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Allan N. Kaufman

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THE LIE TRANSFORM: A NEW APPROACH TO CLASSICAL PERTURBATION THEORY

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ABSTRACT

A survey is presented of the pre-history, discovery, development, and applications of the Lie transform in classical dynamics, with particular attention to its utility in plasma physics.

"Give the world the Lie [transform]."¹

THE AWKWARDNESS OF CLASSICAL-CLASSICAL PERTURBATION THEORY

The classical (pre-Lie) approach² to perturbation theory in classical ($\hbar = 0$) Hamiltonian systems proceeds by the use of a generating function to perform a canonical transformation from old variables q, p to new variables Q, P . This function depends on both old and new variables, e.g., $S(q, P, t)$; as a consequence, the transformation itself, e.g.

$$Q(q, P, t) = \partial S(q, P, t) / \partial P, \quad (1)$$

appears in mixed form, whereas what we need is $Q(q, p, t)$, i.e., the new variables in terms of the old, or vice versa. Again, the relation between the new Hamiltonian $K(Q, P, t)$ and the old Hamiltonian $h(q, p, t)$ appears in a mixed representation:

$$K(Q, P, t) = h(q, p, t) + \partial S(q, P, t) / \partial t; \quad (2)$$

it would be preferable to have a relation directly between the functions K and h , rather than between their values at corresponding points in phase space.

If the old Hamiltonian h is expressible as a power series in a small perturbation parameter ϵ , it is reasonably straightforward to obtain perturbation expansions for S and K . However, even in order ϵ^2 , these expressions are lengthy, and no pattern is manifest. To order ϵ^3 , not only is the amount of algebra disheartening, but any relationships which reside in the physics are hidden. Such relationships would provide new insights and results.

THE SUPERIORITY OF CLASSICAL-QUANTUM PERTURBATION THEORY

Even before the development of the powerful perturbation techniques of quantum electrodynamics in the fifties, quantum theory utilized a systematic perturbation theory³ which led to a set of well-known "rules". The superiority of these rules was so evident,

that it became quite popular in plasma physics to derive purely classical results by quantizing the system and letting $\hbar \rightarrow 0$ in the result. This approach was widely used both for Vlasov (collisionless) plasmas and for plasmas with discreteness (collisional) effects.⁴⁻⁷

Yet it was disconcerting to see that the most expeditious route to a classical result was via a detour through quantum theory. One had the feeling that a classical formalism equal in power to the quantum one was waiting to be discovered.

EVIDENCE FOR THE EXISTENCE OF A BETTER CLASSICAL FORMALISM

Several years ago, S. Johnston and I examined the problem of the interaction of three electromagnetic modes in an arbitrarily nonuniform Vlasov plasma. On the basis of experience with related problems, we were led to the oscillation-center theory, a classical (pre-Lie) canonical formalism developed earlier by R. Dewar⁸ for the study of quasi-linear diffusion, and applied by Johnston⁹ to the problem of induced scattering. After some fifty pages of algebra, utilizing the methods of conventional classical perturbation theory, we succeeded in obtaining a remarkably concise expression¹⁰ for the three-wave coupling coefficient in terms of Poisson brackets (PB) of the single-particle perturbation Hamiltonian and its convective time-integral along unperturbed orbits. In the mixed representation (q, P), these PB did not appear naturally, for they are defined only in terms of conjugate variables. Rather, guided by esthetic principles, we had to extract them from the algebraic mess, and then show that all of the residue cancelled.

The beauty of the concise form thus obtained then led us to a new insight¹¹ as to the essence of the wave coupling and of the Manley-Rowe relations governing such interactions. Thus, it appeared that the interaction Hamiltonian of the three waves was simply the trilinear contribution to the single-particle (new) Hamiltonian K , summed over all the (non-resonant) particles. The Manley-Rowe conditions followed trivially from this expression.

It was then clear to us that a far simpler method must exist for obtaining such a simple result, and we struggled to find it.

THE DEVELOPMENT OF A BETTER CLASSICAL FORMALISM

This "struggle" was remarkably short, from our point of view, for the desired formalism had already been discovered by workers in celestial mechanics (Hori¹², Deprit¹³, Kamel¹⁴, and others), and had even been very clearly presented in the textbook by Nayfeh¹⁵. This formalism was based on the Lie transform, and its hallmark was the PB, as desired.

It had been used and generalized by Dragt and Finn¹⁶ for the study of magnetic moment invariance in a dipole field. More re-

cently, it has been applied by Howland¹⁷ for Kolmogorov's superconvergent perturbation theory, and by McNamara¹⁸ for the treatment of higher-order resonances.

FURTHER DEVELOPMENT OF THE LIE TRANSFORM

The power and beauty of the Lie formalism became even more evident in the non-perturbative Vlasov formulation developed by Dewar¹⁹, who then applied it to renormalized plasma turbulence.

In essence, the idea is to transform the phase space $p, q \equiv \underline{z} \rightarrow \underline{Z}$ by means of a generating function $S(\underline{z}, t)$, which depends only on the old variables; hence it can appear in PB. The function S is chosen so as to simplify the form of the new Hamiltonian K . The old and new Hamiltonians, h and K , each produce the time-evolution of the corresponding phase-space densities f and F , by the respective Liouville equations:

$$\frac{\partial f}{\partial t} + \{f, h\} = 0, \quad \frac{\partial F}{\partial t} + \{F, K\} = 0 \quad (3)$$

These densities are equal at corresponding points:

$$f(\underline{z}; t) = F(\underline{Z}; t). \quad (4)$$

Now if K is a much simpler function than h , the evolution of F is correspondingly simpler than that of f . This simplification is accomplished by proper selection of S , which then has an evolution equation of its own to satisfy. Thus instead of one difficult equation for f , one now has two simpler equations for F and S . The physical content is of course the same, but it may be more apparent in the new variables. In the next sections, we demonstrate these ideas more explicitly.

Older averaging methods^{20,21} also succeeded in simplifying the Hamiltonian. But it appeared that information was lost in the averaging process; and it was not clear (to us at least) how to proceed to higher order. In the Lie method, nothing is lost: what has disappeared from the Hamiltonian is stored in the generating function. Also, the procedure for successive orders appears to be well specified.

THE LIE FORMALISM

"After all, what is a Lie [transform]? 'Tis but the truth in masquerade".²²

A full discussion of the mathematical apparatus has been prepared in a "Lie handbook"²³ by J. Cary. Here we quote the relevant formulae. We begin by associating, with any phase function $A(\underline{z})$, a Lie operator $\tilde{A}$, defined by

$$\tilde{A} \equiv \{A(\underline{z}), \cdot\} \quad (5)$$

$$\equiv \sum_{\mu} \frac{\partial A}{\partial q_{\mu}} \frac{\partial}{\partial p_{\mu}} - \frac{\partial A}{\partial p_{\mu}} \frac{\partial}{\partial q_{\mu}}.$$

For example, the momentum p has the Lie operator $\tilde{p} = -\partial/\partial q$. This is strikingly similar to the association in quantum theory of a Hermitian operator with a classical phase function ($p \rightarrow -i\hbar\partial/\partial q$).

Consider now any phase function, possibly time-dependent and depending also on the perturbation parameter ϵ : $S(\underline{z}, t, \epsilon)$. The corresponding Lie operator $\tilde{S}$ then generates a transformation operator $T(\epsilon)$ by

$$\partial T(\epsilon)/\partial \epsilon = \tilde{S}(\epsilon) T(\epsilon). \quad (6)$$

The latter operator effects a canonical transformation:

$$\underline{Z}(\underline{z}, t, \epsilon) = T(\epsilon) \underline{z}. \quad (7)$$

Corresponding phase functions, e.g., f and F in Eq. (4), are related by the inverse of T :

$$F = T^{-1} f \quad (8)$$

$$\text{or } f = T F$$

The dynamical variables and densities evolve according to the respective Hamiltonians h and K which are related by

$$\frac{\partial K}{\partial \epsilon} = \frac{\partial h}{\partial \epsilon} - T^{-1}(\epsilon) \frac{\partial S}{\partial t}, \quad (9)$$

with

$$h = TH. \quad (10)$$

PERTURBATION EXPANSION

We implement this bare outline with a perturbation expansion:

$$h(\epsilon) = h_0 + \epsilon h_1 + \epsilon^2 h_2 + \dots \quad (11)$$

$$\epsilon S(\epsilon) = 0 + \epsilon S_1 + \epsilon^2 S_2 + \dots$$

Substituting into Eq. (6), we obtain

$$T(\epsilon) = 1 + \epsilon \tilde{S}_1 + \frac{1}{2} \epsilon^2 (\tilde{S}_1^2 + \tilde{S}_2) + \dots \quad (12)$$

We then use Eq. (10) to find $H(\epsilon)$, and Eq. (9) to find $K(\epsilon)$:

$$K(\epsilon) = h_0 + \epsilon K_1 + \epsilon^2 K_2 + \dots \quad (13)$$

In particular, we have

$$K_1 = h_1 - \dot{S}_1, \quad (14)$$

where the dot implies a convective derivative along unperturbed orbits:

$$\dot{A} \equiv \partial A / \partial t + \{A, h_0\}. \quad (15)$$

Now we choose S_1 so as to make K_1 vanish. By Eq. (14):

$$\dot{S}_1 = h_1. \quad (16)$$

We then proceed to K_2 , finding

$$K_2 = h_2 - \frac{1}{2} \dot{S}_2 - \frac{1}{2} \ddot{S}_1 h_1. \quad (17)$$

Suppose h_2 vanishes in the problem studied; we then choose $S_2 \equiv 0$, and obtain

$$K_2 = -\frac{1}{2} \ddot{S}_1 h_1, \quad (18)$$

with S_1 given by (16). One may easily proceed to third order, obtaining

$$K_3 = \frac{1}{3} \ddot{S}_1^2 h_1; \quad (19)$$

this neat result required lengthy algebra¹⁰ by the old method.

OSCILLATION CENTER THEORY

The low frequency force produced non-linearly by a high frequency field has been known for some time²⁴. Its current name is "ponderomotive force" (PMF), and the object on which it acts is called the "oscillation center" (OC). The particle oscillates at high frequency about the orbit of the OC. The concept is quite analogous to the gyration of a particle about its guiding center in a magnetic field.

The PMF concept has been very useful in the study of r.f. confinement²⁴, quasi-static density perturbations due to amplitude

modulation of high-frequency waves²⁵, and parametric instabilities²⁶. Its meaning, however, appeared nebulous until Dewar derived it from a canonical transformation⁸. His pre-Lie formalism led to lengthy algebraic calculations, and now has been superseded in turn by the Lie method, which is astonishingly simple.

Consider a monochromatic electric field

$$\underline{E}(\underline{x}, t) = \tilde{\underline{E}}(\underline{x}) \exp(-i\omega t) + \text{c.c.} \quad (20)$$

acting on a particle in a static field represented by $h_0(\underline{z})$. The linear perturbation in the Hamiltonian is

$$h_1(\underline{z}, t) = -c^{-1} \int d^3x \, \underline{j}(\underline{x}|\underline{z}) \cdot \underline{A}(\underline{x}, t), \quad (21)$$

where $\underline{j}(\underline{x}|\underline{z})$ is the current density at $\underline{x}$ due to a particle at $\underline{z}$, and $\underline{A}$ is the vector potential representation of $\underline{E}$. We insert (21) into (16) and (18), immediately obtaining a formula for the second-order OC Hamiltonian K_2 , in terms of PB of the phase function

$\underline{j}(\underline{x}|\underline{z})$ (at two positions $\underline{x}, \underline{x}'$). We then recognize this PB as having appeared in the Kubo-type formula for the linear Vlasov susceptibility $\chi(\underline{x}, \underline{x}'; \omega)$ of an unperturbed distribution $f(\underline{z})$, representing its linear current response to the field (20). Comparing the expressions for K_2 and χ , we read off the remarkable relation²⁸

$$K_2(\underline{z}) = - (4\pi)^{-1} \int d^3x \int d^3x' \, \tilde{\underline{E}}^*(\underline{x}) \cdot \tilde{\underline{E}}(\underline{x}') : \delta \underline{x}'(\underline{x}, \underline{x}'; \omega) / \delta f(\underline{z}). \quad (22)$$

Hence the lengthy calculations of the past, to deduce second-order forces, are no longer necessary: all one needs is the (generally known) linear response kernel. (Note that $\underline{x}$ is a linear functional of f , so that K_2 is of course independent of f . The prime on $\underline{x}$ denotes Hermitian, or non-resonant, part. To include the resonant response is far more difficult²⁹.)

Relation (22) may be considered as a generalization of the well-known expression³⁰ for the second-order free energy of a dielectric in thermal equilibrium in a static electric field. However, it has a fascinating new feature, namely a momentum dependence, whereas older versions of K_2 ignored this feature.

Suppose that the unperturbed Hamiltonian is q -independent: $h_0(\underline{p})$. Then the OC Hamiltonian reads

$$K(\underline{z}) = h_0(\underline{p}) + K_2(\underline{q}, \underline{p}), \quad (23)$$

to second order. Note that $\underline{z}$ here represents the OC variables. Its dynamics are given by

$$\dot{\underline{p}} = -\partial K/\partial \underline{q} = -\partial K_2/\partial \underline{q}, \quad (24)$$

$$\dot{\underline{q}} = \partial K/\partial \underline{p} = \partial h_0/\partial \underline{p} + \partial K_2/\partial \underline{p}. \quad (25)$$

Eq. (24) states that the OC momentum is acted on by the PMF ($-\partial K_2/\partial \underline{q}$), which generalizes the standard formula for the latter. Eq. (25) distinguishes between the OC velocity $\dot{\underline{q}}$ and the OC momentum $\underline{p}$ (for $h_0 = p^2/2$, $m = 1$). The difference, $\dot{\underline{q}} - \underline{p} = \partial K_2/\partial \underline{p}$, represents the shift in the particle's average velocity, due to its being in the wave field; summed over particles, it represents the particle contribution to the wave momentum³¹.

Another consequence of momentum-dependence in K_2 is that the PMF mimics a magnetic field³². Namely, if we expand K_2 to first order in $\underline{p}$:

$$K_2(\underline{q}, \underline{p}) \equiv e\phi(\underline{q}) - ec^{-1}\underline{p} \cdot \underline{A}(\underline{q}) + O(p^2), \quad (26)$$

the OC equation of motion reads ($m = 1$)

$$\dot{\underline{q}} = e(\underline{E} + c^{-1}\dot{\underline{q}} \times \underline{B}), \quad (27)$$

where the pseudo-potentials ϕ , $\underline{A}$ are defined by Eq. (26), and

$$\underline{B}(\underline{q}) \equiv (\partial/\partial \underline{q}) \times \underline{A}(\underline{q}), \quad (28)$$

$$\underline{E}(\underline{q}) \equiv -\partial\phi/\partial \underline{q} - c^{-1}\partial \underline{A}/\partial t.$$

The pseudofields $\underline{B}$ and $\underline{E}$ satisfy a Faraday law:

$$c \nabla \times \underline{E} = -\partial \underline{B}/\partial t. \quad (29)$$

All these quantities ϕ , $\underline{A}$, $\underline{B}$, $\underline{E}$ are quadratic in the amplitude $\tilde{\underline{E}}$ of the true field.

If the unperturbed motion is in a true magneto-static field $\underline{B}_0$, the interpretation is different, but related. A dependence of K_2 on gyromomentum p_g implies a nonlinear shift in the OC's gyrofrequency $\Omega \equiv \dot{\phi}_g = \partial K/\partial p_g = \partial h_0/\partial p_g + \partial K_2/\partial p_g \equiv \Omega_0 + \delta\Omega$. Since $\Omega_0 = eB_0/mc$, the gyrofrequency shift $\delta\Omega$ may again be interpreted as being due to a magnetic pseudofield $\underline{B}$, quadratic in wave amplitude $\tilde{\underline{E}}$.

SELF-CONSISTENT FIELDS

To determine the Maxwell field $\underline{E}(\underline{x}, t)$ self-consistently, we need the current density

$$\underline{j}(\underline{x}, t) = \int d^6z \underline{j}(\underline{x}|\underline{z}) f(\underline{z}; t) \quad (30)$$

as a source in the Maxwell equations (summation over species implied). It is essential to recognize that the OC current

$$\underline{j}^{OC}(\underline{x}, t) \equiv \int d^6z \underline{j}(\underline{x}|\underline{z}) F(\underline{z}; t) \quad (31)$$

constitutes only part of (30). To see their relation, we substitute (8) into (30):

$$\begin{aligned} \underline{j}(\underline{x}, t) &= \int d^6z \underline{j}(\underline{x}|\underline{z}) TF(\underline{z}, t) \\ &= \int d^6z F(\underline{z}, t) T^{-1} \underline{j}(\underline{x}|\underline{z}) \\ &\equiv \int d^6z F(\underline{z}, t) \underline{j}(\underline{x}|\underline{z}). \end{aligned} \quad (32)$$

We interpret $\underline{j}(\underline{x}|\underline{z})$ as the current at $\underline{x}$ due to a particle whose OC is at $\underline{z}$. Thus $\underline{j}(\underline{x}|\underline{z})$ consists of the "bare" part $\underline{j}(\underline{x}|\underline{z})$, from the OC, and the "polarization" correction $(T^{-1} - 1)\underline{j}(\underline{x}|\underline{z})$, due to the particle's jitter motion. As we know from guiding center theory these separate parts sometimes cancel!

Still guided by that analogy, we expect that the situation for charge density is simpler. Indeed, we find that the OC charge density $\rho(\underline{x}|\underline{z})$ and the slow part of the true charge density $T^{-1}\rho(\underline{x}|\underline{z})$ differ only by order $(\delta r/L)^2$, where $\delta r \sim eE/m\omega^2$ is the first-order displacement due to the wave field, and L is the scale length of the wave amplitude modulation. Hence, we may normally neglect the polarization charge density and use

$$\rho(\underline{x}, t) = \int d^6z F(\underline{z}, t) \rho(\underline{x}|\underline{z}) \quad (33)$$

for the slow charge density source in the slow Poisson equation.

On the basis of such considerations, we have recently derived a simple formula³³ for the quasi-static, quasi-neutral density perturbation caused by spatial modulation of a magnetoplasma wave of arbitrary polarization:

$$\delta n(\underline{x}) = - (4\pi)^{-1} (T_e + T_i)^{-1} [|\tilde{\underline{E}}(\underline{x})|^2 - |\tilde{\underline{B}}(\underline{x})|^2]. \quad (34)$$

This formula (within its range of validity) predicts that a "magnetic" wave ($B > E$) leads to density enhancement, in contrast to the well-known density depression produced by an "electric" wave ($E > B$). Thus, a magnetic wave may contribute to plasma confinement³⁴.

CONCLUSION

On the basis of the results obtained only in the last few years, the Lie approach to classical dynamics would appear to be most promising. It sheds new light on old results, reveals previously unobserved relationships, and leads to new results by extremely economical means. Because the Lie transform preserves Poisson brackets, it is particularly successful in dealing with Hamiltonian systems. Its relation to Lagrangian methods^{21,35-37} has yet to be investigated. Finally, one may hope that dissipative systems³⁸ may be treated by a variant of the Lie method.

In summary, "a Lie [transform] is ... an ever-present help in time of need".³⁹

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