Newtonian adiabatics unified

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Newtonian adiabatics is the consistent truncation of the adiabatic approximation to second order in small velocities. To be complete, it must unify two hitherto disjoint intellectual streams in the study of adiabatic motion. The newer stream focuses on Berry's induced vector potential, or geometric magnetism, and Provost and Vallée's induced scalar potential, reflecting geometry in Hilbert space. The older stream focuses on Inglis' induced inertia, influencing the geometry of adiabatic-parameter space. Starting with the Hamiltonian of the newer stream, unification is simple: A naive or primitive inertia, whose inverse appears in two terms of that Hamiltonian, is replaced by the convention-independent sum of primitive and induced inertia tensors.

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I. INTRODUCTION-NEWTONIAN "TOY MODELS"

The dynamics of electrically charged particles interacting through the electromagnetic field has a natural expansion in the velocities of the particles. An all-order expansion in velocities is at best asymptotic in character, because already at third order in velocity one has radiative processes implying dissipation of the purely particle energies, and hence a nonclosed system. Nevertheless, at second order in velocity there is a consistent truncation of the dynamics involving only the particle degrees of freedom. The electric interactions among particles are given by static Coulomb potentials, while the magnetic interactions are given by a less familiar form, the Darwin Lagrangian [1].

This truncated theory is naturally described as Newtonian electrodynamics, involving as it does kinetic energies quadratic in velocities, and interactions among particles which are instantaneous, so that there is no place for retardation or radiation. In modern parlance, such a theory might be called a "toy model," because important features of the full dynamics still need to be included. Nevertheless, literally for centuries Newtonian theory was a cornucopia of powerful developments in physics, and even today is the basis for presentations of mechanics in introductory physics courses. Thus, this is a toy with great value and useful applications. It is true that for accelerating charged particles, there always will be some radiation. Even for electrically neutral objects interacting through gravity, there also is inevitable, if unobservably small, radiation. Still, the Newtonian approximation for gravitational systems has proven an enormously rich framework, eminently justifying its continued use even though we know it is incomplete (not only omitting radiation but also other relativistic effects such as the Einstein contribution to the precession of the perihelion of Mercury). In the Darwin Lagrangian, among all terms second order in ratios of velocities to the speed of light c is a contribution fourth order in velocity, coming from the velocity-dependence of the inertial mass of each particle. As observed by Coleman and Van Vleck [1], this contribution is essential for a consistent description of the relative motion between a current-loop magnet and an electric charge. Thus we have a demonstration by example that, in cases where there is more than one scale for measuring velocities, a second-order truncation in velocity might not be enough to give a consistent description. This does not contradict the main points of the present paper, that accounting of terms up to second order is at least necessary for consistent truncation, and that there is a systematic way to obtain the unique form of this truncation.

The picture seems quite similar for the case of the adiabatic approximation, giving an effective action for slow degrees of freedom after "integrating out" fast degrees of freedom. In the same sense as for electrodynamics, stopping the adiabatic expansion at second order gives a consistent truncation. Of course, as the terms in the expansion are obtained by perturbation in the velocity, one is entitled to the position that even an internally consistent truncation is logically unjustified, because the perturbation expansion has no finite stopping point. However, the beauty and simplicity of the truncation are so appealing that its internal consistency seems a more than adequate reason to consider it separately. Newtonian dynamics, including Newtonian electrodynamics, provides an alluring indicator of the potential value in such an approach. The main point of the present paper is to provide a complete second-order truncation, because different works in the literature omit one or another part. Let us begin by enumerating those parts (all having geometric interpretations) which go beyond the original Born-Oppenheimer approximation [2].

II. GEOMETRIES OF NEWTONIAN ADIABATICS

Geometry intertwined with dynamics is a pervasive theme in modern physics: General relativity identifies gravity with the geometry of spacetime. Electrodynamics and other gauge theories, as seen in the context of quantum mechanics, are related to the differential geometry of a map between points in spacetime and directions in an abstract space. In this approach, a vector potential is seen as a connection characterizing how the map rotates under infinitesimal motions in spacetime, and the corresponding field strength is simply the curvature of that connection. A second theme receiving con-

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tinually increasing recognition is the importance of approximation schemes based on averaging over fast degrees of freedom to obtain the dynamics for any remaining slow degrees of freedom. In the context of nonrelativistic physics, this usually is described as an adiabatic approximation, while in the context of relativistic quantum field theory, the more common label would be by the result, called an effective field theory. Note that effective field theories generally have actions quadratic in time derivatives of the fields, and thus are examples of the Newtonian truncation in the sense used here, even though of course they are fully relativistic.

A striking connection between the themes of geometry and adiabatics is Berry's discovery [3] that adiabatic variation of parameters in a Hamiltonian induces effective vector potentials appearing in the kinetic momenta conjugate to such parameters or coordinates. Because the structure of the parameter space determines the effective vector potentials and resulting effective magnetic fields, Berry describes the phenomenon as "geometric magnetism." From the perspective of the previous paragraph, it also would be reasonable to use the term "induced (gauge) geometry," as any gauge interaction may be interpreted geometrically.

There is still another kind of geometry found by Provost and Vallée [4] shortly before Berry's work: In addition to the vector potential, there is a scalar potential, which also expresses a geometric structure,

$$\Phi = \hbar^2 Q_{ij} g_{ij}/2, \qquad (1)$$

where in the Hamiltonian for the slow variables the kinetic term is $K = P_i Q_{ij} P_j / 2$. The "metric" g_{ij} measures the infinitesimal distance (in Hilbert space) between instantaneous fast-variable eigenstates corresponding to an infinitesimal change in the values of the adiabatic parameters. As such, g_{ii} of course is intrinsically positive, as is the inverse inertia factor Q_{ii} which multiplies it, so that Φ itself always is positive. A classical interpretation of this potential was given by Aharonov and Stern [5] for the case of a particle with spin and magnetic moment passing through a region in which the magnetic field varies slowly in direction, allowing application of the adiabatic approximation. The scalar potential comes from mean-square oscillation of a component of the spin perpendicular to the magnetic field direction. The reason that in the original discussion [4] this term vanishes with \hbar is that the spin is assumed to be aligned along the magnetic field as well as quantum mechanics can allow, so that the mean-square perpendicular components of the spin are proportional to \hbar , and would disappear in the classical limit. An amusing technical point is that in this example, the second factor \hbar in Eq. (1) is compensated by a large magnetic quantum number to give a nonvanishing classical spin.

The existence of these beautiful if exotic geometrical structures raises the question of whether adiabaticity generically induces or perhaps modifies more conventional geometry, namely that of the space of slow parameters. This space is analogous to the space of possible locations of a particle, in which geodesic paths are the trajectories followed if no explicit forces are acting. In other words, the metric is given by the inertia tensor for the slow parameters. There are two key aspects of this inertia. First, it must be large, so that motion is slow enough to make the adiabatic approximation accurate, but not so large that the effects of adiabatically induced forces are negligible. Secondly, the large inertia may be primitive, i.e., associated with explicit degrees of freedom in the full action, or induced, i.e., a consequence of the velocity-dependent coupling associated with the adiabatic variation of parameters.

It will be seen a little later that at least one prominent case of the latter type has been known for decades. Nevertheless, the simplicity, universality, and especially the geometry associated with induced inertia seem yet to be accorded the wide recognition they deserve.

To compute induced inertia, we need to consider systematically contributions to the energy through second order in the velocity of slow coordinates, i.e., beyond what is needed for the scalar potential (zeroth order in velocity) or the vector potential (first order in velocity, though locally ambiguous because of gauge freedom). Let us examine a little more carefully the orders in small parameters of the relevant geometric contributions to the Hamiltonian. Berry [6] considered the limit $|\mathbf{V}|T$ fixed, $T \rightarrow \infty$, where T is the time for completion of a cycle in parameter space. However, one may also take T fixed and finite, so that the area enclosed by the cyclic orbit becomes small in the limit of small velocity. In that case, assuming that the fast variables (such as a large but slowly precessing spin) are of macroscopic or classical magnitude, it is straightforward to show that the (quantum) scalar potential contribution to the action is $\propto \hbar^2 T$, that of the induced Berry flux is $\propto V^2 T^2$, and the quadratic contribution to be discussed below is $\propto V^2 T$. Thus for fixed T the inertial term and the Berry term are comparable, and clearly both should be included in a consistent scheme. Clearly if the fast variables are quantum in scale, then all three terms should be taken into account.

Second-order terms in velocity have the same form as conventional kinetic energies, so that if the slow variables specify coordinates of a massive particle, there already is such a term present. If there is no such primitive quadratic term, but one wishes to identify the slow parameters as collective variables, then it is essential to obtain from the adiabatic evolution itself precisely such a kinetic term. Even if there were a primitive contribution, one should expect it to be supplemented by an induced contribution.

Berry [6] discussed the systematic expansion of the total phase associated with an arbitrarily slow cyclic motion in powers of the velocity. He observed that, unlike the case of ordinary time-independent perturbation theory for a finite system, the adiabatic expansion is an asymptotic series, rather than a Taylor series with a finite radius of convergence: There is an exponentially small probability of nonadiabatic jumps, and this implies an essential singularity at zero velocity. Nevertheless, for sufficiently small velocity, the first few terms of the series can give an accurate description of the evolution. These considerations imply that for a self-contained dynamics, one at least should go to second order in the expansion, so as to determine completely the inertia tensor of the slow degrees of freedom: The inertia is a prerequisite for obtaining observable consequences from the vector and scalar potentials.

III. INDUCED INERTIA, THE FINAL PIECE IN NEWTONIAN ADIABATICS

Consider the general problem specified by a time-dependent Hamiltonian,

$$H(t)|\psi\rangle = i\hbar(d|\psi\rangle/dt).$$
⁽²⁾

If the rate of change for H is slow (and its eigenvalues do not change), then in the vicinity of any time t_0 we may write

$$|\psi(t)\rangle = U(t)|\psi'(t)\rangle,\tag{3}$$

where one has by definition $U(t_0)=1$, and $U^{\dagger}HU$ is timeindependent. This gives a familiar time-independent perturbation theory problem to determine $|\psi'(t_0)\rangle$. The equivalent "perturbed" Hamiltonian is

$$H' = H(t_0) + \mathbf{V} \cdot \mathbf{P},\tag{4}$$

where the matrix elements of the operators P_i are defined by

$$\langle m|P_i|n\rangle = -i\hbar\langle m|\partial_{\chi i}|n\rangle, \tag{5}$$

with $n \neq m$, and $V^i = \partial_i X^i$, the (slow) velocity of motion in the space of parameters X^i .

To first order in **V**, the wave function is given by

$$|\psi(t_0)\rangle = |\psi'(t_o)\rangle = |n\rangle + \sum \alpha_m |m\rangle, \tag{6}$$

with again $m \neq n$, and

$$\alpha_m = \mathbf{V} \cdot \langle m | \mathbf{P} | n \rangle / (E_n - E_m). \tag{7}$$

This means that the instantaneous eigenfunction to first order in **V** is **not** simply the eigenfunction of the instantaneous Hamiltonian. What we want to know is the shift in energy to second order in **V** implied by this shift in the wave function. We have arrived at the crucial juncture in the calculation. Although ψ is not an eigenstate of *H*, it is *H* which appears in the Schrödinger equation, and therefore the desired energy must be computed from the expectation value $\langle \psi | H(t_0) | \psi \rangle$,

$$\Delta E_n = \sum |\alpha_m|^2 (E_m - E_n), \qquad (8)$$

which evidently is positive if $|n\rangle$ is the ground state with respect to the fast variables. Using the definition of α_m , one may rewrite the energy shift in a suggestive form,

$$\Delta E_n = \sum_m |\langle m | \mathbf{V} \cdot \mathbf{P} | n \rangle|^2 / (E_m - E_n).$$
(9)

This should look very familiar, as it differs only in sign from the well-known expression for the second-order energy shift in conventional time-independent perturbation theory. Just as the negative sign in the latter case may be understood as a consequence of level repulsion by mixing potentials, so the positive sign here makes excellent physical sense: If one "wobbles" the slow parameters for a system in its instantaneous ground state with respect to fast variables, that wobbling can only raise the energy. It might be interesting to study the relationship between the different behaviors for time-independent perturbation theory and adiabatic perturbation theory of the shifts in neighboring energy levels (repulsive or attractive) and the behaviors of the corresponding series (convergent or divergent). Let us rewrite the expression one more time, as

$$\Delta E_n = \mathcal{I}_{ij} V^i V^j / 2, \qquad (10)$$

where this implies

$$\mathcal{I}_{ij} = 2 \operatorname{Re} \sum_{m, m \neq n} n |P_i| m \langle m | P_j | n \rangle / (E_m - E_n).$$
(11)

The inertia tensor \mathcal{I}_{ii} plays the role of a metric in the space of coordinates X^i , as the principle of least action implies that in the absence of explicit forces the motion follows a geodesic path as determined by \mathcal{I} . Of course, if there were also a primitive quadratic term in the velocities, then it would be the sum of the primitive and the induced contributions to the inertia which would constitute the metric. Equation (11) represents the key result. It implies, as asserted earlier, that for motion of an instantaneous ground state, the inertia tensor or spatial metric receives an intrinsically positive contribution. Near a crossing point of two instantaneous energy levels, where of course the adiabatic approximation must fail, the Berry vector potential diverges as the inverse first power of distance from the crossing, while the scalar potential diverges as the inverse second power [7]. Because of the extra energy denominator, the inertia tensor diverges as the inverse third power (slowing the response to applied forces).

All these effects combine to protect the ground state from too close an approach to any such crossing, giving a selfenforcement of the adiabatic approximation. On the other hand, for the higher of two states near a level crossing, the vector and scalar potentials continue to give positive or repulsive $1/r^2$ effects, but the induced contribution to the inertia now is negative, by itself generating what with repulsive forces becomes an acceleration towards the level crossing, and therefore a possibility of breakdown rather than preservation of adiabaticity.

The above discussion is quantum-mechanical, whether the slow variables are collective or are those of massive "elementary" particles. When adiabatic motion is associated with classical collective variables, for example degrees of freedom characterizing a soliton configuration of classical fields, then there is a well-known procedure for computing the kinetic energy in terms of the classical action for the fields and identifying this kinetic energy as a quadratic form in the time derivatives of the collective coordinates [8]. This gives a nice continuity between quantum and classical treatments of such phenomena. In both regimes, of course, the inertia is intrinsically positive if the associated structure for zero velocity is stable.

An illustration of the quantum procedure for the case of collective coordinates is the Inglis cranking model, introduced to describe the low-lying rotational bands in deformed nuclei [9]. The general formula (11) was evaluated for slow rotation of the symmetry axis of a spheroidal harmonicoscillator potential containing a Fermi gas of nucleons, with the result that the moment of inertia takes its rigid-body value. Later work on the collective model of nuclei introduced an attractive pairing force between nucleons, yielding substantially lower and more phenomenologically acceptable values of this inertia [10]. A systematic algebraic formulation of the Inglis cranking model was described by Lipkin, de Shalit, and Talmi [11], who obtained a refinement taking account of the "center-of-mass" correction—the orientation of the nuclear deformation axis is redundant with the full set of coordinates of all the individual nucleons. This of course becomes irrelevant if the slowly varying coordinate is associated with an elementary particle of large mass.

A case of the latter sort was treated by Littlejohn and Weigert (LW) [12], who pursued further the considerations of Aharonov and Stern [5] on a neutral particle with spin (and parallel magnetic moment) moving through a region in which a strong magnetic field varies slowly both in magnitude and direction. LW found a term in the energy proportional to the square of the momentum, in addition to the usual kinetic energy of the massive particle. Thus the kinetic energy is changed, though only slightly, from the case without the variable field. Let us use Eq. (11) to obtain the LW result. In terms of the particle coordinates, the operator we need is

$$\delta H = (\mathbf{V} \cdot \boldsymbol{\nabla}) \hat{\mathbf{B}} \cdot \mathbf{S}, \qquad (12)$$

where **V** is the particle velocity, $\hat{\mathbf{B}}$ is a unit vector in the direction of the magnetic field **B**, and **S** is the particle spin. Substituting into the formula (9), for a state labeled by spin projection *m* onto the direction of **B**, we obtain

$$\Delta E(m) = [(\mathbf{V} \cdot \mathbf{\nabla}) \hat{\mathbf{B}}]^2 (1/gB)$$
$$\times [|\langle m-1|S_x|m\rangle|^2 - |\langle m+1|S_x|m\rangle|^2], \quad (13)$$

where the bracket has the value $\hbar^2 m/2$, and -gBm is the interaction energy of the spin with the magnetic field. This expression is identical to that obtained by LW, except for the sign. In their analysis, the sign of the extra term is negative for positive *m*. That apparent discrepancy has a trivial explanation: Their expansion uses momentum rather than velocity, and because the mass appears in the denominator when kinetic energy is expressed in terms of momentum, an increase in effective mass becomes a negative contribution to the energy expressed in terms of momentum. They, like Berry in his discussion of asymptotic expansions in powers of the velocity [6], do not discuss explicitly the significance of the sign of the quadratic energy term. Therefore, we may consider the argument here as explaining in terms of basic principles a sign which was an issue of no special concern in their work.

For Inglis, of course, the sign was crucial, as a net negative moment of inertia yields an instability against increase of angular momentum, and is physically unacceptable as well as clearly unrelated to experiment. Thus he obtained the correct sign because he knew what it should be, and tacitly reversed the sign of the standard, negative, stationary-state second-order perturbation energy. The arbitrariness was noted and corrected afterwards, in a manner outlined by Goeppert-Mayer [13]. Actually the result mentioned earlier of a rigid-body value for the inertia only was worked out explicitly in [13]. This discussion makes clear that the "new term" of LW represents an independent discovery of induced inertia, nearly 40 years after it was introduced by Inglis. Perhaps because they did not identify this effect as induced inertia, they did not use it also to modify the Provost-Vallée scalar potential, as is advocated in the next section of the present paper.

A simple application of induced inertia comes from the almost trivial problem of the free motion of a hydrogen atom. By Galilean invariance, the kinetic energy is $K=(M + m)V^2/2$, where the two masses are those of the proton and the electron, respectively. In the adiabatic formulation, the first term is primitive, and the second must be induced by the motion of the center of the Coulomb potential influencing the electron. According to the general formula (11), this gives

$$m\delta_{ij} = 2\hbar^2 \operatorname{Re} \sum \langle -i\partial_{X^i}(n)|m\rangle\langle m| - i\partial_{X^j}|n\rangle/(E_m - E_n),$$
(14)

where X_i is the proton coordinate. Because of translation invariance, we may substitute for the gradient with respect to the proton coordinate the negative gradient with respect to the electron coordinate. Consequently, with a little rearrangement the relation may be expressed in the form

$$\delta_{ij} = (2m/\hbar^2) \sum \langle n|x^i|m\rangle \langle m|x^j|n\rangle (E_m - E_n).$$
(15)

This is nothing but the well-known Thomas-Reiche-Kuhn energy-weighted sum rule for electric dipole transitions, the ancestor of a host of sum rules extending all the way to high-energy physics in the the analysis of phenomena such as deep inelastic lepton scattering. The TRK sum rule is easily derived by elementary commutation relations of the position coordinate operator with the Hamiltonian and the momentum. For an atom with Z electrons, the left-hand side of the sum rule would be multiplied by Z, so that it counts the number of constituents of the atom contributing to photoexcitation [14].

The analysis presented above indeed rounds out the picture of induced geometry associated with adiabatic interactions, adding to gauge geometry and Hilbert space geometry the even more venerable geometry of ordinary coordinate space. In general, all these geometrical effects may appear in any system. They all do in the LW case, but even models of collective nuclear rotation include examples with a nonzero projection of the nuclear angular momentum onto the deformation axis, and hence a Berry vector potential. (There is also a scalar potential, but it is independent of the slow variables, and therefore at best could be observed in transitions between instantaneous fast-variable eigenstates.) Formally, the calculation of \mathcal{I} appears to be higher order in the slow velocity than the (linear) construction of the Berry vector potential. However, as the effect of that potential on motion of the slow particles requires understanding of the kinetic energy for its manifestation, the second-order terms surely are necessary for a self-contained description of the geometry of adiabatic phenomena.

Having acknowledged this principle, we still should note a quantitative aspect which is so important that it is tantamount to a qualitative distinction: Unless the entire inertia tensor is generated adiabatically, the adiabatic modification of the metric may be unobservably small, being clearly of higher order in its effects than the Berry vector potential. For example, in the LW case, if the spinning particle has approximately a Dirac gyromagnetic ratio, then the induced shift in the metric will be

$$\delta \mathcal{I}/\mathcal{I} = \mathcal{O}(2\pi (\nabla \hat{\mathbf{B}})^2 / |\mathbf{B}|), \qquad (16)$$

where here $|\mathbf{B}|$ is measured in units of an Aharonov-Bohm quantum of flux. This quantity inevitably is much smaller than unity for any reasonable setup. That may well be the reason why its existence was overlooked for so long before LW. An open question is whether there exist systems where the primitive and the induced contributions to the inertia are comparable, so that both must be taken into account for an accurate description of the motion. A promising place to look for such comparable contributions might be the motion of quasiparticle excitations in a strongly correlated medium. Whatever the general answer to the question may be, the induction in adiabatic processes of all conceivably relevant types of geometry (including ordinary spatial geometry) appears inescapable.

IV. FULL NEWTONIAN ADIABATIC HAMILTONIAN

Let us conclude with a comprehensive scheme for computation of adiabatic quantum dynamics through second order in velocity. To weave together the discussion here with previously identified elements, one begins with the computation of the induced inertia, and uses the total $\tilde{\mathcal{I}} = \mathcal{I}_{\text{primitive}}$ $+\mathcal{I}_{induced}$ to compute the inverse inertia $\tilde{Q}=\tilde{\mathcal{I}}^{-1}$. An interesting point here is that in some cases there may be ambiguity about what is primitive and what is induced inertia (for example, one might choose to redefine fast variables as describing, instead of motion with respect to a fixed frame, rather motion with respect to slow variables), but the sum should be unambiguous. In terms of adiabatic perturbations, this statement seems quite natural: The primitive inertia is simply an explicit (diagonal) second-order perturbation of the zerovelocity Hamiltonian, while the induced inertia comes from iterating a first-order off-diagonal perturbation. By changing choices of basis, one may shuffle contributions to the second-order diagonal part between primitive and induced.

The total adiabatic Hamiltonian in the context of the newer (induced-potential) stream of adiabatics was presented by Berry [15],

$$H_{eff} = V_{B-O} + (P - A_B)_i Q_{ij} (P - A_B)_j / 2 + \hbar^2 g_{ij} Q_{ij} / 2,$$
(17)

where V_{B-O} is the Born-Oppenheimer potential, including all potential energies and also the kinetic energies corresponding to fast degrees of freedom, averaged over those fast variables for specified values of the slow variables. The vector potential \mathbf{A}_B is the connection associated with the Berry phase, which to this point in the present paper was kept hidden in the path-dependent transformation factor U(t). The scalar po-

tential also comes from gradients of the path-dependent U.

The effect of including induced inertia should be obvious at this point: One rewrites Eq. (17) as

$$H_{eff} = V_{B-O} + (P - A_B)_i \tilde{Q}_{ij} (P - A_B)_j / 2 + \hbar^2 g_{ij} \tilde{Q}_{ij} / 2,$$
(18)

having exchanged the primitive and convention-dependent \mathcal{I} for the complete quantity $\tilde{\mathcal{I}}$, hence replacing Q by $\tilde{Q} = \tilde{\mathcal{I}}^{-1}$.

Thus the Newtonian adiabatic Hamiltonian is determined by the ordinary geometry (both primitive and induced) of the space of slow parameters, as well as by the induced or geometric vector and scalar potentials, all in a coherent and consistent pattern.

V. OUTLOOK

While it is worth recording the complete Newtonian adiabatic "package," the really interesting question is whether this package could provide any new insights into physical systems, and thus be something more than a mere catalogue entry. The best prospect for such a development may be in analysis of strongly correlated systems, their ground states, and simple excitations. Here is an analogy: In classical electrodynamics, the hydrogen atom would be unstable against collapse, but quantum effects stabilize its ground state. This makes the Newtonian approximation quite accurate for the ground-state structure.

Similarly, perhaps the exponentially suppressed jumps in adiabatic dynamics would simply disappear if one were using the adiabatic approximation to describe a stable structure, such as a many-body ground state, or a state built on that ground state with some fixed number of quasiparticles, each carrying a conserved charge. Again, the evident stability of these configurations suggests that the Newtonian description may become accurate, once one treats the adiabatic parameters as quantum variables. In particular, for such an enterprise in the case of the fractional quantum Hall effect, where with interactions neglected there is no inertia, induced inertia clearly becomes essential to the description.

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