partial v_{\ell}}\right)_{\mathbf{J},\mathbf{I}} = v_i \left(\frac{\partial P_i}{\partial v_{\ell}}\right)_{\mathbf{J},\mathbf{I}} + P_{\ell} - \left(\frac{\partial \tilde{\mathcal{L}}}{\partial v_{\ell}}\right)_{\mathbf{J},\mathbf{I}}.$$
(16)

By definition of P_{ℓ} , the latter pair sums up to zero, so

$$\dot{\boldsymbol{\rho}} = \boldsymbol{\Omega}_{0} + \left(\frac{\partial U}{\partial \mathbf{J}}\right)_{\mathbf{I},\mathbf{v}} + v_{i} \left\{ \left(\frac{\partial P_{i}}{\partial \mathbf{J}}\right)_{\mathbf{I},\mathbf{v}} + \left(\frac{\partial P_{i}}{\partial v_{\ell}}\right)_{\mathbf{J},\mathbf{I}} \left(\frac{\partial v_{\ell}}{\partial \mathbf{J}}\right)_{\mathbf{I},\mathbf{P}} \right\}.$$
(17)

The expression in the curly brackets equals $(\partial P_i/\partial \mathbf{J})_{\mathbf{I},\mathbf{P}} \equiv 0$. Then, one obtains from Eq. (17) and a similar equation for $\dot{\boldsymbol{\theta}}$ that the frequency shifts $\delta \boldsymbol{\Omega} = \boldsymbol{\Omega} - \boldsymbol{\Omega}_0$ and $\delta \boldsymbol{\omega} = \boldsymbol{\omega} - \boldsymbol{\omega}_0$ satisfy

$$\delta \boldsymbol{\Omega} = \left(\frac{\partial U}{\partial \mathbf{J}}\right)_{\mathbf{I},\mathbf{v}}, \qquad \delta \boldsymbol{\omega} = \left(\frac{\partial U}{\partial \mathbf{I}}\right)_{\mathbf{J},\mathbf{v}}.$$
 (18)

Particularly, notice that the derivatives are taken at fixed \mathbf{v} , not at fixed \mathbf{P} .

Eqs. (18) represent the main result of this section, showing how the effective potential U seen by the OC can be derived from the eigenfrequencies of the particle–field system, in analogy with the dressed-atom approach in quantum mechanics [28–31]. In Ref. [10], we studied how this allows calculating the effective potential for nonlinear oscillators under the assumption that U is independent of **v**. Below, we focus on linear coupling but allow for arbitrary $U(\mathbf{v})$.

3. Ponderomotive potential

Suppose sufficiently weak, *linear* waves, so that, to the leading order in I, Eqs. (18) yield $U \approx \Phi$, where

$$\boldsymbol{\Phi} = \delta \boldsymbol{\omega} \cdot \mathbf{I} \tag{19}$$

is called the ponderomotive potential. (Here $\delta \boldsymbol{\omega}$ is independent of **I** but may depend on **J**, so $\delta \boldsymbol{\Omega} = \partial \boldsymbol{\Phi} / \partial \mathbf{J}$, in agreement with Ref. [2].) As waves at multiple frequencies yield additive $\boldsymbol{\Phi}$, we now focus on a single mode with some frequency $\boldsymbol{\omega}$. Suppose such a wave propagates through plasma, of volume \mathcal{V} , comprised of species *s* with densities $N_s = \mathcal{N}_s / \mathcal{V}$. (Particles with different **v** are also considered different species here.) Then, from Eq. (19), the ponderomotive potential on a particle of type *s* is $\boldsymbol{\Phi}_s = I(\delta \boldsymbol{\omega} / \delta \mathcal{N}_s) = (I/\mathcal{V})(\partial \boldsymbol{\omega} / \partial N_s)$. On the other hand, $I = \mathcal{E}\mathcal{V}/\boldsymbol{\omega}$, where \mathcal{E} is the wave energy density. Thus,

² The scalar product of any $\mathbf{a} = (a_1 \dots a_M)$ and $\mathbf{b} = (b_1 \dots b_M)$ is henceforth understood as $\mathbf{a} \cdot \mathbf{b} \equiv \sum_{i=1}^M a_i b_i$.

$$\Phi_{\rm s} = \frac{\mathcal{E}}{\omega} \frac{\partial \omega}{\partial N_{\rm s}},\tag{20}$$

with a corollary that, for a positive-energy mode ($\mathcal{E} > 0$), Φ_s and $\partial \omega / \partial N_s$ have the same sign.

One can also rewrite Eq. (20) in terms of the local field amplitude as follows. Consider (Section 4.2 in Ref. [32])

$$\mathcal{E} = \frac{1}{16\pi} \mathbf{E}^* \cdot \frac{\partial(\hat{\boldsymbol{\epsilon}}\omega)}{\partial\omega} \cdot \mathbf{E} + \frac{|B|^2}{16\pi},\tag{21}$$

where **E** and **B** are the complex envelopes of the wave electric and magnetic fields.³ From the Faraday's law, one has

$$|\mathbf{B}|^2 = |\mathbf{n} \times \mathbf{E}|^2, \tag{22}$$

where $\mathbf{n} = c\mathbf{k}/\omega$, with \mathbf{k} being the wavevector, and c being the speed of light. On the other hand, from the homogeneous-wave equation (Section 1.3 in Ref. [32]),

$$\mathbf{n} \times (\mathbf{n} \times \mathbf{E}) + \hat{\boldsymbol{\epsilon}} \cdot \mathbf{E} = 0, \tag{23}$$

one obtains

$$|\mathbf{n} \times \mathbf{E}|^2 = \mathbf{E}^* \cdot \hat{\boldsymbol{\epsilon}} \cdot \mathbf{E}.$$
(24)

Then,

$$\mathcal{E} = \frac{1}{16\pi} \left[\mathbf{E}^* \cdot \left(\omega \frac{\partial \hat{\boldsymbol{\epsilon}}}{\partial \omega} \right) \cdot \mathbf{E} + 2|\mathbf{n} \times \mathbf{E}|^2 \right].$$
(25)

Notice, though, that differentiating Eq. (24) with respect to N_s at constant **k** (in which case $\mathbf{n} \propto \omega^{-1}$) yields

$$\frac{1}{\omega} \frac{\partial \omega}{\partial N_s} \left[\mathbf{E}^* \cdot \left(\omega \frac{\partial \hat{\boldsymbol{\epsilon}}}{\partial \omega} \right) \cdot \mathbf{E} + 2|\mathbf{n} \times \mathbf{E}|^2 \right]$$
$$= -\mathbf{E}^* \cdot \frac{\partial \hat{\boldsymbol{\epsilon}}}{\partial N_s} \cdot \mathbf{E}.$$
(26)

Therefore, Φ_s , as given by Eq. (20), equals

$$\Phi_{s} = -\frac{1}{16\pi} \mathbf{E}^{*} \cdot \frac{\partial \hat{\boldsymbol{\epsilon}}}{\partial N_{s}} \cdot \mathbf{E}.$$
(27)

Yet, for an ideal gas or plasma, one can write

$$\hat{\boldsymbol{\epsilon}} = 1 + \sum_{s} \hat{\boldsymbol{\chi}}_{s}, \qquad \hat{\boldsymbol{\chi}}_{s} = 4\pi N_{s} \hat{\boldsymbol{\alpha}}_{s}, \qquad (28)$$

where $\hat{\boldsymbol{\alpha}}_{s}(\mathbf{x}, \mathbf{v}_{s}, t; \mathbf{J}_{s})$, given by

$$\hat{\boldsymbol{\alpha}}_{s} = \frac{1}{4\pi} \frac{\delta \hat{\boldsymbol{\chi}}_{s}}{\delta N_{s}},\tag{29}$$

are understood as the polarizability tensors of individual particles of type *s*. Then, omitting the index *s*, one has

$$\Phi = -\frac{1}{4}\mathbf{E}^* \cdot \hat{\boldsymbol{\alpha}} \cdot \mathbf{E},\tag{30}$$

in agreement with an alternative derivation in Ref. [10]. Correspondingly, Φ can be understood as the average energy of the particle–field dipole interaction, with one factor $\frac{1}{2}$ in Eq. (30) being due to time averaging, and another $\frac{1}{2}$ being due to the fact that the particle dipole moment is linear in **E**. (Similarly, the ponderomotive potential due to the particle spin [33] can be introduced.)

4. Ponderomotive Hamiltonian

Consider now how Φ enters the OC Hamiltonian

$$\mathcal{H} = \mathbf{P} \cdot \mathbf{v} - \mathcal{L},\tag{31}$$

where \mathcal{L} [Eq. (8)] is given by

$$\mathcal{L} = \mathcal{L}_0(\mathbf{x}, \mathbf{v}, \mathbf{J}, t) - \Phi(\mathbf{x}, \mathbf{v}, \mathbf{J}, t).$$
(32)

Suppose henceforth that Φ itself is a weak perturbation to the OC dynamics. First, this allows one to expand the dependence between the OC velocity **v** and the OC canonical momentum **P** as

$$\mathbf{v} = \mathbf{v}_0 + \delta \mathbf{v},\tag{33}$$

where $\mathbf{v}_0(\mathbf{x}, \mathbf{P}, \mathbf{J}, t)$ is the corresponding dependence at zero Φ , and $\delta v \ll v_0$. Then, Eq. (31) rewrites as

$$\mathcal{H} \approx \mathbf{P} \cdot (\mathbf{v}_0 + \delta \mathbf{v}) - \mathcal{L}_0(\mathbf{v}_0) - \delta \mathbf{v} \cdot \frac{\partial \mathcal{L}_0(\mathbf{v}_0)}{\partial \mathbf{v}_0} + \Phi,$$
(34)

where we can take $\Phi \approx \Phi(\mathbf{x}, \mathbf{v}_0, \mathbf{J}, t)$, neglecting higher-order corrections. The combination

$$\mathcal{H}_0(\mathbf{x}, \mathbf{P}, \mathbf{J}, t) \equiv \mathbf{P} \cdot \mathbf{v}_0 - \mathcal{L}_0(\mathbf{x}, \mathbf{v}_0, \mathbf{J}, t)$$
(35)

is the Hamiltonian function evaluated at $P(\mathbf{x}, \mathbf{v}_0, \mathbf{J}, t)$. Thus, $\partial \mathcal{L}_0 / \partial \mathbf{v}_0 = \mathbf{P}$ in Eq. (34), so the latter yields

$$\mathcal{H} \approx \mathcal{H}_0(\mathbf{x}, \mathbf{P}, \mathbf{J}, t) + \boldsymbol{\Phi}(\mathbf{x}, \mathbf{P}, \mathbf{J}, t), \tag{36}$$

implying Φ [**x**, **v**₀(**x**, **P**, **J**, *t*], [When Φ is independent of **v**, Eq. (36) also holds for arbitrarily large Φ .]

Finally, consider the particle–field Hamiltonian *H* [Eq. (11)]. Using Eq. (12) together with Eqs. (7), (8), and (31), one gets $H = \mathcal{H} + \mathfrak{E}_0$, where $\mathfrak{E}_0 \equiv -\bar{L}_f(I)$ is the energy of the unperturbed field (Section 2.1). For linear field modes, one has $\mathfrak{E}_0 = \omega_0 \cdot \mathbf{I}$; hence,

$$H = \boldsymbol{\omega}_0 \cdot \mathbf{I} + \boldsymbol{\Phi}(\mathbf{x}, \mathbf{P}, \mathbf{J}, t) + \mathcal{H}_0(\mathbf{x}, \mathbf{P}, \mathbf{J}, t).$$
(37)

On the other hand, Eq. (19) permits rewriting the sum of the two former terms as $\boldsymbol{\omega} \cdot \mathbf{I}$, which equals the wave total energy $\mathfrak{E} = \mathcal{EV}$; then,

$$H = \mathfrak{E} + \mathcal{H}_0(\mathbf{x}, \mathbf{P}, \mathbf{J}, t). \tag{38}$$

In other words, in the weak-field limit considered in this section, the total energy of the particle–field system is a sum of the wave energy \mathfrak{E} and the OC kinetic energy defined as $K = \mathcal{H}_0(\mathbf{x}, \mathbf{P}, \mathbf{J}, t)$. Correspondingly, for multiple particles, one gets

$$H = \mathfrak{E} + \sum_{i} K_{i}.$$
(39)

In the continuous limit, the sum can be replaced with an integral over the OC distribution function; then, a result reported in Ref. [4] is reproduced.

5. Discussion

Eq. (36) states that the second-order (in *E*) "ponderomotive Hamiltonian" $K^{(2)} \equiv \mathcal{H} - \mathcal{H}_0$ satisfies $K^{(2)} = \Phi$, with the latter proportional to $\hat{\boldsymbol{\alpha}} \propto \delta \hat{\boldsymbol{\chi}} / \delta N$ [Eq. (30)]. For specific \mathcal{H}_0 and waveparticle interactions via Lorentz forces, this result has been known as the K- $\boldsymbol{\chi}$ theorem [2,4,11–16]. However, what we showed here is that the properties of the Lorentz force are irrelevant to Eqs. (30) and (36) and that these equations hold equally for arbitrary dipole interactions and any \mathcal{H}_0 . (For how to produce exotic \mathcal{H}_0 , see, e.g., Refs. [6,18,19].) Hence, the K- $\boldsymbol{\chi}$ theorem is not specific to motion

³ Here we used the fact that, since the wave is assumed to propagate without dissipation, $\hat{\epsilon}$ [Eq. (28)] is Hermitian.

of plasma particles, yet is a general property of Hamiltonian dynamics. $^{\rm 4}$

Notice also that, behind the $K-\chi$ theorem, there exists a stronger statement, Eq. (32); as it describes the "ponderomotive Lagrangian" $\mathcal{L}^{(2)} \equiv \mathcal{L} - \mathcal{L}_0$, we call this result the $\mathcal{L}-\chi$ theorem. For Eq. (32) to be valid, even **v**-dependent Φ is not required to be a small perturbation to the OC motion; instead, it is only the dipole approximation (i.e., that *U* is quadratic in *E*) that needs to hold. Unlike in Ref. [4], where the $\mathcal{L}-\chi$ theorem is derived from the motion equations, it is seen now that the details of the particle motion are irrelevant to this result as well.

In summary, the main points of this Letter are in generalizing the $K-\chi$ theorem [the combination of Eqs. (36) and (30)] and the $\mathcal{L}-\chi$ theorem [the combination of Eqs. (32) and (30)] to any Hamiltonian dipole interactions. The generalization is performed by extending the classical dressed-particle approach [10] to velocity-dependent ponderomotive potentials. As a spin-off, we also put forth Eq. (20), which yields a nonconventional representation of the ponderomotive potential.

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