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Geometrical mechanics for particles in dissipative systems

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The quantum-mechanical problem of motion of particles in dissipative systems is considered. Ray theory is applied to cases where systems change slowly in space and time. Although complex momentum and energy are necessary to describe the physical situation, real space-time paths and group velocity are imposed. The analogy to geometrical optics in absorbing systems is striking and a nonrelativistic as well as relativistic treatment is possible.

INTRODUCTION

The formulation of geometrical mechanics by Synge[1] and his extended Fermat principle for lossless systems have inspired the study of real space-time rays in absorbing media.[2,3] This approach serves as an alternative to other real space-time rays formalisms, especially Suchy's[4-6] approach. The latter has been criticized by Bennett to be nonunique.[6-8] But, even though this objection is clarified,[9,10] Suchy's formalism for ray tracing is very difficult to implement because a bundle of rays must be traced simultaneously.[4,9] The present formalism, on the other hand, facilitates the tracing of individual real rays. The feasibility of the model for machine computations of ray tracing in an absorbing ionosphere has been demonstrated recently.[11] There exist also formalisms which use complex space and time concepts; for further references see the above-cited studies.

The above-mentioned studies have been motivated by problems in the realm of electromagnetic wave propagation, especially for ionospheric applications. The initial analogy of geometrical mechanics and geometrical optics is now revisited, with the aim of understanding the motion of particles in a general class of dissipative systems. This is done here by using the theory of real rays in dissipative systems.[2,3]

The formulation of classical mechanics in a general way which includes dissipation is an old problem whose difficulties are notorious. Some linkage to the literature is provided by mentioning the works of Denman,[12] van der Vaart,[13] Gossick,[14] Denman and Kupferman,[15] and Denman and Buch,[16] who essentially strive to define a Lagrangian or Hamiltonian formalism for nonconservative systems. Quite naturally this led researchers to consider quantum-mechanical problems in dissipative systems. See Kostin,[17] Buch and Denman,[18] and Hasse.[19] However, as the latter mentions, the general problem of quantal dissipative systems is still open. In any case, the above-mentioned studies do not elaborate on the problem of ray tracing in the broad class of media considered here.

Without analyzing specific microscopic models, dissipation is admitted into the present formalism by allowing complex momentum- and energy-dependent functions, slowly varying in space and time. The introduction of complex potentials into quantum-mechanical problems is well known, especially in nucleon-nucleon interactions where energy-dependent potentials are mandatory. This optical potential or optical model, as it is called, can be found in any general survey on nuclear physics; see for example Lock and Measday,[20] who cite recent specialized studies by Hodgson[21] and Austern.[22] In the present case, although momentum and energy are complex, the group velocity of the particles is real, hence complex space-time coordinates are avoided. Similarly to the results in nuclear physics[21,22] and unlike Buch and Denman,[18] the present analysis reveals how the probability of the particles is dissipated as they move along the real trajectories.

Finally some simple examples are considered to demonstrate the theory. An appendix gives a simplified derivation of the rigorous ray formalism, derived elsewhere.[3]

HOMOGENEOUS TIME-INVARIANT SPACE

First we consider the problem of a particle moving in a homogeneous time-invariant isotropic space. The appropriate wave-mechanical equation must be given. For the nonrelativistic case Schrödinger's equation

$$\left(-\frac{\hbar^2}{2m}\nabla^2+V-i\hbar\frac{\partial}{\partial t}\right)\Psi(\bar{x},t)=0 \qquad (1)$$

is chosen, where V cannot be a function of either space or time; otherwise the above assumptions are violated.

On the other hand, V can depend on momentum and energy without introducing inhomogeneity or anisotropy into the equation. This implies in (1), $V(\partial/\partial\vec{x}, \partial/\partial t)$, i.e., a differential operator. The possibility of including differential operators provides the loss terms in the equations governing the motion of the particle. It is interesting to note, in this context, that Rayleigh's dissipation function (see Goldstein,[23] for example) describes viscous (i.e., velocity-dependent) frictional forces can be used to extend the Lagrangian equations because of its velocity dependence, similar to the present momentum and energy dependence.

Now let Ψ be represented as a superposition of plane waves, which will be interpreted subsequently as a wave packet

$$\Psi(\vec{x}, t) = \int d^3\vec{k}\, d\omega\, \Psi(\vec{k}, \omega) e^{i\vec{k}\cdot\vec{x} - i\omega t}. \tag{2}$$

It must be emphasized that (2) is *not* a Fourier integral, since $\vec{k}, \omega$ are not necessarily real; therefore an inverse transformation is not available. However, in the present case it is not needed.

By combining (1) and (2) and exploiting $\partial/\partial\vec{x} \equiv i\vec{k}$, $\partial/\partial t \equiv -i\omega$ we derive the dispersion relation between $\vec{k}$ and ω,

$$F = \frac{\hbar^2 k^2}{2m} + V(\vec{k}, \omega) - \hbar\omega = 0\,, \tag{3}$$

and, by identifying the momentum and energy by $p = \hbar\vec{k}$, $E = \hbar\omega$, respectively, we get the corresponding classical expression for the energy balance. The function $V(\vec{k}, \omega)$ need not be real; therefore in general, F and also $\vec{k}, \omega$ are complex.

The concepts of complex momentum and energy are not new in physics (e.g., complex power in oscillatory electrical networks, or complex potentials in nuclear physics, as mentioned above); however, it needs physical interpretation before it can be accepted here. This is done below, after clarifying the concept of a wave packet.

The choice of $\vec{k}, \omega$ satisfying (3) is not unique even for real V. It is the stipulation that the group velocity must be real which determines the allowed values of $\vec{k}, \omega$ satisfying (3). Writing $F = 0$ in the form $\omega = \Omega(\vec{k})$ and expanding Ω as a Taylor series about a central value $\vec{k}_0$, retaining only the first derivative, yields

$$\omega = \Omega(\vec{k}_0) + \frac{\partial\Omega}{\partial\vec{k}_0}\cdot(\vec{k} - \vec{k}_0)\,. \tag{4}$$

Substituting (4) in (2) yields

$$\Psi(\vec{x}, t) = e^{i\vec{k}_0\cdot\vec{x} - i\omega_0 t} f(\vec{k}_0, \vec{x} - \vec{v}t)\,,$$
$$\vec{v} = \frac{\partial\Omega}{\partial\vec{k}_0}, \quad \omega_0 = \Omega(\vec{k}_0)\,, \tag{5}$$

where f is the integral after the complex plane wave is pulled out. This is a description of a wave packet with a carrier wave $e^{i\vec{k}_0\cdot\vec{x} - i\omega_0 t}$ and an envelope f which is constant on $\vec{x} = \vec{v}t$. However, in the present case $\vec{k}_0, \omega_0$ are in general complex. Since real $\vec{x}, t$ are stipulated, we must choose those values $\vec{k}_0, \omega_0$ satisfying $\mathrm{Im}\vec{v} = 0$.

We can now return to the concepts of complex momentum and energy. According to (5), the probability density is defined as

$$\Psi\Psi^* = e^{-2\,\mathrm{Im}\vec{k}\cdot\vec{x} + 2\,\mathrm{Im}\omega t} ff^*\,. \tag{6}$$

The fact that $\vec{k}, \omega$ are allowed to be complex leads to a function (6) which is dependent on $\vec{x}, t$. If we move in space with the group velocity prescribed by (5), then ff^* is a constant and the exponential becomes

$$e^{-2(\mathrm{Im}\vec{k}\cdot\vec{v} - \mathrm{Im}\omega)t}\,. \tag{7}$$

If in addition $\mathrm{Im}\vec{k}\cdot\vec{v} > \mathrm{Im}\omega$, then we have, as we move in space, a time-dependent exponentially decaying function which describes the absorption of the stream of particles. The opposite situation $\mathrm{Im}\vec{k}\cdot\vec{v} < \mathrm{Im}\omega$ describes a situation where owing to the stream of particles the medium is stimulated to generate more particles. In some respects this brings to mind the avalanche effects in electrical discharge and stimulated emission of radiation in lasers. However, the present linear theory is more adequate for description of stable systems, and therefore limiting the discussion to dissipative systems leads us on firmer ground.

INHOMOGENEOUS TIME-VARYING SPACE

In inhomogeneous time-varying space we allow V to change slowly in space and time. (The precise meaning of "slowly changing" functions is not further elaborated here. It suffices to say that over a distance k^{-1} and time ω^{-1}, V is approximately constant.) The particle is described by means of the eikonal approximation

$$\Psi = f(\vec{x}, t) e^{i\phi(\vec{x}, t)}\,,$$
$$\phi(\vec{x}, t) = \int_{P_1}^{P_2} (\vec{k}\cdot d\vec{x} - \omega\, dt)\,, \tag{8}$$

where $f(\vec{x}, t)$ is the amplitude and $\phi(\vec{x}, t)$ is the phase of the de Broglie wave packet. The phase is described as a line integral in four-space between events P_1 and P_2. For (8) to be a unique representation we prescribe[24]

$$\nabla\times\vec{k} = 0\,,$$
$$\frac{\partial\omega}{\partial\vec{x}} + \frac{\partial\vec{k}}{\partial t} = 0\,. \tag{9}$$

Synge[1] considers ϕ as the extended action (this corresponds to Fermat's principle in its extended form for optics), hence we prescribe $\delta\phi=0$, where δ denotes the variation. However, this variation vanishes subject to the constraints that $F(\vec{k},\omega,\vec{x},t)=0$ [similar to (3), but includes the slow variation in $\vec{x},t$]; furthermore, all along the trajectory $\mathrm{Im}\vec{v}=0$. It has been shown[2,3] that the equation of motion are given by

$$\begin{aligned}\vec{v}&=\frac{d\vec{x}}{dt}=-\frac{F_{\vec{k}}}{F_\omega},\quad \mathrm{Im}\vec{v}=0,\\ \frac{d\omega}{dt}&=-\frac{F_t}{F_\omega}+i\vec{v}\cdot\vec{\beta},\\ \frac{d\vec{k}}{dt}&=\frac{F_{\vec{x}}}{F_\omega}+i\vec{\beta},\\ \vec{\beta}&=-\left[\mathrm{Re}\left(\frac{\partial\vec{v}}{\partial\vec{k}}+\frac{\partial\vec{v}}{\partial\omega}\vec{v}\right)\right]^{-1}\\ &\quad\cdot\mathrm{Im}\left(\frac{\partial\vec{v}}{\partial\vec{k}}\cdot\frac{F_{\vec{x}}}{F_\omega}-\frac{\partial\vec{v}}{\partial\omega}\frac{F_t}{F_\omega}+\frac{\partial\vec{v}}{\partial\vec{x}}\cdot\vec{v}+\frac{\partial\vec{v}}{\partial t}\right),\end{aligned}\tag{10}$$

where $F_\omega=\partial F/\partial\omega$, $F_{\vec{x}}=\nabla F$, etc. and $\partial\vec{v}/\partial\vec{k}$ is a matrix $\partial v_i/\partial k_j$, $i,j=1,2,3$, etc. See the appendix. The new term $\vec{\beta}$, which vanishes in conservative systems, is necessary to keep $\vec{x},t$ real, i.e., $\mathrm{Im}\vec{v}=0$, not only at the boundary, where $\mathrm{Im}\vec{v}=0$ is a boundary condition, but all along the trajectory.

The above given theory is not limited to the wave equation (1). In fact, any function $F(\vec{k},\omega,\vec{x},t)=0$ can be used, provided it leads to group velocities not larger than c, otherwise special relativity theory is violated. Thus for example Schrödinger's zero-spin relativistic equation or Dirac's relativistic equation (see Schiff,[25] for example) may be used. The latter leads for a free particle to a determinant $E^2-c^2p^2-m^2c^4=0$ which is identical to the dispersion relation of Schrödinger's relativistic equation, therefore for a free particle the equations of motion are independent of spin. This is not the case if electromagnetic potentials are added.

SIMPLE EXAMPLES

Homogeneous time-invariant media

For simple examples we choose the nonrelativistic equation (3) and a homogeneous time-invariant and isotropic system. Thus we take $V=V(\hbar^2k^2,\hbar\omega)$. It follows that in (10) $\vec{\beta}=d\omega/dt=d\vec{k}/dt=0$ and the group velocity is a constant given by

$$\vec{v}=2\hbar\vec{k}\left(\frac{1}{2m}+\frac{\partial V}{\hbar^2\partial k^2}\right)\Big/\left(1-\frac{\partial V}{\hbar\partial\omega}\right),\quad \mathrm{Im}\vec{v}=0.\tag{11}$$

As a simple representative of this class we may take

$$V=\alpha\hbar^2k^2/(2m),\tag{12}$$

where α is a complex constant. Hence (3) becomes

$$F=\frac{\hbar^2k^2}{2m}\gamma-\hbar\omega=0,\quad \gamma=1+\alpha\tag{13}$$

and (11) yields

$$\vec{v}=\hbar\gamma\vec{k}/m,\quad \mathrm{Im}(\gamma\vec{k})=0.\tag{14}$$

Since k_i, $i=1,2,3$ and γ are phasors in the complex plane, we have $\arg\gamma=-\arg k_i$, and consequently from (13) we have

$$\arg k_i=\arg\omega=-\arg\gamma.\tag{15}$$

Since there is only one direction of interest in space, we may drop the vector notation in (14). According to the argument following (7), dissipation exists for $(\mathrm{Im}k)k\gamma\hbar/m>\mathrm{Im}\omega$, but the imaginary part of (13) prescribes $(\mathrm{Im}k)k\gamma\hbar/(2m)=\mathrm{Im}\omega$; hence, provided $\mathrm{Im}k\neq0$, $\gamma\neq0$, the inequality is identically satisfied. This is a very interesting result, showing that the present system cannot give rise to amplification (as opposed to dissipation). Another interesting result is the fact that the group velocity (14) is a constant of space and time, but (7) still prescribes an exponential decay. This implies that individual particles are not slowed down by dissipation, as one would expect from classical mechanics consideration (see also Buch and Denman[18]), but are simply "disappearing" from the stream of particles, i.e., their energy is either finite or zero.

If we take $V=\alpha\omega$, with α a complex constant, then (13) can be written again, with $\gamma=(1-\alpha)^{-1}$, hence we arrive at the same results. Classically, in both cases V is proportional to the square of the velocity, hence this result is not surprising.

Anisotropy can be introduced by making V a function of $\vec{k}$ instead of k^2. Although the problem of spin is not considered now, Dirac's approach inspires one to try $V=(\hbar^2/m)\vec{\alpha}\cdot\vec{k}$, where here $\vec{\alpha}$ is taken as a constant complex vector. Now (3) becomes

$$\frac{\hbar^2\vec{k}\cdot(\vec{k}+2\vec{\alpha})}{2m}-\hbar\omega=0\tag{16}$$

and

$$\vec{v}=\frac{\hbar}{m}(\vec{k}+\vec{\alpha}),\quad \mathrm{Im}\vec{k}=-\mathrm{Im}\vec{\alpha}.\tag{17}$$

The condition for dissipation becomes $(\hbar/m)\mathrm{Im}\vec{k}\cdot(\mathrm{Re}\vec{k}+\mathrm{Re}\vec{\alpha})>\mathrm{Im}\omega$ but the imaginary part of (16) leads to $(\hbar/m)\mathrm{Im}\vec{k}\cdot\mathrm{Re}\vec{\alpha}=\mathrm{Im}\omega$. Combining these relations, the inequality becomes

$$\mathrm{Im}\vec{\alpha}\cdot\mathrm{Re}\vec{k}<1,\tag{18}$$

and therefore $\mathrm{Im}\vec{\alpha}\cdot\mathrm{Re}\vec{k}>1$ means amplification.

Space and time slowly varying media

In order to avoid complicated problems requiring machine computations, we again consider very simple problems. Let V be independent of $\vec{k},\omega$, but a slowly varying function of space and time.

From (10),

$$\vec{v} = \hbar\vec{k}/m\,, \quad \mathrm{Im}\vec{k} = 0\,. \tag{19}$$

But if V is allowed to be complex, then ω must be complex although $\vec{k}$ is real. The condition $\mathrm{Im}\vec{k}\cdot\vec{v} \gtrless \mathrm{Im}\omega$ implies $\mathrm{Im}\omega < 0$, $\mathrm{Im}\omega > 0$ for dissipation and amplification, respectively. From (19) we have $\partial\vec{v}/\partial\vec{k} = \vec{I}\hbar/m$, where $\vec{I}$ is the idemfactor dyadic, therefore (10) prescribes

$$\vec{\beta} = \frac{1}{\hbar}\,\mathrm{Im}\frac{\partial V}{\partial \vec{x}}\,,$$

$$\frac{d\vec{k}}{dt} = -\frac{1}{\hbar}\,\mathrm{Re}\frac{\partial V}{\partial \vec{x}}\,, \tag{20}$$

$$\frac{d\omega}{dt} = \frac{1}{\hbar}\frac{\partial V}{\partial t} + \frac{i\vec{k}}{m}\cdot\mathrm{Im}\frac{\partial V}{\partial \vec{x}}\,.$$

Consider first $V(t)$ depending on time only. Then $\vec{\beta} = d\vec{k}/dt = 0$, hence only ω can change according to $\omega = V(t)$. This is less interesting than a space-dependent function $V(\vec{x})$. Here (20) prescribes that $\vec{k}$ will change as a function of $\mathrm{Re}\nabla V$, while $\mathrm{Re}(d\omega/dt) = 0$ and $\mathrm{Im}\,d\omega/dt = (\vec{k}/m)\cdot\mathrm{Im}\nabla V$. Hence $\mathrm{Re}\omega$ is a constant and $\mathrm{Im}\omega$, connected with the time dependence according to (7), depends on $\mathrm{Im}\nabla V$ in the direction tangent to the trajectory.

DISCUSSION

The question of dissipative systems has been discussed within the realm of ray mechanics, and simple examples were given. Synge[1] in his book proceeds by a method he calls "primitive quantization" to discuss notorious physical phenomena, e.g., the hydrogen atom. His approach is admittedly a somewhat more precise version of the Bohr-Sommerfeld quantum theory. A similar transition for dissipative systems, if suggested, could perhaps indicate the way in which dissipation can be incorporated into wave mechanics (as opposed to ray mechanics). This seems to be an open problem at present.

APPENDIX

A simplified derivation of (10) is given. Since $F(\vec{k}, \omega, \vec{x}, t) = 0$ must be satisfied always and everywhere, we must have $dF = 0$, hence for $\partial F/\partial\omega \neq 0$

$$\frac{1}{\partial F/\partial\omega}\frac{dF}{dt} = 0 = \frac{\partial F/\partial k_i}{\partial F/\partial\omega}\frac{dk_i}{dt} + \frac{d\omega}{dt} + \frac{\partial F/\partial x_i}{\partial F/\partial\omega}\frac{dx_i}{dt} + \frac{\partial F/\partial t}{\partial F/\partial\omega}\,. \tag{A1}$$

The real part of (A1) is satisfied by

$$\mathrm{Re}\frac{dk_i}{dt} = \mathrm{Re}\frac{\partial F/\partial x_i}{\partial F/\partial\omega}\,,\qquad \mathrm{Re}\frac{d\omega}{dt} = -\mathrm{Re}\frac{\partial F/\partial t}{\partial F/\partial\omega}\,, \tag{A2}$$

subject to

$$v_i = \frac{dx_i}{dt} = -\frac{\partial F/\partial k_i}{\partial F/\partial\omega}\,, \quad \mathrm{Im}v_i = 0\,. \tag{A3}$$

Postulating

$$\mathrm{Im}\frac{dk_i}{dt} = \mathrm{Im}\frac{\partial F/\partial x_i}{\partial F/\partial\omega} + \beta_i\,, \quad \mathrm{Im}\beta_i = 0$$
$$\mathrm{Im}\frac{d\omega}{dt} = -\,\mathrm{Im}\frac{\partial F/\partial t}{\partial F/\partial\omega} + \alpha\,, \quad \mathrm{Im}\alpha = 0 \tag{A4}$$

and substituting in the imaginary part of (A1) yields

$$\alpha = \beta_j v_j\,. \tag{A5}$$

Therefore only β_j are undetermined yet. But in order that v_i remains real along the ray path we have to add the constraint $(d/dt)\mathrm{Im}v_i = 0$, yielding

$$\mathrm{Im}\left(\frac{\partial v_i}{\partial k_j}\frac{dk_j}{dt} + \frac{\partial v_i}{\partial\omega}\frac{d\omega}{dt} + \frac{\partial v_i}{\partial x_j}\frac{dx_j}{dt} + \frac{\partial v_i}{\partial t}\right) = 0\,. \tag{A6}$$

Substitution of (A2)–(A5) in (A6) yields β_j and completes the derivation of (10).

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