PHYSICAL REVIEW B

SOLID STATE

THIRD SERIES, VOL. 1, NO. 8 15 APRIL 1970

Transport in a Magnetic Field. I. The Gauge-Independent Formalism*

L. L. VAN ZANDT

Department of Physics, Purdue University, Lafayette, Indiana 47907

(Received 17 March 1969)

The problem of the dynamics of a system of charged particles in a constant magnetic field is transformed into one from which the constant field gauge has been removed. The Liouville equation assumes a different form in this formalism. A variational principle for generating approximate solutions to complex problems is presented.

I. INTRODUCTION

THE subject of this discussion is the theory of a plasma of identical charged interacting particles in the presence of a magnetic field. While some of our results apply to this system without further specialization, nonetheless, we shall gradually reduce the scope to consider transport phenomena in a degenerate electron gas. Our principal effort is a demonstration of a general procedure for generating equations of transport of various quantities in the presence of magnetic fields.

The customary approach to this problem is via the Boltzmann equation[1,2] or a related form; the states of the particles of the plasma are described by wave packets. The magnetic field is taken into account by the use of the Lorentz force acting on the packet.

We shall criticize and circumvent two aspects of this procedure. First, its treatment of particle motion is essentially classical in that the packets are spatially localized, and so too are the forces acting upon them. This localization restricts the Boltzmann equation approach to the description of long-wavelength phenomena. Our final transport equations will contain correction terms for shorter wavelengths. Second, the construction of packets, each considered by itself, makes a collection of one-particle problems out of a single many-body system. The use of the Lorentz force on each packet actually means that one is using a different gauge for each particle of the plasma. This is a more serious difficulty than the first, for it leads to transport equations which are actually different at all wavelengths from those derived from the fully quantum-mechanical gauge-independent theory we develop here.

Our argument in this paper is devoted to the total elimination of reference to gauge in the equations of motion of physically meaningful quantities. Our final formalism will thus achieve gauge invariance by being gauge independent.

In this paper we shall develop a gauge-independent modified form of the Liouville equation appropriate to many-body systems. We shall show how the solutions of this equation may be used to find values for physical quantities such as particle density, current, current density, spin density, etc. Finally, we shall show how solutions of our modified equation may be obtained variationally and thus give a means for generating approximate solutions for many-body interacting systems.

We wish to emphasize that the construction of the formalism is carried out without approximation. The applications we shall subsequently display are approximate, and we shall identify and discuss the approximations as they are made, but there are no fundamental limitations on our basic equations.

In Sec. II we develop the gauge-independent density matrix. To remove reference to gauge, we follow a procedure given by Thomas[3] for single particles. We extend his method to many-body interacting systems.

In Sec. III we show how the expectations of various operators referring to physical quantities may be obtained, as well as a transformed Liouville equation. Again, the results are cast in gauge-independent form. Gauge independence is explicitly demonstrated.

In Sec. IV, we develop a variational principle useful

* Supported by Advanced Research Projects Agency.

[1] V. P. Silin, Zh. Eksperim. i Teor. Fiz. **33**, 495 (1957) [English transl.: Soviet Phys.—JETP 6, 945 (1958)].

[2] A. H. Wilson, *Theory of Metals* (Cambridge University Press, Cambridge, England, 1953), 2nd ed., p. 51.

[3] R. B. Thomas, Jr., Phys. Rev. **171**, 827 (1968).

for obtaining approximate solutions of the modified Liouville equation. The principle is structurally similar to Frenkel's[4] variational principle on the Schrödinger equation used and discussed elsewhere.[5,6] The use which we make of this principle in the following paper is the equivalent of the time-dependent Hartree-Fock approximation.[5–7]

II. TRANSFORMATION OF DENSITY MATRIX

Measurable values for physical quantities are obtained by evaluating the trace of the product of the appropriate operators with the statistical density operator or density matrix,

$$\langle O\rangle=(\mathrm{Tr}O\rho)(\mathrm{Tr}\rho)^{-1}. \tag{1}$$

The density matrix ρ satisfies the Liouville equation,

$$ih\frac{\partial\rho}{\partial t}=[H,\rho]. \tag{2}$$

In this, H is the Hamiltonian operator for the complete system:

$$H=\sum_{i=1}^{N}\left\{\left[-ih\nabla_i-\frac{e}{c}\mathbf{A}(\mathbf{r}_i)\right]^2\frac{1}{2m}+U(\mathbf{r}_i,\boldsymbol{\sigma}_i)+\tfrac{1}{2}\sum_{j\neq i}^{N}V(\mathbf{r}_i,\mathbf{r}_j)\right\}. \tag{3}$$

The sums run over all the particles of the system. $\mathbf{A}(\mathbf{r}_i)$ is the vector potential at the point $\mathbf{r}_i$.

The Hamiltonian contains explicit reference to the vector potential and is hence gauge dependent. All wave functions, must have a complementary gauge dependence so that the values of physical quantities, various matrix elements and their sums which the theory leads us to construct, shall be gauge invariant. Equations (1) and (2) then imply that ρ is gauge dependent. If we were to change the gauge in the Hamiltonian, (3), without making a corresponding transformation on ρ, the values of "physical" quantities calculated from (1) would be changed. It is thus important that the gauge used in H and ρ be consistent.

It is possible to obtain exact solutions of (2) and (3) for noninteracting systems, the well-known Landau states.[8] But it is our intention here to make contact eventually with the semiclassical Boltzmann-like theory of transport as given by Silin.[1] For this purpose the use of the exact solutions is awkward.

Localized wave packets describing the motion of single particles may be constructed and used to obtain a Boltzmann equation.[2] In attempting to apply the procedure suggested in Ref. 2 to our many-particle systems, however, we immediately encounter the difficulty of having to use a different gauge for every particle. We proceed instead by transforming to a formalism from which the vector potential has been eliminated. This transformation, applied to Eqs. (1) and (2) leaves them explicitly dependent on **B** but not **A**.

The existence of a useful gauge-independent formalism is suggested by the work of Thomas.[3] For a one-particle gas, he finds a gauge-independent expression for the particle current. We broaden the system to many particles and the class of operators from just the current to include tensor densities of many kinds.

The density matrix ρ is a function of all the $\mathbf{p}_i$, $\mathbf{r}_i$, $\boldsymbol{\sigma}_i$, **B**, and t. Gauge invariance of all measurable quantities imposes the requirement that $\mathbf{p}_i$ and $\mathbf{A}(\mathbf{r}_i)$ shall appear only in the combination $\mathbf{p}_i-(e/c)\mathbf{A}(\mathbf{r}_i)$. We may, therefore, express ρ as a Fourier integral,

$$\rho=\int\exp\left[i\sum_{s=1}^{N}\left(\mathbf{p}_s-\frac{e}{c}\mathbf{A}_s\right)\cdot\boldsymbol{\xi}_s\right]\times R(\boldsymbol{\xi}_1\cdots\boldsymbol{\xi}_N,\mathbf{r}_1\cdots\mathbf{r}_N,\mathbf{B},t)d\boldsymbol{\xi}_1\cdots d\boldsymbol{\xi}_N, \tag{4}$$

in which $\mathbf{A}_s$ means $\mathbf{A}(\mathbf{r}_s)$. In the symmetric gauge,

$$\mathbf{A}(\mathbf{r})=\tfrac{1}{2}B(x\hat{\mathbf{y}}-y\hat{\mathbf{x}}). \tag{5}$$

In this gauge, $\mathbf{p}_s\cdot\boldsymbol{\xi}_s$ and $\mathbf{A}_s\cdot\boldsymbol{\xi}_s$ commute. The integrand can then be written as

$$\exp\left[-i\sum_s(e/c)\mathbf{A}_s\cdot\boldsymbol{\xi}_s\right]\exp\left[i\sum_{s'}\mathbf{p}_{s'}\cdot\boldsymbol{\xi}_{s'}\right]R=\prod_{s=1}^{N}\left\{\sum_{n_s=0}^{\infty}\frac{[-i(e/c)\mathbf{A}_s\cdot\boldsymbol{\xi}_s]^{n_s}}{n_s!}\right\}\times\{\exp(i\sum_{s'}\mathbf{p}_{s'}\cdot\boldsymbol{\xi}_{s'})R\}. \tag{6}$$

Now the factors of $(\boldsymbol{\xi}_s)_{x,y}$ appearing in the first terms in braces can be replaced by $-i\partial/\partial(\mathbf{p}_s)_{x,y}$ operating on the second term. This derivative can in turn be expressed as a commutator of the second term with $(\mathbf{r}_s)_{x,y}$. By this sequence of operations, the terms in $\mathbf{A}_s$ can be removed from under the integrations over $\boldsymbol{\xi}_s$, and ρ expressed as an N-fold series of commutators of $\mathbf{r}_s$ and $\tilde{\rho}$, where

$$\tilde{\rho}\equiv\int\exp(\sum_{s=1}^{N}i\mathbf{p}_s\cdot\boldsymbol{\xi}_s)Rd\boldsymbol{\xi}_1\cdots d\boldsymbol{\xi}_N. \tag{7}$$

Thus

$$\rho=\prod_{s=1}^{N}\prod_{s'=1}^{N}\sum_{n_s=0}^{\infty}\sum_{n_{s'}=0}^{\infty}\frac{(ieBx_s/2\hbar c)^{n_s}}{n_s!}\frac{(-ieBy_{s'}/2\hbar c)^{n_{s'}}}{n_{s'}!},$$

[4] J. Frenkel, *Wave Mechanics, Advanced General Theory* (Clarendon Press, Oxford, England, 1934), p. 253.
[5] A. D. Mclachlan and M. A. Ball, Rev. Mod. Phys. **36**, 844 (1964).
[6] L. L. Van Zandt, Phys. Rev. **172**, 372 (1968).
[7] L. L. Van Zandt, Phys. Rev. **162**, 399 (1967).
[8] For example, C. Kittel, *Quantum Theory of Solids* (John Wiley & Sons, Inc., New York, 1963), p. 218ff.

$$[x_1^{[n_{1'}]},[x_2^{[n_{2'}]},\ldots,[y_1^{[n_1]},[y_2^{[n_2]},\ldots,\tilde{\rho}]\cdots]$$
$$\equiv\exp\left[-\sum_{s'=1}^{N}\frac{e}{c}\mathbf{A}_{s'}\cdot\left(\frac{\partial}{\partial\mathbf{p}_{s'}}\right)_{op}\right]\tilde{\rho}\equiv\tilde{U}\tilde{\rho}. \quad (8)$$

In this expression,

$$[a^{[n]},b]\equiv[a,[a,\ldots(n\text{ times}),b]]\cdots(n\text{ times})]$$

and

$$[a^{[0]},b]\equiv b. \quad (9)$$

The x_s and y_s all commute so that the successive commutations in (8) could be performed in any order.

Now we assume that ρ (and thereby $\tilde{\rho}$) vanishes at infinite $\mathbf{r}$ or infinite $\mathbf{p}$ faster than any power of $\mathbf{r}$ or $\mathbf{p}$. Then $\mathrm{Tr}[x^n,\tilde{\rho}]=0$; from Eq. (8) we then obtain

$$\mathrm{Tr}\rho=\mathrm{Tr}\tilde{\rho}, \quad (10)$$

for only the term in the sums with

$$n_1=n_{1'}=n_2=n_{2'}=\cdots=0$$

contributes. Thus, if ρ is normalized the transformation of Eq. (8) conserves this normalization.

III. EQUATIONS OF MOTION

Let us now consider the operator product $O_0\rho$. Clearly, if O_0 does not involve any of the $\mathbf{p}_s$ we have

$$O_0[x^{[n]},\tilde{\rho}]=[x^{[n]},O_0\tilde{\rho}]. \quad (11)$$

Hence we can convert $O_0\rho$ to the transformation in (8) acting on $O_0\tilde{\rho}$. In particular

$$\mathrm{Tr}O_0\rho=\mathrm{Tr}O_0\tilde{\rho}. \quad (12)$$

Now consider O_1, proportional to $mv_{sx}=[\mathbf{p}_s-(e/c)\mathbf{A}_s]_x$ and functions of $\mathbf{r}_s,\mathbf{r}_{s'}$,

$$O_1=mv_{sx}f(\mathbf{r}). \quad (13)$$

Then we form

$$O_1\rho=[\mathbf{p}_s-(e/c)\mathbf{A}_s]_x f\tilde{U}\tilde{\rho}=[\mathbf{p}_s-(e/c)\mathbf{A}_s]_x\tilde{U}f\tilde{\rho}$$

and by manipulation of commutators of the form $[p_{sx},x^n]$ obtain

$$O_1\rho=\int\exp\left(-i\sum\frac{e}{c}\mathbf{A}_{s'}\cdot\xi_{s'}\right)\left(p_{sx}+\frac{eB}{2c}y-\hbar\frac{eB}{2c}\xi_{sy}\right)$$
$$\times\exp[i\sum\mathbf{p}_{s'}\cdot\xi_{s'}]R(\xi)d\xi. \quad (14)$$

Again we convert factors of $i\xi_{s'}$ into $(\partial/\partial\mathbf{p}_{s'})_{op}$ as in the construction of $\tilde{\rho}$ and $\tilde{U}$ in Eq. (8). However, if $i\xi_{sx}$ in the first exponent is replaced by $\partial/\partial p_{sx}$, this differentiation will act not only on $\exp[i\sum\mathbf{p}_s\cdot\xi_s]$ but also on the intermediate factor of p_{sx}. Correcting for this additional differentiation introduces a factor $-(eB/2c)y$, cancelling the term in y already present and giving finally

$$O_1\rho=\tilde{U}\tilde{O}_1\tilde{\rho}, \quad (15)$$

where

$$\tilde{O}_1=\left[p_{sx}+i\frac{eB}{2c}\hbar\left(\frac{\partial}{\partial p_{sy}}\right)_{op}\right]f. \quad (16)$$

A similar process converts $mv_{sy}\rho$ into $\tilde{U}[p_{sy}-i(eB/2c)\hbar\times(\partial/\partial p_{sx})_{op}]f\tilde{\rho}$. Clearly, successive factors of mv_x and mv_y may be commuted with $\tilde{U}$ seriatim. Equation (15) is then a general result, and $\tilde{O}$ is obtained from O by replacing

$$p_x+\frac{eB}{2c}y=p_x+\frac{eB}{2c}i\hbar\frac{\partial}{\partial p_y}$$

with

$$p_x+\frac{eB}{2c}i\hbar\left(\frac{\partial}{\partial p_y}\right)_{op}$$

and making the corresponding changes for mv_y.

Note that v_x and v_y do not commute. The value of their commutator is preserved under the transformation to $\tilde{v}_x$ and $\tilde{v}_y$.

The procedure we have followed depends only on the properties of $\tilde{U}$ and could, in fact, be carried out without reference to ξ.

Let us now consider the form ρO. Clearly

$$\rho O_0=\tilde{U}(\tilde{\rho}O_0), \quad (17)$$

where the commutators in $\tilde{U}$ [cf. Eq. (8)] now include O_0. One may perform a series of steps as led to (15) to obtain a corresponding relation for ρO. However, a general expression is not needed, since (15) is adequate for finding expectations. We do need to transform $[H,\rho]$ to obtain an equation of motion for $\tilde{\rho}$. In light of (17), this means we need to find $\sum_s[(mv_s^2),\rho]$.

This commutator is conveniently found by expanding $\exp[-i\sum(e/c)\mathbf{A}_s\cdot\xi_s]$ as in (6) and (8), and rewriting factors of ξ_s in terms of $(\partial/\partial\mathbf{p}_s)_{op}$. The manipulations are straightforward but lengthy. One obtains

$$[H,\rho]=\tilde{U}\left\{\sum_s\left[\frac{1}{2m}\mathbf{p}_s^2,\tilde{\rho}\right]\right.$$
$$+\frac{eB}{2mc}(p_{sx}[y_s,\tilde{\rho}]+[y_s,\tilde{\rho}]p_{sx}$$
$$-p_{sy}[x_s,\tilde{\rho}]-[x_s,\tilde{\rho}]p_{sy})$$
$$\left.+\left[U(\mathbf{r}_s,\boldsymbol{\sigma}_s)+\tfrac{1}{2}\sum_{s'\neq s}V(\mathbf{r}_s,\mathbf{r}_{s'}),\tilde{\rho}\right]\right\}. \quad (18)$$

Equation (8) may be differentiated by time. Combining the result with (18) gives

$$\left\{i\hbar\frac{\partial\rho}{\partial t}-[H,\rho]\right\}=0$$
$$=\tilde{U}\left\{[\bar{H},\rho]+\tfrac{1}{2}\omega_c\sum_s(p_{sx}[y_s,\tilde{\rho}]+[y_s,\tilde{\rho}]p_{sx}\right.$$
$$\left.-p_{sy}[x_s,\tilde{\rho}]-[x_s,\rho]p_{sy})-i\hbar\frac{\partial\tilde{\rho}}{\partial t}\right\}, \quad (19)$$

in which

$$\bar{H}\equiv\sum_s\left\{\frac{\mathbf{p}_s^2}{2m}+U(\mathbf{r}_s,\boldsymbol{\sigma}_s)+\tfrac{1}{2}\sum_{s'\neq s}V(\mathbf{r}_s,\mathbf{r}_{s'})\right\}. \quad (20)$$

Since $\tilde{U}$ operating on functions which vanish exponentially at infinite $\mathbf{r}$ and $\mathbf{p}$ is nonsingular, the expression inside the braces in (19) is the desired equation of motion of $\tilde{\rho}$.

Let O_1 be some operator of physical interest. We take the trace of Eq. (15). But since $\mathrm{Tr}(\partial/\partial\mathbf{p}_s)_{op}{}^n\tilde{O}_1\tilde{\rho}=0$, we have only

$$\mathrm{Tr}O_1\rho=\mathrm{Tr}\tilde{O}_1\tilde{\rho}. \quad (21)$$

Thus in place of (1) we have (21) and in place of (2) we have

$$i\hbar\frac{\partial\tilde{\rho}}{\partial t}=[\bar{H},\tilde{\rho}]-\frac{e}{2mc}\sum_s\{\mathbf{p}_s\times\mathbf{B}\cdot[\mathbf{r}_s,\tilde{\rho}]+[\mathbf{r}_s,\tilde{\rho}]\cdot\mathbf{p}_s\times\mathbf{B}\}. \quad (22)$$

To carry out the manipulations above, we have made a gauge choice described in Eq. (5). It is of some interest to see where the gauge dependence of ρ has gone and to generalize somewhat our original gauge choice.

Any vector potential of the form

$$A=B(a_1x\hat{\mathbf{y}}-a_2y\hat{\mathbf{x}}) \quad (23)$$

represents an acceptable gauge as long as $a_1+a_2=1$. Our particular gauge choice was made so that $[\mathbf{p}\cdot\boldsymbol{\xi},\mathbf{A}\cdot\boldsymbol{\xi}]=0$. In the more general gauge of (23),

$$[\mathbf{p}\cdot\boldsymbol{\xi},\mathbf{A}\cdot\boldsymbol{\xi}]=i\hbar\xi_x\xi_yB(a_2-a_1). \quad (24)$$

We then have

$$e^{i[\mathbf{p}-(e/c)\mathbf{A}]\cdot\boldsymbol{\xi}}=e^{-i(e/c)\mathbf{A}\cdot\boldsymbol{\xi}}e^{-\hbar\xi_x\xi_yeB(a_2-a_1)/2c}e^{i\mathbf{p}\cdot\boldsymbol{\xi}}. \quad (25)$$

We convert $i\boldsymbol{\xi}$ to $(\partial/\partial\mathbf{p})_{op}$ as before and obtain

$$\exp\left\{\frac{eB}{c}\left[-a_1x\left(\frac{\partial}{\partial p_y}\right)_{op}+a_2y\left(\frac{\partial}{\partial p_x}\right)_{op}\right]+i\hbar^{\frac{1}{2}}(a_2-a_1)\left(\frac{\partial}{\partial p_x}\right)_{op}\left(\frac{\partial}{\partial p_y}\right)_{op}\right\}e^{i\mathbf{p}\cdot\boldsymbol{\xi}}=\tilde{U}(a_1,a_2)e^{i\mathbf{p}\cdot\boldsymbol{\xi}}. \quad (26)$$

Now we construct, for example,

$$mv_x\rho=mv_x\tilde{U}(a_1,a_2)\tilde{\rho}=[p_x+(eB/c)a_2y]\tilde{U}(a_1a_2)\tilde{\rho}. \quad (27)$$

The term $(eB/c)a_2y$ commutes with $\tilde{U}(a_1,a_2)$. Moving p_x through the first factor in (27) adds a correction term

$$\frac{eB}{c}a_1(i\hbar)\left(\frac{\partial}{\partial p_y}\right)_{op} \quad (28)$$

and from the second factor we get another term

$$(-eB/c)a_2y \quad (29)$$

and from the third factor, we get a term

$$\frac{eB}{c}i\hbar^{\frac{1}{2}}(a_2-a_1)\left(\frac{\partial}{\partial p_y}\right)_{op}. \quad (30)$$

Thus, altogether, we have

$$\left(p_x+\frac{eB}{c}a_2y\right)\tilde{U}(a_1,a_2)=\tilde{U}(a_1,a_2)\left[p_x+\frac{i\hbar eB}{2c}(a_1+a_2)\left(\frac{\partial}{\partial p_y}\right)_{op}\right]. \quad (31)$$

But since $a_1+a_2=1$, we regain the expression (16), independent of the gauge. Higher powers of v_x as well as v_y are handled similarly. Our use of Eqs. (21) and (22) instead of (1) and (2) thus achieves the total elimination of the gauge from the formalism. All gauge effects are incorporated into the operator $\tilde{U}$ which effects the transformation.

These equations must be used with extreme care, however, for the transformation (8) has some very strange properties. In particular, we know that ρ must have only positive eigenvalues. This requirement leads to *negative* as well as positive eigenvalues for $\tilde{\rho}$. Also, if we treat a single system, rather than an ensemble, i.e., a "pure" state, then $\rho^2=\rho$. This property is also destroyed by the nonsimilarity transformation (8). We elaborate on these oddities in the following paper where solutions of (19) are exhibited appropriate to more specific circumstances.

IV. VARIATIONAL PRINCIPLE

The equation of motion for $\tilde{\rho}$ is in an unusual form. While still bearing a resemblance to the Liouville equation in some terms, it contains additional terms. It cannot necessarily be cast into the form of an ordinary Liouville equation for $\tilde{\rho}$ with an effective Hamiltonian.

We mean for the formalism developed here to be of quite general utility, however. Hence, we wish to display a general method for solving dynamical problems cast in this form. In fact, in the next paper, we succeed in rephrasing our specific problem in the form of the ordinary Liouville equation by means of a time-dependent transformation. For cases in which such transformations are not available or of excessive complexity, we present the following general procedure.

Our goal is the solution of the operator equation (22), but since part of $\bar{H}$ is the interaction operator $\frac{1}{2}\sum_{i\neq j}V(\mathbf{r}_i-\mathbf{r}_j)$ an exact solution is clearly out of the question. At some initial instant, however, we may choose ρ—or $\tilde{\rho}$—arbitrarily without loss of generality (requiring that $\tilde{\rho}^+=\tilde{\rho}$). This corresponds to the freedom to prepare an ensemble in any initial state. From this initial state we have thus to determine the state at later times in accord with the Schrödinger equation, or equivalently, from the initial $\rho(0)$, to find subsequent

$\rho(t)$ from the Liouville equation, or again equivalently, from a starting $\tilde{\rho}(0)$, to find subsequent $\tilde{\rho}(t)$ from Eq. (22).

We have elsewhere[6] discussed the solving of the Schrödinger equation by a variational approximation due to Frenkel. We show here how an analogous procedure can lead to approximate solutions of (2) or (22).

At some starting instant, $t=0$, let $\rho=\rho(0)$. A time Δt later,

$$\rho=\rho(0)+\frac{\partial\rho}{\partial t}\Delta t$$

$$=\rho(0)+\frac{1}{i\hbar}[H,\rho]\Delta t, \tag{32}$$

from Eq. (2).

Now we are free to choose a simple expression for $\rho(0)$, but in general, $[H,\rho]$ will still be of uncomputable complexity. We must, therefore, approximate $\partial\rho/\partial t\cong\Xi$. This function Ξ will depend on $\mathbf{v}_i$ and $\mathbf{r}_i$ in general, and may also contain adjustable parameters b_i. We construct for Ξ as general a function as we can, consistent with carrying out the operations we shall have to perform on it. The b_i are then chosen to make Ξ the "best" approximation to $\partial\rho/\partial t$ out of the set of functions determined by the ranges of the b_i; the b_i are determined variationally.

Consider the difference $(\partial\rho/\partial t-\Xi)$. Clearly,

$$\left\langle\left(\frac{\partial\rho}{\partial t}-\Xi\right)^{\dagger}\left(\frac{\partial\rho}{\partial t}-\Xi\right)\right\rangle\geq 0. \tag{33}$$

The expectation signs in (33) are meant to refer to any diagonal element of the operator. Let

$$I\equiv\mathrm{Tr}\left|\frac{\partial\rho}{\partial t}-\Xi\right|^{2}\geq 0. \tag{34}$$

The equality sign holds only where $\partial\rho/\partial t$ and Ξ are strictly equal [consider the representation in which $(\partial\rho/\partial t)-\Xi$ is diagonal].

We minimize I with respect to the b_i to obtain the best approximate Ξ. Thus

$$\frac{\delta I}{\delta b_i}=-\mathrm{Tr}\left\{\left(\frac{\partial\rho}{\partial t}-\Xi\right)\frac{\delta\Xi^{\dagger}}{\delta b_i}+\frac{\delta\Xi}{\delta b_i}\left(\frac{\partial\rho^{\dagger}}{\partial t}-\Xi^{\dagger}\right)\right\}$$

$$=-2\,\mathrm{Re}\,\mathrm{Tr}\frac{\delta\Xi^{\dagger}}{\delta b_i}\left(\frac{\partial\rho}{\partial t}-\Xi\right)$$

$$=0. \tag{35}$$

Now ρ must be Hermitian to describe a physical state. Then $\partial\rho/\partial t$ is likewise Hermitian. If our approximate $\partial\rho/\partial t$ is not, we can make it so by forming $\frac{1}{2}(\Xi^{\dagger}+\Xi)$ and proceeding; we will lose no generality in this. Then $\delta\Xi$ will also be Hermitian, and since the b_i can always be taken as real, any imaginary part of (35) will have no physical content. In particular, we could set the complete expression

$$\mathrm{Tr}\frac{\delta\Xi^{\dagger}}{\delta b_i}\left(\frac{\partial\rho}{\partial t}-\Xi\right)=0. \tag{36}$$

Frequently (36) is useful even when care is not taken to make $\delta\Xi$ Hermitian. The imaginary part of (36) is trivially satisfied. Usually a combination of $\delta/\delta b_i$ and $\delta/\delta b_i^*$ can be chosen to make $\delta\Xi$ Hermitian. Since half of the resulting equations are trivial, the use of (36) instead of (35) only introduces redundant expressions. This could be anticipated; Eq. (34) contains all the physics of Eq. (32), which latter equation yields a complete dynamics. The apparent ambiguity of (35) hides no new physics.

Equations (35) and (36) relate simply to the Frenkel variational principle[4] on the wave functions. Let us define a new operator θ by

$$\Xi=[\theta,\rho]. \tag{37}$$

Since $\partial\rho/\partial t=(i\hbar)^{-1}[H,\rho]$, Eq. (36) can be written

$$\mathrm{Tr}\frac{\delta\Xi^{\dagger}}{\delta b_i}([H-i\hbar\theta,\rho])=0. \tag{38}$$

Let us write ρ in terms of some basis vectors $|\epsilon_i\rangle$:

$$\rho=|\epsilon_i\rangle\rho_{ij}\langle\epsilon_j|. \tag{39}$$

Now,

$$\frac{\partial\rho}{\partial t}=\sum_{i,j}\left\{\frac{\partial}{\partial t}|\epsilon_i\rangle\rho_{ij}\langle\epsilon_j|+|\epsilon_i\rangle\rho_{ij}\frac{\partial}{\partial t}\langle\epsilon_j|\right\}. \tag{40}$$

Now $\partial\rho/\partial t$ is expressed in terms of $\partial|\epsilon_j\rangle/\partial t$ and thus Ξ, the approximate $\partial\rho/\partial t$, may be expressed in terms of approximate $\partial|\epsilon_j\rangle/\partial t$ which we shall call $|\theta_j\rangle$:

$$\Xi=\sum_{ij}\{|\theta_i\rangle\rho_{ij}\langle\epsilon_j|+|\epsilon_i\rangle\rho_{ij}\langle\theta_j|\}. \tag{41}$$

The operator θ of Eq. (37) therefore replaces $|\epsilon_j\rangle$ with an approximation to $\partial|\epsilon_j\rangle/\partial t$. Taking variations,

$$\delta\Xi=\sum_{ij}\{(\delta|\theta_i\rangle)\rho_{ij}\langle\epsilon_j|+|\epsilon_i\rangle\rho_{ij}\delta\langle\theta_j|\}. \tag{42}$$

By rearranging operators under the Tr we can now write (38) as

$$\sum_{j,l,m}\rho_{jl}\{\delta\langle\theta_l|\}(H-i\hbar\theta)|\epsilon_m\rangle\rho_{mj}$$
$$+\sum\langle\epsilon_j|\{\delta|\theta_i\rangle\}\rho_{il}\langle\epsilon_l|(H-i\hbar\theta)|\epsilon_m\rangle\rho_{mj}$$
$$+\sum\rho_{jl}\langle\epsilon_l|H-i\hbar\theta\{\delta|\theta_m\rangle\}\rho_{mj}$$
$$+\sum\langle\epsilon_j|H-i\hbar\theta|\epsilon_l\rangle\rho_{lm}\langle\epsilon_m|\{\delta\theta_i\rangle\}\rho_{ij}=0. \tag{43}$$

Choosing a set of $|\epsilon_i\rangle$ which diagonalize ρ, we obtain

$$\sum_j \rho_j^2\{\delta\langle\theta_j|\}(H|\epsilon_j\rangle - i\hbar|\theta_j\rangle) + \sum_j \rho_j^2(\langle\epsilon_j|H + i\hbar\langle\theta_j|)\{\delta|\theta_j\rangle\} = 0. \quad (44)$$

If we further specialize ρ to describe a pure state ($\rho^2=\rho$), we obtain

$$\mathrm{Re}\int \delta\theta^*(H\psi - i\hbar\theta)dv = 0, \quad (45)$$

which is Frenkel's variational equation.

Thus as long as we work with the Liouville equation, application of either Frenkel's principle or Eq. (35) will produce the same results. In the modified formalism of Sec. II, however, $\partial\tilde{\rho}/\partial t$ is not expressed as a commutator, $[\tilde{\rho},H]$, but includes additional terms which are not manifestly of the form $[\tilde{\rho},\tilde{H}']$.

Our demonstration of the equivalence of the two variational principles depends on the expression of $\partial\rho/\partial t$ as $(1/i\hbar)[H,\rho]$, a simple commutator. We therefore relinquish Frenkel's simpler form in favor of the more generally applicable Eqs. (35) or (36).

To make (35) or (36) useful, we assume a form for an approximate ρ in which the time appears explicitly. At some starting instant, $t=0$, the true density matrix may be taken as $\rho(0)$ without loss of generality. We calculate $\partial\rho/\partial t$ on the basis of our assumed time dependence and use this for Ξ. Also for the true, or exact $\partial\rho/\partial t$ as it appears in (35) we can use Eq. (2) or Eq. (22). Thus we have

$$\mathrm{Tr}\left[\frac{\delta}{\delta b_i}\left(\frac{\partial\rho}{\partial t}\right)^{\dagger}\right]\left[[H,\rho]\frac{1}{i\hbar} - \frac{\partial\rho}{\partial t}\right] = 0,$$

using Eq. (2) for simplicity, or

$$\mathrm{Tr}\left[\frac{\delta}{\delta b_1}\left(\frac{\partial\tilde{\rho}}{\partial t}\right)\right]\left[[\bar{H},\tilde{\rho}] - \frac{e}{2mc}\sum_s \{\mathbf{p}_s\times\mathbf{B}\cdot[\mathbf{r}_s,\tilde{\rho}] + [\mathbf{r}_s,\tilde{\rho}]\cdot\mathbf{p}_s\times\mathbf{B}\} - i\hbar\frac{\partial\tilde{\rho}}{\partial t}\right] = 0.$$

We make ρ or $\tilde{\rho}$ as general as we can consistent with solving the variational Eq. (35) or (36). It should finally be pointed out that Eq. (35) or (36) may also be useful as a variational approach to thermodynamic problems.

V. CONCLUSIONS

We have developed a formal structure for the study of the dynamics of a plasma in a magnetic field. Beginning with the Liouville equation, we have transformed the basic equations into forms from which the ambiguities of various gauges have been entirely removed. We have shown how Thomas's transformation can be extended to systems of arbitrary numbers of interacting particles. Also, we have given the forms of expectations of all operators describing gauge invariant, physically meaningful quantities. We have thus given the prescriptions for a complete many-body dynamics in gauge-independent form.

We have furthermore shown how approximate solutions of the operator equations of motion may be generated variationally. We shall use this method in the second paper of this series to obtain what is essentially the time dependent Hartree-Fock approximation.

We have not yet shown why the gauge-independent formalism is advantageous to use as compared to the ordinary Liouville equation. This is best shown, however, by application of the formalism to the construction of transport equations. In fact, the formalism is ideally suited to this problem; it describes plasma dynamics in just the right way for making contact with the semiclassical, Boltzmann equation approach to transport.

It should finally be mentioned that although we have developed the formalism for systems of identical particles, the extension to plasmas of arbitrary constitution is trivial. The manipulations here presented are, in fact, only a reformulation of the Schrödinger equation. This reformulation has been carried out without approximation and preserves the full generality of the original gauge-dependent form.