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Quantum Theory of Non Relativistic: Adiabatic Charged-Particle Motion in Inhomogeneous Electric and Magnetic Fields

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ABSTRACT

A quantum mechanical theory of non-relativistic adiabatic charged particle motion in inhomogeneous electric and magnetic fields is presented. The calculations are based on a kinetic equation for the density matrix operator in the prescribed fields.

INTRODUCTION

A quick perusal of literature reveals that to date there has been no clear attempt at solving the problem concerning quantum effects on particle motion in inhomogeneous electric and magnetic fields. However, numerous papers have been published regarding the classical relativistic and nonrelativistic theories of charged-particle motion[1,2]. In the present communication, we concentrate our study to nonrelativistic particle motion in inhomogeneous electric and magnetic fields. We do so simply because particle motion is elementary if electric and magnetic fields are constants in time and are either zero or uniform in space.

We know that the motion of each particle in a collection of charged particles is determined by the fields due to the other particles plus the field due to external forces. Thus in order to understand the behaviour of the collection, it is necessary to understand first the behaviour of a single particle in the prescribed fields[3,4]. In the classical domain, the particle orbit theory is well described by a distribution function $f(r,vt)$ in the six dimensional coordinate $\vec{r}$ plus the force $\vec{F}$ acting on the particle[5,6]. In order to handle quantum effects, we solve an initial value problem for a kinetic equation for the density matrix[7]. In coordinate space, we are concerned with traces of the type

$$\int Y(\phi,\theta)(<\phi,\theta|p(t)|\phi,\theta> \sin\phi \; d\varphi d\theta,$$

where $<\phi,\theta|\rho(t)|\phi,\theta>$ is the diagonal matrix element of the density matrix in a coordinate representation.

There exists a need even from a purely conceptual point of view, for a simple quantum kinetic model, even if schematic, in order to explain the importance of quantum mechanical effects on charged particle motion and the properties of plasma. In the present paper, our calculations will be based on the quantum analog of Vlasov's equation for the density matrix operator (collisionless assumption). An analogous study is however, being contemplated in which the effect of collisions will be taken into account or a detailed balance system will be treated.

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DENSITY MATRIX IN EXTERNAL FIELDS

For quantum mechanical treatment, however, the system is described by a density matrix operator $\rho(t)$ obeying a kinetic equation of the form

$$\frac{\partial \rho}{\partial t} + \frac{i}{h}[H(rt), \rho(t)] = 0 \tag{1}$$

The Hamiltonian $H(r,t)$ consists of a free particle term H_0 and the interaction of the particle with external electric $E(r,t)$ and magnetic $B(r,t)$ fields.

$$H(r,t) = H_o + V_E + M_H \tag{2}$$

where

$$H_O = \frac{p^2}{2m} = \frac{-\hbar^2}{2m}\nabla^2 \text{ unperturbed system}$$

$$V_E = \frac{e}{m}E(t), \text{ and } M_H = \frac{1}{2}\frac{B^2}{\mu}.$$

A static electric field perpendicular to the magnetic field produces no net electric current in a neutral plasma. However, a time-dependent electric field does produce a current in plasma, which therefore behaves like a dielectric. Thus our Hamiltonian will take the form below:

$$H(t) = H_o + V_E(t) + M_H(t) \tag{3}$$

and the corresponding equation of motion is given by

$$\frac{\partial \rho}{\partial t} + \frac{i}{h}[H(t), \rho(t)] = 0 \tag{4}$$

where $V_E(t)$ is purely time-dependent electric energy, and $M_H|t|$ is purely time dependent magnetic energy.

This equation is easier to study on the basis where H_o is diagonal[8]. Let ℓ, ℓ' stand for a set of quantum numbers specifying an eigenfunction of H_o such that

$$E_l - E_{l'} = \hbar\omega_{ll'} = \exp\left(-\beta E_{l'}\right) / \mathrm{Tr}\ \mathrm{ex}\left[\left(-\beta H_{l'}\right)\right]$$

In order to include the effects of inhomogeneity in space with respect to electric and magnetic fields, we shall consider a three dimensional space with eigenfunction $Y(\theta, \phi)$ and eigenvalues $E_\ell = \frac{\hbar^2}{2m}\ell(\ell+1)$ since in such a space, distribution of charged particles and direction of charged particle motion is given by angles and thus

$$
\begin{aligned}
\rho &= \rho(\phi,\theta,t) \\
V_E &= V(\phi,\theta,t) \\
M_H &= M(\phi,\theta,t)
\end{aligned}
\tag{5}
$$

Equation (4) will then take the following form:

$$\frac{\partial p}{\partial t}+\frac{i}{\hbar}\left[H_o,\rho(\phi,\theta,t)\right]=-\frac{i}{\hbar}\left[V(\phi,\theta,t)\rho(\phi,\vartheta,t)\right]-\frac{i}{\hbar}\left[M(\phi,\theta,t),\rho(\phi,\theta,t)\right] \tag{6}$$

where $V(\phi,\theta,t)$ is both time and space dependent electric energy, and $M(\phi,\theta,t)$ is both time and space dependent magnetic energy.

Thus, in a more explicit notation for the three dimensional case, equation (6) above takes the form below:

$$
\begin{aligned}
&\frac{\partial\rho}{\partial t}+\frac{i}{\hbar}\left[H_o,\rho\right]= \\
&-\frac{i}{\hbar}\{<\phi\theta|V|\phi'\theta'><\phi'\theta'|\rho|\phi'\theta'>-<\phi\theta|\rho|\phi'\theta'><\phi'\vartheta'|V|\phi'\theta'>\} \\
&-\frac{i}{\hbar}\{<\phi\theta|M|\phi'\theta'><\phi'\theta'|\rho|\phi'\theta'>-<\phi'\theta'|\rho|\phi'\theta'><\phi'\theta'|M|\phi\theta'>\}
\end{aligned}
\tag{7}
$$

The above equation can be handled in a number of ways. Let us form $\langle\phi'\,\theta'|l'\,m'\rangle$ to the right and $<\ell m|\phi\vartheta>$ to the left thereby move into energy representation[9]

$$
\begin{aligned}
&(\frac{\partial}{\partial t}+\omega_{\ell\ell'})<\ell m|\phi\theta><\phi\theta|\rho|\phi'\theta'><\phi'\theta'|\ell'm'> = \\
&\iint-\frac{i}{\hbar}\{<\ell m|\phi\theta><\phi'\theta'|V|\phi'\theta'><\phi'\theta'|\rho|\phi'\theta'> \\
&<\phi'\theta'|\ell'm'>\sin\phi d\phi d\theta\sin\phi' d\phi' d\theta'- \\
&\iint\frac{i}{\hbar}\{\ell m|\phi\theta><\phi\theta|M|\phi'\theta'><\phi'\theta'|\rho|\phi'\theta'> \\
&<\phi'\theta'|\ell m'>\sin\phi d\phi d\theta\sin\phi' d\phi' d\theta'\}
\end{aligned}
\tag{8}
$$

where $\omega_{\ell\ell'}=\frac{1}{\hbar}E_{0\ell\ell'}$

The other terms simply drop out because $V\left(\phi,\theta,t\right)$ and $M\left(\phi,\theta,t\right)$ have no diagonal elements.

Our immediate problem now concerns rigorous treatment of the two terms in the curly brackets contained in the integrals in equation (10)

The first term namely:

$$-\frac{i}{\hbar}\int_0^{2\pi}\int^{\pi} < \ell m|\phi\theta >< \phi\theta|V|\phi'\theta' >< \phi'\theta'|\rho|\phi'\theta' > \\ < \phi'\theta'|\ell' m' > \sin\phi d\phi d\theta \sin\phi' d\phi' d\theta' \tag{9}$$

has been given a thorough treatment in ref. (5) and it reduces finally to the following form

$$2\pi V_{\ell\ell'}\int\int \sin\phi\, d\theta\, d\phi < \ell m|\phi\theta >< \phi\theta|\rho|\phi\theta > < \phi\theta|\ell' m' > \tag{10}$$

Multiplying equation (10) by $\langle\phi\theta|\ell m\rangle$ to the left and by $< \ell' m'|\phi'\theta' >$ to the right then using the addition theorem for spherical harmonics to re-express (10), we come back to coordinate representation of the form

$$4\pi\sum_{\ell\ell'} V_{\ell\ell'}\frac{(2\ell+1)(2\ell'+1)}{(4\pi)^2}\int\int P_\ell(\cos\alpha)P_{\ell'}(\cos\alpha')\sin\phi d\phi\, d\theta \quad < \phi\theta|\rho|\phi'\theta' > \tag{11}$$

where $\cos\alpha = \cos\vartheta\cos\vartheta' + \sin\vartheta\sin\vartheta'\cos\left(\phi-\phi'\right)$, $P_\ell(\cos\alpha)$ and $P_{\ell'}(\cos\alpha')$ are the associated Legendre polynomials.

Equation (11) is also very familiar from ref. (8) and has been given a thorough consideration in ref. (7). It reduces to the form below

$$\frac{\pi}{4}\sum_{\ell\ell'} V_{\ell\ell'}(2\ell+1)(2\ell'+1)T(\ell\ell'|1) \tag{12}$$

where

$$T\left(\ell\ell'|1\right) = \frac{3(\ell+1)}{2(2\ell+1)}\phi_\ell(\ell+1) + \frac{3(\ell-1)}{2(2\ell+1)}\phi_{\ell'}(\ell'-1)\ .$$

Similarly, the second term namely

$$-\frac{i}{\hbar}\int_0^{2\pi}\int_0^{\pi}<\ell m|\phi\theta><\phi\theta|M|\phi'\theta'|\rho|\phi\theta'><\phi'\theta'|\ell'm'>\sin\phi d\phi d\psi \sin\phi' d\theta' d\varphi' \quad (13)$$

can be reduced to

$$\frac{\pi}{4}\sum_{\ell\ell'} M_{\ell\ell'}(2\ell+1)(2\ell'+1)T(\ell\ell'|1) \quad (14)$$

Thus the right hand side of equation (8) will take the form below:

$$\frac{\pi}{4}\sum_{\ell\ell}(V_{\ell\ell'}+M_{\ell\ell'})(2\ell+1)(2\ell'+1)T(\ell\ell'|1) \quad (15)$$

and the left hand side of equation (8) will have the form below

$$\Delta_{\ell\ell}<\ell m|\phi\theta><\phi\theta|\rho|\phi\theta><\phi\theta|\ell' m> \quad (16)$$

Where $\Delta_{\ell\ell'}=(\frac{\partial}{\partial t}+w_{\ell\ell'})$

Now multiplying the above expression (16) to the left by $\langle\phi\theta|\ell m\rangle$ and to the right by $\langle\ell' m'|\phi\theta\rangle$ and finally summing over ℓm and $\ell' m'$, we form coordinate diagonal elements of the density matrix

$$<\phi\vartheta|\rho|\phi\theta> \quad (17)$$

To go back to energy representation of the diagonal elements we multiply (17) to the left by $\langle\ell m|\phi\theta\rangle$ and to the right by $\langle\phi\theta|\ell m\rangle$ thereby forming

$$<\ell m|\rho|\ell m> \quad (18)$$

Thus equation (8) will take the following form in energy representation

$$<\ell m|\rho|\ell m>=\frac{\pi}{4_{\ell\ell'}}\sum_{\ell\ell'}(V_{\ell\ell'}+M_{\ell\ell'})(2\ell+1)(2\ell'+1)T(\ell\ell'|1)\Delta_{\ell\ell'}^{-1} \quad (19)$$

From (19), we can compute several expectation values or velocity moments by taking the trace of the above density matrix multiplied with relevant parameters. By direct calculations it can be shown easily that the average particle population per level with respect to diagonal element of the density matrix is zero. Thus we have to concentrate our study on the off-diagonal elements in order to include the effects of the prescribed electric and magnetic fields.

Performing integration with respect to $\phi\theta$ and $\phi'\theta'$ on the left hand side of equation (8), we form the off-diagonal elements of the density matrix in energy representation.

$$< \ell m|\rho|\ell' m'> \quad (20)$$

In order to form the off-diagonal elements of the density matrix in equation (11), we will first multiply $\langle\phi\theta|\rho|\ell m\rangle$ (diagonal elements) to the left by $\langle\ell m|\phi\theta\rangle$ and to the right by $\langle\phi\theta|\ell m\rangle$ and form the diagonal elements in energy representation

$$\langle\ell m|\rho|\ell m\rangle \quad (21)$$

Then now multiplying equation (21) to the left by $\langle\phi\theta|\ell m\rangle$, and to the right by $\langle\ell m|\phi'\theta'\rangle$, we obtain the off-diagonal elements of the density matrix in coordinate representation

$$<\phi\theta|\rho|\phi'\theta'>= \Sigma_{\ell=0}\rho_{\ell'} <\phi\theta|\ell m>< \ell m|\phi'\theta'> \quad (22)$$

where

$$\rho_{\ell'} = \exp(-\beta E_{\ell'})|Q$$

and

$$Q = \sum_{\ell=o}(2\ell+1)\exp)(-\rho E_{\ell}) \quad (23)$$

$$E_{\ell} = \frac{\hbar^2}{2m}\ell(\ell+1)$$

$$\beta = 1|kT$$

Putting equation (22) into equation (11) and treating it as before in ref. (7,8), we finally obtain the following expression instead of equation (12)

$$\frac{\pi}{4}\sum_{\ell\ell}\rho_{\ell'}V_{\ell\ell'}(2\ell+1)(2\ell'+1)T(\ell\ell'|1) \quad (24)$$

The second term in equation (8) is to be given the same treatment and in the circumstances reduces to the form

$$\frac{\pi}{4}\sum_{\ell\ell'}{}_{\ell\ell'}\rho_{\ell'}M_{\ell\ell'}(2\ell+1)(2\ell'+1)T(\ell\ell'|1) \quad (25)$$

Thus, the equation for the off-diagonal elements of the density matrix in energy representation has the form

$$<\ell m|\rho|\ell' m'>=\frac{\pi}{4}\sum_{\ell\ell'}\Delta_{\ell\ell'}^{-1}\rho_{\ell'}(2\ell+1)(2\ell'+1)(V_{\ell\ell'}+M_{\ell\ell'})T(\ell\ell'|1) \quad (26)$$

From the above, the average particle population per level is no longer zero. We are therefore in a position to compute the following:

1. The average particle velocity is

$$<v>=\Sigma_{\ell\ell'}<\ell|v|\ell'><\ell|\rho|\ell'>=\frac{n}{4}\Sigma_{\ell\ell'}<\ell|v|\ell'>\Delta_{\ell\ell'}^{-1}\rho_e(2\ell+1)(2\ell'+1)x(V_{\ell\ell'}+M_{\ell\ell'})T(\ell\ell'|1)$$

2. Momentum

$$<p>=\Sigma_{\ell\ell'}m[<\ell|v-<v>|\ell'>]^2<\ell|\rho|\ell'>=\frac{\pi m}{4}\Sigma_{\ell\ell'}<\ell[v-<v>|\ell'>]^2\Delta_{\ell\ell'}^{-1}\rho_{\ell'}(2\ell+1)x(2\ell'+1)(V_{\ell\ell'}+M_{\ell\ell'})T(\ell\ell'|1)$$

3. Heat flux tensor

$$<Z>=\Sigma_{ee'}m[<\ell|v-<v>|\ell'>]^3<\ell|\rho|\ell'>=\frac{\pi m}{4}\Sigma_{ee'}[<\ell|v-<v>|\ell'>|]^3\Delta_{\ell\ell}^{-1}\rho_{e'}$$

$$x(2_\ell+1)(2_{\ell'}+1)(V_{\ell\ell'}+M_{\ell\ell'})T(\ell\ell'|1)$$

GUIDING CENTER MOTION

It is a well established fact in the classical theory that in a uniform magnetic field that is constant in time, a charged particle moves in a helical path. To a good approximation, such motion may be described as a motion about a circle whose center is moving along a line of force. In cases where the field is not quite uniform and not quite independent of time, we expect the motion not to be quite helical but rather something approximating helical motion is expected. Thus, a good approximation in the circumstances will contain gyration about a center that now may move at right-angles to and along a line of force [(11)]. The particle spirals rapidly while its center of rotation moves slowly and therefore the drift velocity is much smaller compared to the orbital velocity [(12)]

The classical equation of motion of the particle is the following[(14)]:

$$m\frac{d^2r}{dt^2}=\frac{e}{m}\dot{r}+B(r,t)+eE(r,t) \quad (27)$$

If we now replace $r=R+g$ where g is the radius of gyration and R the distance from point of origin or observation and taking average over a period of gyration [(13,14)], we obtain

$$\ddot{R}=\frac{e}{m}E(R,t)+\frac{R}{e}+B(R,t)-\frac{M}{m}\nabla B(R)+ \quad (28)$$

where $M = \frac{eg^2\omega}{2c} = \frac{mv_1^2}{2B}$ is the magnetic moment, v_1 is the particle velocity perpendicular to the magnetic field.

In formulating the quantum analog of the above classical theory we shall assume the unperturbed or stationary states correspond to cases in which both magnetic and electric fields are constant in time and also uniform in space. A natural consequence of such an assumption classically is that the radius of gyration g remains constant during motion and the obvious quantum analogy is that we are dealing with a system at fixed energy levels.

Motion of such a system is given by the unperturbed Hamiltonian, and the stationary states (fixed energy levels) is obtained from the solution of the following eigenvalue problem

$$ih\frac{\partial\psi_o}{\partial t} = H_o\psi_o \tag{29}$$

To include the effects of the fields, we shall assume therefore that the system is perturbed and that the fields are no longer static and uniform. The corresponding Hamiltonian is given by

$$H_o = H(t) = H_0 + H^1(t) \tag{30}$$

where

$$H^1(rt) = \frac{e}{m}E(R,t) + \frac{R}{c}xB(R,t),\ H_0\frac{-h^2}{2m}\nabla^2 = \frac{-h^2}{2m^3} < p >^2 \text{, and } < p > = m < v >,$$

<v> is the average particle velocity already computed at the end of previous section, H_o is the unperturbed Hamilton, $H^1(t)$ is the effect of the fields-perturbation.

Solution of equation (29) has the form

$$\psi_0 = \sum_n \alpha_o^n \phi_o^n \exp(\frac{i}{h}E_0^n t) \tag{31}$$

where α_0^n are constant coefficients, ϕ_0^n are the eigenfunctions of the following eigenvalue problem

$$H_0\,\phi_0^n = E_0^n\,\phi_0^n \tag{32}$$

Our main problem is to find a solution for Schroedinger equation with Hamiltonian $H(r,t) = H_0 + H^1(t)$. An exact solution of such an equation cannot be found, however, for an approximate solution, we shall apply the method of non stationary perturbation theory.

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Let us consider the following Schroedinger equation.

$$ih\frac{\partial\psi}{\partial t} = [H_0 + H'(t)]\psi \qquad (33)$$

and seek the solution of the above equation in the form

$$\psi = \sum_n \alpha_n(t)\phi_0^n \exp\left(+\frac{1}{\hbar}E_o^m t\right) \qquad (34)$$

where $\alpha_n(t)$ are the expansion coefficients to be defined.

Now putting equation (34) into equation (33) and multiplying the resulting expression to the left by ϕ_o^{+n} and using orthonormal property of functions ϕ_o^n and ϕ_0^{+n} together with equation (32), we obtain

$$\alpha_m = -\frac{i}{h}\sum_n \alpha_n < m|H'|n > \exp\left[\frac{1}{\hbar}(E_o^n - E_o^m)t\right] \qquad (35)$$

where

$$< m|H'|n >= \phi_0^{+m} H' \phi_0^n dX = H'_{mn} \qquad (36)$$

Expression (36) indicate that the matrix element H'_{mn} causes transition from n to m energy states.

CONCLUSION

The primary aims in writing this paper are two fold. One is to trigger off research in this area which has been left rather dormant for years and the other is to present an approach for solving such problems based on the author's previous works. We know that macroscopic theory is very well covered in numerous papers and books dealing with classical electromagnetic field. [15] These theories consider physical quantities averaged over elements of volume which are physically infinitesimal. Thus, they ignore the microscopic variations of quantities which result from the molecular structure of matter. In these considerations the actual microscopic value of electric field is always replaced by its averaged value E. However, it must be stressed that in the present communication, we are not directly concerned with the microscopic value of the electric field as such, but are rather interested in the effects of its averaged value on the motion of a charged particle. We have also limited our consideration to a completely rarified system in which collisions can be assumed absent. This no doubt simplifies our treatment in the sense that we do not take into account the kind of redistribution after impact [16] that often result in polarization. Static and uniform fields in this respect, correspond to states in which the particle is perturbed by the diagonal elements of electric and magnetic fields. These elements are all zero and therefore have no effect on the particle motion. Classically this is a motion about a circle of constant radius of gyration whose center moves along a line of force and the obvious quantum analog is that the particles have fixed energy levels. However, the effects of nonstationary and nonuniform fields is to cause transition to different energy levels. Finally in order to consider relativistic effect, we will introduce the proper covariant forms of electromagnetic field equations and relativistic mass for the particles in later communication.

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