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Approximate Solutions of the Liouville Equation. III. Variational Principles and Projection Operators[1]

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Aspects of stationary variational principles for the Laplace-transformed Liouville equation are discussed. Projection techniques are used to derive new stationary principles applicable to the space orthogonal to the space spanned by functions occurring in the conservation laws. As a result, any trial function automatically leads to results satisfying the conservation laws. The procedure is also applied to the parity-even and parity-odd distributions which obey equations governed by the square of the Liouville operator. The technique is extended to eliminate the one-body additive contribution to the solution exactly. Finally, the ideas of the moment method, which leads to the continued-fraction representation of autocorrelation functions, are applied to variational principles. We find continued-fraction variational principles such that a zero trial function yields the usual representation. However, a trial function representing noninteracting particles contains the results of the moment method and in addition yields the exact analytic behavior for free particles.

KEY WORDS: Liouville equation; variational principles; projection operators.

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1. INTRODUCTION

In the two previous papers of this series[1,2] we discussed an approach to finding approximate solutions of the Liouville equation. We worked directly with trial functions, i.e., approximations to the N-particle distribution function that fit initial conditions exactly in the linear response domain. Each assumption as to the form of the N-particle distribution fixes the reduced distribution functions and the relations between them. This then amounts to a truncation of the hierarchy, although, of course, *all* the reduced distributions are determined and are exact at $t = 0$.

In the first paper we worked with approximations to F_N that were ordered according to a scheme of one-body additive, two-body additive terms, etc., in the particle variables. We showed how this led to closures of the BBGKY hierarchy[3] for time-dependent distribution functions. In addition, we were able to use the exact hierarchy for the equilibrium correlation functions to eliminate the interparticle potential energy from the equations for the time-dependent correlation functions. This provides "renormalized" theories where the time-dependent functions are expressed in terms of the static correlation functions.

In the second paper the theory was reformulated by using a stationary variational principle for the Laplace-transformed Liouville equation. The renormalized theories are an immediate consequence of integration by parts in the variational functional. In addition, it was shown that the one-body additive part could always be exactly eliminated from the functional, resulting in a modified propagator for the part of the distribution function that is orthogonal to the one-body additive terms.

A second line of development was initiated in Part II. In the absence of external magnetic fields, at any instant the distribution function consists of a symmetric or even-parity part that is unchanged under the operation $p_\alpha \to -p_\alpha$ (or alternatively under the operation $q_\alpha \to -q_\alpha$), and of an odd-parity part that changes sign. Either one of these parts can be exactly eliminated in favor of the other. We arrive at a variational principle for one of the parts that is governed by the operator L^2. We showed that the one-body additive approximation can be improved when the assumption is made only on the even-parity (or symmetric) part of the distribution function.

In the present paper we continue the formal analysis of the stationary variational principles. The strategy is to use projection operators to find modified principles that incorporate exact features of the problem automatically. It is then impossible to make approximations that violate the exact features. In Section 2 we work with the odd-parity part of the distribution functions and project out the vectors that guarantee satisfaction of the conservation laws. The modified principle applies then to trial functions in an orthogonal space. In Section 3 we present a general treatment of the one-body theory with arbitrary initial conditions. In Section 4 we project out the entire one-body additive part in the even- and odd-parity functionals. We construct the modified operator that acts in the orthogonal space. We carried out the elimination of the one-body part for the renormalized form of the theory involving the Liouville operator in Ref. 2, Section 3.

In Section 5 we introduce continued-fraction variational principles. Following Mori,[4] we use the ideas of the analysis of the classical moment problem.[5] We construct a finite vector space by starting with the initial distribution function and applying powers of the Liouville operator or of its square to generate a sequence of vectors. The vectors are then normalized and made orthogonal to each other. This is an approach that explicitly accounts for the short-time behavior of the distribution function, i.e., the first few frequency moments of the autocorrelation function. The distribution function can then be written as a linear combination of the vectors of the finite space, together with an orthogonal part. By varying the amplitudes of the vectors of the finite space for an arbitrary orthogonal part we gain a new form for the variational principle. The new form can be written as a continued fraction.

If the trial distribution is to take the orthogonal part equal to zero at any stage, we have the Mori approximant to the autocorrelation function. There is, however, a great advantage to the variational approach. For example, one can start with a noninteracting distribution as the trial distribution and find the projection orthogonal to the finite vector space. The resulting autocorrelation function has the correct free-streaming behavior, i.e., a branch cut in the σ plane in addition to the Lorentzian-type structure of the usual moment method. In the summary in Section 6 we outline further extensions of the present approach.

2. CONSERVATION LAWS

In the analysis of the Laplace-transformed Liouville equation, namely

$$(\sigma + L) F = F_0 \tag{1}$$

the conservation laws are of paramount importance. Let

$$\rho(\mathbf{k}) = \sum_{\alpha=1}^{N} e^{ikq_\alpha}$$

be the Fourier component of the density. Then the continuity equation is

$$\langle \rho^*, (\sigma + L) F \rangle = \langle \rho^*, F_0 \rangle \tag{2}$$

Here the notation is $\langle A, B\rangle \equiv \int d\Gamma\,(A \cdot B)\,\Phi$. In like manner, the current density has the Fourier components

$$j_\mu(\mathbf{k}) = \sum (p_{\alpha\mu}/m)\, e^{ik\cdot q_\alpha}, \qquad \mu = 1, 2, 3 \tag{3}$$

and obeys the three conservation laws

$$\langle j_\mu{}^*, (\sigma + L)\,F\rangle = \langle j_\mu{}^*, F_0\rangle \tag{4}$$

There is also a conservation law for the energy density which is somewhat arbitrary because of the ambiguity in the localization of potential energy.

We would like to find an improved variational principle in which the conservation laws are automatically satisfied. By this we mean that if a trial function is inadequate, we find it impossible to obtain a stationary value. If the trial function is general enough, the procedure should reject the part of the trial that is not compatible with the conservation laws.

It is easiest to satisfy the conservation laws when we use the odd-parity (antisymmetric) part of the distribution function. Here F^A is varied. For any approximate F^A the symmetric part of the distribution is given as

$$F^S = -(1/\sigma)\,LF^A + (1/\sigma)\,F_0{}^S \tag{5}$$

The exact F^A obeys

$$(\sigma^2 - L^2)\,F^A = \sigma F_0{}^A - LF_0{}^S \tag{6}$$

Now let $Q^S(\mathbf{p}_1 \cdots \mathbf{q}_N)$ be an even-parity function. Then

$$\sigma\langle Q^{S*}, F^S\rangle + \langle Q^{S*}, LF^A\rangle = \langle Q^{S*}, F_0{}^S\rangle \tag{7}$$

is the transport equation for Q^S. We see that with any approximate form for F^A the use of the associated F^S implies that the transport equation is automatically satisfied. In particular, the continuity equation and the energy density transport equation are automatically obeyed. It only remains to find approximations to F^A such that the momentum transport equations

$$\langle j_\mu{}^*(\mathbf{k}), (\sigma^2 - L^2)\,F^A\rangle = \langle j_\mu{}^*, \sigma F_0{}^A - LF_0{}^S\rangle \tag{8}$$

are obeyed. The trial functions must satisfy the initial condition

$$\sigma \to \infty: \qquad F^A \to (F_0{}^A/\sigma) - (LF_0{}^S/\sigma^2)$$

In certain cases it is easy to satisfy the momentum transport equation. For example, in the density autocorrelation function problem $F_0{}^A = 0$:

$$-LF_0{}^S = i\mathbf{k}\cdot\mathbf{j}(\mathbf{k}) \tag{9}$$

The trial

$$F^A = B(\mathbf{k}, \sigma)\, i\mathbf{k} \cdot \mathbf{j} \tag{10}$$

satisfies the balance equation if

$$B\langle j_\mu{}^*(\mathbf{k}), (\sigma^2 - L^2)\, \mathbf{k} \cdot \mathbf{j}(\mathbf{k})\rangle = \langle j_\mu{}^*, \mathbf{k} \cdot \mathbf{j}\rangle \tag{11}$$

The rotational invariance of L^2 makes it possible to satisfy the equation with a scalar B. Taking $\mathbf{k} = (0, 0, k)$, we find a satisfactory B.

For work with general trial functions it is important to incorporate momentum conservation in a variational principle. Consider the case where $F_0{}^A = 0$, and start from the normalized principle

$$J^A = \langle F^{A*}, LF_0\rangle\langle F^A, LF_0{}^*\rangle/\langle F^{A*}, (\sigma^2 - L^2)\, F^A\rangle \tag{12}$$

When F^A satisfies Eq. (6) exactly, the value of this functional is

$$[J^A] = \langle F^A, LF_0{}^*\rangle \tag{13}$$

For example, if $F_0 = \rho(\mathbf{k}) = F_0{}^S$, we have

$$LF_0{}^* = -i\mathbf{k} \cdot \mathbf{j}(-\mathbf{k}), \qquad [J^A] = \langle -F^A, \mathbf{k} \cdot \mathbf{j}(-\mathbf{k})\rangle$$

Thus we have an estimate of the Laplace transform of the longitudinal current Fourier component. In the present form, where F^A is varied, F^S is limited to F^A by Eq. (5). Consequently,

$$[J^A] = \sigma\langle F, \rho^*(\mathbf{k})\rangle - \langle \rho(\mathbf{k}), \rho^*(\mathbf{k})\rangle \tag{14}$$

Thus $[J^A]$ allows one to compute the Laplace transform of the density autocorrelation function. For an approximate trial F^A the quantity J^A gives an estimate of this quantity in the sense afforded by a stationary variational principle.

The current components have the normalization and orthogonality properties

$$\langle J_\mu{}^*(\mathbf{k}), j_\nu(\mathbf{k})\rangle = \delta_{\mu,\nu}(m/\theta), \qquad \theta = 1/KT \tag{15}$$

Let us introduce three normalized vectors

$$\Psi_\mu = j_\mu(\mathbf{k})(\theta/m)^{1/2} \tag{16}$$

We now write

$$F^A = \sum_{\mu=1}^{3} B_\mu \Psi_\mu + G^A \tag{17}$$

where G^A is orthogonal to each of the Ψ_μ. It will be convenient to take $\mathbf{k} = (0, 0, k)$.

Let us now introduce the form for F^A into the variational principle. The numerator contains a factor (for the density autocorrelation function case)

$$\langle F^A, LF_0{}^*\rangle = ikB_3(m/\theta)^{1/2} \tag{18}$$

together with its complex conjugate. We have used the orthogonality of G^A to the Ψ_μ. The denominator may be written as

$$\Delta \equiv \langle F^{A*}, (\sigma^2 - L^2)\, F^A\rangle = \sum_{\mu=1}^{3} B_\mu{}^* B_\mu M_{\mu\mu} - \sum_{\mu=1}^{3} B_\mu{}^*\langle \Psi_\mu{}^*, L^2 G^A\rangle$$
$$- \sum_{\mu=1}^{3} B_\mu \langle \Psi_\mu, L^2 G^{A*}\rangle + \langle G^{A*}, (\sigma^2 - L^2)\, G^A\rangle \tag{19}$$

Here

$$M_{\mu\mu} \equiv \sigma^2 - \langle \Psi_\mu{}^*, L^2 \Psi_\mu\rangle$$
$$\langle \Psi_\nu{}^*, L^2\Psi_\mu\rangle = -N\delta_{\mu,\nu} k^2\overline{p^4} - \tfrac{1}{3}\overline{p^2}\delta_{\mu\nu}\Big\langle \sum_{\alpha,\beta} (\partial^2 V/\partial q_{\beta\nu}\, \partial q_{\alpha\mu})\, e^{ik(q_\alpha - q_\beta)}\Big\rangle$$

Let us now require stationarity of J^A under variations of $B_1{}^*$ and $B_2{}^*$. It suffices to study $\partial\Delta/\partial B_1{}^* = \partial\Delta/\partial B_2{}^* = 0$. This yields

$$B_1 = -\langle \Psi_1{}^*, L^2 G^A\rangle / M_{11}\,, \qquad B_2 = -\langle \Psi_2{}^*, L^2 G^A\rangle / M_{22} \tag{21}$$

We can therefore rewrite Δ, eliminating B_1 and B_2, and

$$\Delta = B_3{}^* B_3 M_{33} - B_3{}^*\langle \Psi_3{}^*, L^2 G^A\rangle - B_3\langle G^{A*}, L^2\Psi_3\rangle + Z^A \tag{22}$$
$$Z^A = \langle G^{A*}, (\sigma^2 - L^2)\, G^A\rangle - \sum_{i=1,2} (|\langle \Psi_i{}^*, L^2 G^A\rangle|^2 / M_{22}) \tag{23}$$

Finally we vary J^A with respect to $B_3{}^*$. The result is

$$B_3\langle G^{A*}, L^2\Psi_3\rangle = Z^A \tag{24}$$

We have a new form for the variational principle

$$J_C{}^A = \frac{-k^2}{m^2}\left[M_{33} - \frac{\langle G^{A*}, L^2\Psi_3\rangle\langle \Psi_3{}^*, L^2 G^A\rangle}{Z^A}\right]^{-1} \tag{25}$$

Recall from Eq. (20) that M_{33} is an explicitly known function. The trial function enters in the quantity Z^A as well as in $\langle G^{A*}, L^2\Psi_3\rangle$.

This principle has been arrived at by varying the amplitude of the three current states for arbitrary G^A orthogonal to these states. To achieve this orthogonality, we start with an arbitrary trial distribution F^T and project out the part that lies in the space of the current states. Thus

$$G^A = F^T - \sum_{\mu=1}^{3} \Psi_\mu \langle \Psi_\mu{}^*, F^T \rangle \tag{26}$$

Now if $J_C{}^A$ is stationary, the quantity $(J_C{}^A)^{-1}$ plus a constant is also stationary. Hence it suffices to vary the structure

$$J_1{}^A \equiv -\langle G^{A*}, L^2\Psi_3\rangle\langle\Psi_3{}^*, L^2G^A\rangle/Z^A \tag{27}$$

We summarize what is involved in a practical calculation of the Laplace transform of the density autocorrelation function. One starts with a trial distribution, containing parameters or functions of a restricted class. One forms the antisymmetric part and then constructs the part G^A that is orthogonal to the current vectors. The parameters or functions involved in G^A are varied to make $J_1{}^A$ stationary. The quantity

$$J_C{}^A = -(k^2/m^2)[M_{33} - J_1{}^A]^{-1} \tag{28}$$

is then an estimate of the Laplace transform of the longitudinal current, and thus of the density autocorrelation function.

The above procedure has been carried out for the initial condition corresponding to the density autocorrelation function where LF_0 is a linear combination of the Ψ_μ. For the more general initial condition the numerator contains

$$\langle F^A, LF_0\rangle = ikB_3(mKT)^{1/2} + \langle G^A, LF_0\rangle \tag{29}$$

and the denominator is unchanged. We therefore find the same values for B_1 and B_2. The value of B_3 is now

$$B_3 = (\langle G^{A*}, LF_0\rangle - ik(mKT)^{1/2}\, Z)/M_{33}\langle G^{A*}, LF_0\rangle - ik(mKT)^{1/2}\, \langle G^{A*}, L^2\Psi_3\rangle \tag{30}$$

and

$$J = -ik(mKT)^{1/2}\,(ikB_3(mKT)^{1/2} + \langle G^A, LF_0{}^*\rangle)/(B_3M_{33} - \langle\psi_3{}^*, L^2G^A\rangle)$$

3. GENERAL SOLUTION FOR ONE-BODY ADDITIVE FUNCTIONS

To eliminate the one-body additive part in Section 4, we will first need a more general solution than that given in Ref. 2. Let

$$F^s = \sum_{\alpha=1}^{N} \psi(\mathbf{p}_\alpha/\mathbf{k})\, e^{ikq_\alpha}$$

with the general initial condition $\psi(\mathbf{p}_\alpha/\mathbf{k}/t = 0) = \psi_0(\mathbf{p}_\alpha/\mathbf{k})$. We let

$$\rho_2(k) = P_2(k)/N.$$

Then the functional is

$$\frac{J}{N} = \int \left\{\sigma^2 + \left(\frac{\mathbf{kp}}{m}\right)^2\right\} \psi^*\psi\phi\, d^3p + \sigma^2\rho_2(k)\, \Lambda^*(k)\, \Lambda(k)$$
$$+ V_0 \int \phi \frac{\partial\psi^*}{\partial\mathbf{p}} \cdot \frac{\partial\psi}{\partial\mathbf{p}}\, d^3p - \int (\psi^* s_0 + \psi s_0^*)\, \phi\, d^3p \qquad (31)$$

Here

$$\Lambda(k) = \int \phi\psi(\mathbf{p}/\mathbf{k})\, d^3p, \qquad \Lambda_0(k) = \int \phi\psi_0(\mathbf{p}/\mathbf{k})\, d^3p$$
$$s_0(\mathbf{p}/\mathbf{k}) = \psi_0(\mathbf{p}/\mathbf{k}) + \rho_2(k)\, \Lambda_0(k) \qquad (32)$$

To get this into a more familiar form, put $\psi = g/\sqrt{\phi}$. Then

$$\frac{J}{N} = V_0 \int \frac{\partial g^*}{\partial\mathbf{p}} \frac{\partial g}{\partial\mathbf{p}}\, d^3p + \int g^* g \left\{\frac{p^2}{(2mKT)^2} V_0 + \left(\frac{\mathbf{kp}}{m}\right)^2 + \sigma^2 - \frac{3V_0}{2mKT}\right\}$$
$$\times\, d^3p + \sigma^2\rho_2(k)\, \Lambda^*\Lambda - \int \{g^* s_0 + g s_0^*\} \sqrt{\phi}\, d^3p \qquad (33)$$

The terms on the first line correspond to the functional for an anisotropic oscillator. Choose $k = \{0, 0, k\}$ and set

$$\epsilon = \frac{1}{2}\left(\frac{\sigma^2}{V_0} - \frac{3}{2mKT}\right), \quad \omega^2 = \frac{1}{(2mKT)^2} + \frac{k^2}{m^2 V_0}, \quad \omega_0 = \frac{1}{2mKT} \qquad (34)$$

Then

$$\frac{J}{N} = V_0 \int \frac{\partial g^*}{\partial\mathbf{p}} \frac{\partial g}{\partial\mathbf{p}}\, d^3p + \int g^* g[\omega^2 p_3^2 + \omega_0^2(p_1^2 + p_2^2) + 2\epsilon]\, d^3p$$
$$+ \sigma^2\rho_2\Lambda^*\Lambda - \int \{g^* s_0 + g s_0^*\} \sqrt{\phi}\, d^3p \qquad (35)$$

Let $\Psi(n_1n_2n_3)$ be the eigenfunctions of the three-dimensional oscillator

$$-\tfrac{1}{2}(\partial^2/\partial\mathbf{p}^2)\, \Psi(n_1n_2n_3) + \tfrac{1}{2}\{\omega^2 p_3^2 + \omega_0^2(p_1^2 + p_2^2)\}\, \Psi(n_1n_2n_3) \qquad (36)$$
$$= \lambda(n_1n_2n_3)\, \Psi(n_1n_2n_3)$$

where

$$\lambda(n_1n_2n_3) = (n_3 + \tfrac{1}{2})\, \omega + (n_1 + n_2 + 1)\, \omega_0 \qquad (37)$$

We may expand g as

$$g = \sum A(n_1n_2n_3)\, \Psi(n_1n_2n_3) \qquad (38)$$

Then we define

$$\epsilon(n_1n_2n_3) = 2V_0(\epsilon + \lambda(n_1n_2n_3)) \tag{39}$$

$$\begin{aligned}\frac{J}{N} = \sum A^*(n_1n_2n_3)\, A(n_1n_2n_3)\, \epsilon(n_1n_2n_3) + \sigma^2\rho_2(k)\, \Lambda^*\Lambda \\ - \int \{g^*s_0 + gs_0{}^*\} \sqrt{\phi}\, d^3p\end{aligned} \tag{40}$$

With this expansion we have

$$\begin{aligned}\Lambda = \int g \sqrt{\phi}\, d^3p = \sum A(n_1n_2n_3)\, T(n_1n_2n_3) \\ T(n_1n_2n_3) = \int \Psi(n_1n_2n_3) \sqrt{\phi}\, d^3p \\ \int g^*s_0 \sqrt{\phi}\, d^3p = \sum A^*(n_1n_2n_3)\, s^0(n_1n_2n_3) \\ s_0(n_1n_2n_3) = \int \Psi^*(n_1n_2n_3)\, s_0 \sqrt{\phi}\, d^3p\end{aligned} \tag{41}$$

We now have a degenerate quadratic form. The variation of J with respect to $A^*(n_1n_2n_3)$ yields

$$A(n_1n_2n_3)\, \epsilon(n_1n_2n_3) + \sigma^2\rho_2 T^*(n_1n_2n_3)\, \Lambda = s_0(n_1n_2n_3) \tag{42}$$

with

$$\Lambda\left\{ 1 + \sigma^2\rho_2 \sum \frac{|\, T(n_1n_2n_3)|^2}{\epsilon(n_1n_2n_3)} \right\} = \sum \frac{T^*(n_1n_2n_3)\, s_0(n_1n_2n_3)}{\epsilon(n_1n_2n_3)} \tag{43}$$

The theory can be put in a more useful form by introducing the bilinear generating function

$$g(\tilde{p}/\tilde{p}') = \sum_{n_1n_2n_3} [\Psi(n_1n_2n_3/\mathbf{p})\, \Psi^*(n_1n_2n_3/\mathbf{p}')/\epsilon(n_1n_2n_3)] \tag{44}$$

We will later exhibit the explicit closed (Mehler) form. Associated with it are the functions

$$K(\mathbf{p}) = \int g(\mathbf{p}/\mathbf{p}')[\phi(p')]^{1/2}\, d^3p' \tag{45}$$

and

$$Z = \int \phi^{1/2} K(\mathbf{p})\, d^3p = \iint \phi^{1/2} g(\mathbf{p}/\mathbf{p}')(\phi')^{1/2}\, d^3p\, d^3p' \tag{46}$$

The value for Λ is then given as

$$\Lambda\{1 + \sigma^2\rho_2 Z\} = \int K(\mathbf{p})\, s_0(\mathbf{p}) \sqrt{\phi}\, d^3p \tag{47}$$

The solution for $\psi(\mathbf{p})$ is

$$\sqrt{\phi}\ \ \psi(\mathbf{p}) \equiv g(\mathbf{p}) = \int H(\mathbf{p}/\mathbf{p}')\, s_0(\mathbf{p}')[\phi(p')]^{1/2}\, d^3p' \tag{48}$$

Here $H(\tilde{p}/\tilde{p}')$ is

$$H(\mathbf{p}/\mathbf{p}') = g(\mathbf{p}/\mathbf{p}') - [\sigma^2\rho_2(k)/(1 + \sigma^2\rho_2 Z)]\, K(\mathbf{p})\, K(\mathbf{p}') \tag{49}$$

The additional, separable part of the kernel represents the effect of the term $\sigma^2\rho_2\Lambda^*\Lambda$ in the functional J. The optimum $\psi(\mathbf{p}/\mathbf{k})$ for given $\psi_0(\mathbf{p}/\mathbf{k})$ gives J the value

$$\begin{aligned}[J/N] &= -\int \psi s_0{}^*\phi\, d^3p \\ &= -\iint \sqrt{\phi}\, s_0{}^* H(\mathbf{p}/\mathbf{p}')\, s_0(p')[\phi(\mathbf{p}')]^{1/2}\, d^3p\, d^3p' \end{aligned} \tag{50}$$

This represents the solution of the one-body additive approximation for a general $s_0(p)$. For the special case of the density autocorrelation function $s_0(p) = 1 + \rho_2$ and

$$[J/N] = -\sigma^2(1 + \rho_2)^2\, Z/(1 + \sigma^2\rho_2 Z) \tag{51}$$

We now write $g(\mathbf{p}/\mathbf{p}')$ in a more compact form. We define

$$\begin{aligned} G(p_1/p_1' \,\|\, \omega\gamma) \equiv (2\pi \sinh \gamma\omega)^{-1/2} \exp[&-\tanh(\tfrac{1}{2}\gamma\omega)\, \tfrac{1}{4}(p_1 + p_1')^2 \\ &- \coth(\tfrac{1}{2}\gamma\omega)\, \tfrac{1}{4}(p_1 - p_1')^2] \end{aligned} \tag{52}$$

The Mehler bilinear generating function[6] is

$$e^{-\gamma/2} \sum_{n=0}^{\infty} e^{-\gamma n} \Psi_n(\omega_0^{1/2} p_1)\, \Psi_n(\omega_0^{1/2} p_1') = G(p_1 p_1' \,\|\, \omega_0\gamma) \tag{53}$$

Using the parametric form

$$1/\epsilon(n_1 n_2 n_3) = \int_0^\infty e^{-\gamma\epsilon(n_1 n_2 n_3)}\, d\gamma \tag{54}$$

we write

$$\begin{aligned} g(\mathbf{p}/\mathbf{p}') = \int_0^\infty & e^{-\gamma\epsilon} G(p_1/p_1' \,\|\, \omega_0\gamma) \\ & \times\ G(p_2/p_2' \,\|\, \omega_0\gamma)\, G(p_3/p_3' \,\|\, \omega\gamma)\, d\gamma \cdot 2V_0 \end{aligned} \tag{55}$$

4. ELIMINATION OF THE ONE-BODY PART

We now take up the question of improving the one-body theory for the L^2 variational principles. We first write

$$F^s = \int \hat{N}(\mathbf{p}/\mathbf{k})\, \psi(\mathbf{p}/\mathbf{k})\, dp + G^s(\mathbf{p}_1 \cdots \mathbf{q}_N/\sigma), \qquad \psi(\mathbf{p}/\mathbf{k}) = \psi(-\mathbf{p}/\mathbf{k}) \quad (56)$$

with no restrictions on G^s. Then our functional is

$$J = \langle F^{s*}, (\sigma^2 - L^2)\, F^s\rangle - \sigma\langle F^s, F_0{}^*\rangle - \sigma\langle F^{s*}, F_0\rangle \quad (57)$$

It takes the form

$$J = J_{11} + \langle G^{s*}, (\sigma^2 - L^2)\, G^s\rangle - \langle G^s, F_0{}^*\rangle\, \sigma - \sigma\langle G^{s*}, F_0\rangle$$
$$- \int \{\psi^*(p/k)\, s_0(\mathbf{p}/\mathbf{k}) + \text{c.c.}\}\, \phi\, d^3p \quad (58)$$

Here

$$s_0(p/k) = [1/\phi(p)]\langle \hat{N}^*(\mathbf{p}/\mathbf{k}), -(\sigma^2 - L^2)\, G^s + \sigma F_0\rangle$$
$$J_{11} = N \int \{\sigma^2 + (\mathbf{k}\cdot\mathbf{p}/m)^2\}\, \psi^*\psi\phi\, d^3p + \sigma^2\rho_2(k)\, A^*A$$
$$+ V_0 \int \phi\, (\partial\psi/\partial\mathbf{p})(\partial\psi/\partial\mathbf{p})\, d^3p \quad (59)$$

We use the solution of the one-body problem to eliminate $\psi(p/k)$. It is useful to introduce the phase-space operator

$$\hat{C}(\mathbf{pk}/\mathbf{p}'\mathbf{k})\, H^s(\mathbf{p}_1 \cdots \mathbf{q}_N) \equiv \hat{N}(\mathbf{p}/\mathbf{k})\langle \hat{N}^*(\mathbf{p}'/\mathbf{k}), H^s\rangle \quad (60)$$

The key operator in the analysis is

$$\hat{Q} \equiv \frac{1}{N} \iint 1/[\phi(p)]^{1/2}\, \mathscr{H}(\mathbf{p}/\mathbf{p}')\, \hat{C}(\mathbf{pk}/\mathbf{p}'\mathbf{k})\, 1/[\phi(p')]^{1/2}\, d\tilde{p}\, d\tilde{p}' \quad (61)$$

It incorporates the one-body analysis in the kernel $\mathscr{H}(p/p')$. We will also use the operators

$$\hat{M} = (\sigma^2 - L^2)\, \hat{Q}(\sigma^2 - L^2) \quad (62)$$

and the source function

$$D_0 = F_0 - (\sigma^2 - L^2)\, \hat{Q}F_0 \quad (63)$$

The solution of the one-body problem then allows us to write

$$[J] = -\sigma^2\langle F_0{}^*, \hat{Q}F_0\rangle + \langle G^{s*}, (\sigma^2 - L^2 - \hat{M})\, G^s\rangle$$
$$- \sigma\langle G^s, D_0{}^*\rangle - \sigma\langle G_2{}^*, D_0\rangle \quad (64)$$

The first term is the one-body estimate of the autocorrelation function. In the second term the operator L^2 is replaced by $L^2 + \hat{M}$. F_0 represents a new source term for G^s. In order to improve the one-body theory systematically, we now restrict the trials G^s to be orthogonal to one-body additive functions in the sense that

$$\langle G^{s*}, \hat{N}(\mathbf{p}/\mathbf{k})\rangle = 0 \tag{65}$$

for any $\mathbf{p}$. We will discuss the construction of such G^s from general trial functions later. Assuming that we have orthogonal G^s, it follows that

$$\hat{Q}G^s = 0 \tag{66}$$

Hence

$$\langle G^{s*}, D_0\rangle = \langle G^{s*}, F_0\rangle + \langle G^{s*}, L^2\hat{Q}^*F_0\rangle, \qquad \langle G^{s*}, \hat{M}G^s\rangle = \langle G^{s*}, L^2\hat{Q}L^2G^s\rangle \tag{67}$$

Our functional can be replaced by the normalized functional

$$[J] = -\sigma^2\langle F_0{}^*, \hat{Q}F_0\rangle - \sigma^2(\langle G^s, D_0{}^*\rangle\langle G^{s*}, D_0\rangle/\langle G^{s*}, (\sigma^2 - L^2 - \hat{M})\, G^s\rangle) \tag{68}$$

It is obtained in the usual way by replacing G^s by AG^s and varying the amplitude A. This is the goal of our analysis. The one-body estimate is the first term and is not subject to variation. Varying G^s leads to an improvement of the estimate of the correlation function $-\sigma\langle F^{s*}, F_0\rangle$, which is the exact stationary value of J.

Functions G^s that are orthogonal to all one-body functions may be generated by a simple projection technique. We start with a general trial function $F_T(\mathbf{p}_1 \cdots \mathbf{q}_N/\sigma)$ and form

$$G^s = F_T - \int B(\mathbf{p}_1/\mathbf{k})\, \hat{N}(\mathbf{p}_1/\mathbf{k})\, d\mathbf{p}_1 \tag{69}$$

We impose the condition

$$\begin{aligned} 0 &= \langle N^*(\mathbf{p}/\mathbf{k}), G^s\rangle \\ &= \langle \hat{N}^*(\mathbf{p}/\mathbf{k}), F_T\rangle - \int \langle \hat{N}^*(\mathbf{p}/\mathbf{k})\, \hat{N}(\mathbf{p}_1/\mathbf{k})\rangle\, B(\mathbf{p}_1/\mathbf{k})\, d\mathbf{p}_1 \end{aligned} \tag{70}$$

Since

$$\langle \hat{N}^*(\mathbf{p}/\mathbf{k})\, \hat{N}(\mathbf{p}_1/\mathbf{k})\rangle = \delta(\mathbf{p} - \mathbf{p}_1)\, N\phi(p) + \phi(p)\, \phi(p_1)\, P_2(k) \tag{71}$$

we have a soluble integral equation for $B(\mathbf{p}/\mathbf{k})$. The result is

$$NB(\mathbf{p}/\mathbf{k})\, \phi(p) = \langle \hat{N}^*(\mathbf{p}/\mathbf{k}), F_T\rangle - \phi(p)\, P_2(k)\langle \rho(\mathbf{k}), F_T\rangle/[N + P_2(k)] \tag{72}$$

We note that the previous considerations apply almost verbatim when we put the antisymmetric (odd-parity) part of the distribution function at the center of the theory. We have

$$(\sigma^2 - L^2) F^A = \sigma F_0^A - (LF_0^s/\sigma) \equiv \sigma T_0^A, \qquad T_0^A = F_0^A - (LF_0^s/\sigma^2) \tag{73}$$

with the symmetric part given by

$$F^s = (F_0^\sigma/\sigma) - (1/\sigma) LF^A \tag{74}$$

The starting point is the stationary variational principle

$$J^A = \langle F^{A*}, (\sigma^2 - L^2) F^A \rangle - \sigma\langle F^{A*}, T_0^A \rangle - \sigma\langle F^A, T_0^{A*} \rangle \tag{75}$$

The stationary value is

$$[J^A] = -\sigma\langle F^A, T_0^{A*} \rangle = -\sigma\langle F^A, T_0^A \rangle + (1/\sigma)\langle F^A, LF_0^s \rangle \tag{76}$$

If the initial condition is $F_0^A = 0$, $F_0^s = \rho(\mathbf{k})$, $[J^A]$ is the longitudinal current.

From J^A we now put

$$F^A = \int \hat{N}(\mathbf{p}/\mathbf{k})\, \psi^A(\mathbf{p}/\mathbf{k})\, d\tilde{p} + G^A(\mathbf{p}_1 \cdots \mathbf{q}_N/\sigma) \tag{77}$$

where

$$\psi^A(\mathbf{p}/\mathbf{k}) = -\psi^A(-\mathbf{p}/\mathbf{k})$$

The steps are the same. We replace F_0 by T_0^A, D_0 by

$$D_0^A = T_0^A - (\sigma^2 - L^2)\, \hat{Q} T_0^A \tag{78}$$

and

$$[J^A] = -\sigma^2 \langle T_0^{A*}, \hat{Q} T_0 \rangle - \sigma^2 \frac{\langle G^A, T_0^{A*} \rangle \langle G^{A*}, T_0^A \rangle}{\langle G^{A*}, (\sigma^2 - L^2 - \hat{M})\, G^A \rangle} \tag{79}$$

with the same operators $\hat{Q}$ and $\hat{M}$.

Considerable analysis is thus contained in the operators $\hat{M}$ and $\hat{Q}$ that occur in Eqs. (63), (66), (78), and (79). The function $\mathscr{H}(\tilde{p}/\tilde{p}')$ occurring in $\hat{M}$ and $\hat{Q}$ summarizes the explicit effect of eliminating the one-body part of the distribution function. We can easily find better estimates of the correlation function. For example, the function F_T that is used in Eq. (44) may be constructed by the moment method as a series of powers of L^2 operating on F_0. The leading term already contains two-body additive terms. The result is given in terms of a few (complicated) integrals. However, we do not enter into the details of such calculations here.

5. CONTINUED-FRACTION VARIATIONAL PRINCIPLE

In the previous sections we discussed the construction of modified variational principles using projection operator techniques. In the Section 2 we paid explicit attention to projecting out the vectors corresponding to the conservation laws in the odd-parity theory. In the Sections 3 and 4 we showed that it was possible to project out the entire one-body additive space of functions. This corresponds to an infinite number of linearly independent functions in phase space. The strategy of projection operators is at the basis of Mori's continued-fraction representation of the Laplace transform of correlation functions. A series of linearly independent functions is formed by successive operations of the Liouville operator in the initial distribution. One projects out the portion of the space orthogonal to the (finite-dimensional) vector space that is formed. We will now show that this technique can be used in conjunction with stationary variational principles.

The advantage of the variational approach lies in the residual term after a finite number of projections have been formed. This term has the same structure as the original variational functional. Thus a termination can be performed, for example, with a free-particle trial. The resulting autocorrelation functions then have the correct branch cut characteristic of free-particle streaming.

To simplify the discussion, let us study the inhomogeneous equation

$$\hat{K}f = \Psi_0 \tag{80}$$

where $\hat{K}$ is a linear, self-adjoint operator. For simplicity let

$$\langle \Psi_0{}^*, \Psi_0 \rangle = \int \Phi \Psi_0{}^* \Psi_0 \, d\Gamma = 1 \tag{81}$$

In the usual moment method we seek to approximate the inverse operator $\hat{K}^{-1}$ by constructing a finite vector space from the vectors $\Psi_0, \hat{K}\Psi_0, \ldots, \hat{K}^{n-1}\Psi_0$. Consider the norm-independent principle

$$J = -\langle f^* \Psi_0 \rangle \langle f_0{}^*, f \rangle / \langle f^*, \hat{K}f \rangle \tag{82}$$

Put

$$f = A_0 \Psi_0 + f_1 \tag{83}$$

with f_1 orthogonal to Ψ_0 in the sense $\langle \Psi_0{}^*, f_1 \rangle = 0$. We can construct a suitable f_1 from an unrestricted function G_1 by writing the projection

$$f_1 = G_1 - \Psi_0 \langle \Psi_0{}^*, G_1 \rangle \tag{84}$$

Now vary A_0 and $A_0{}^*$ in the Schwinger principle for any F_1. Then $\delta J / \delta A_0{}^* = 0$ yields

$$A_0 = -\langle f_1{}^*, \hat{K} f_1 \rangle / \langle f_1{}^*, \hat{K} \Psi_0 \rangle \tag{85}$$

and

$$J = [K_{00} - (\langle \hat{K}\Psi_0{}^*, f_1\rangle\langle f_1{}^*, \hat{K}\Psi_0\rangle/\langle f_1{}^*, \hat{K}f_1\rangle)]^{-1} \tag{86}$$

where

$$K_{00} \equiv \langle \Psi_0{}^*, \hat{K}\Psi_0\rangle \tag{87}$$

In the next step we define a new normalized vector constructed from $\hat{K}F_0$ and made orthogonal to F_0. Let

$$\Psi_1 = (\hat{K}\Psi_0 - \Psi_0\hat{1}K_{00})/\| \hat{K}\Psi_0 - \Psi_0\hat{1}K_{00} \| \tag{88}$$

We define matrix elements as

$$K_{ij} = \langle \Psi_i{}^*, \hat{K}\Psi_j\rangle \tag{89}$$

We now write

$$f_1 = A_1\Psi_1 + f_2 \tag{90}$$

with

$$\langle f_2{}^*, \Psi_0\rangle = \langle f_2{}^*, \Psi_1\rangle = 0 \tag{91}$$

Inserting this into J and performing $\delta J/\delta A_1{}^* = 0$, $\delta J/\delta A_1 = 0$,

$$A_1 = -\langle f_2{}^*, \hat{K}f_2\rangle/\langle f_2{}^*, \hat{K}\Psi_1\rangle \tag{92}$$

$$J = \left[K_{00} - \frac{K_{10}K_{10}^*}{K_{11} - (\langle \hat{K}\Psi_1{}^*, f_2\rangle\langle f_2{}^*, \hat{K}\Psi_1\rangle/\langle f_2{}^*, \hat{K}f_2\rangle)}\right]^{-1} \tag{93}$$

It is clear that one can repeat this procedure. The actual variation is made by choosing a trial G_M and constructing the associated f_M that is orthogonal to the moment vectors

$$f_M = G_M - \sum_{n=0}^{M-1} \Psi_n\langle \Psi_n{}^*, G_M\rangle \tag{94}$$

The only part that needs to be varied is the last structure

$$\langle \hat{K}\Psi_{r-1}^*, f_n\rangle f_r{}^*, \hat{K}\Psi_{r-1}\rangle/\langle f_r{}^*, \hat{K}f_r\rangle \tag{95}$$

We can put the matrix elements into a more succinct form. Introducing

$$\hat{B} = \hat{K} - K_{00}\hat{1}, \qquad \langle \Psi_0{}^*\hat{A}\Psi_0\rangle \equiv \bar{A} \tag{96}$$

we have

$$K_{01} \equiv \langle \Psi_0{}^*\hat{K}\Psi_1\rangle = \overline{A^2}/\|\hat{B}\Psi_0\|, \qquad K_{11} = 1/\|B\Psi_0\|^2[\overline{B^3} + K_{00}\overline{B^2}] \tag{97}$$

Let us now apply the continued-fraction variational principles to the antisymmetric formulation of the density autocorrelation problem. We take $F_0{}^A = 0$, $F_0{}^s = \rho(\mathbf{k})$, and

$$(\sigma^2 - L^2) F^A = -L\rho(\mathbf{k})/\sigma \tag{98}$$

Toget this into the standard form, put

$$\hat{K} = \sigma^2 - \hat{L}^2, \qquad f = \sigma F^A/\||\ L\rho\ \||, \qquad \Psi_0 = -\hat{L}\rho/\|\ L\rho\ \| \tag{99}$$

Let us look at the principles in sequence. If we work with the variational functional J_1, we make a trial f_1 starting with an unrestricted G_1 from

$$f_1 = G_1 - \Psi_0\langle\Psi_0{}^*, G_1\rangle \tag{100}$$

This corresponds to a total distribution function

$$f = \{A_0 - \langle\Psi_0{}^*, G_1\rangle\}\,\Psi_0 + G_1 \tag{101}$$

Let us now suppose that the trial G_1 is one-body additive. Since Ψ_0 is one-body additive, so is f. Thus with functional variations of G_1 the theory would not be better than a one-body functional variation using the starting functional J.

On the other hand, if we work at the level of the functional J_2, we start with an unrestricted G_2 and construct

$$f_2 = G_2 - \Psi_1\langle\Psi_1{}^*G_2\rangle - \Psi_0\langle\Psi_0{}^*G_2\rangle \tag{102}$$

This corresponds to a trial distribution for the starting functional

$$f = \{A_0 - \langle\Psi_0{}^*, G_2\rangle\}\,\Psi_0 + \{A_1 - \langle\Psi_1{}^*G_2\rangle\}\,\Psi_1 + G_2 \tag{103}$$

Now Ψ_1 is proportional to $(\hat{K} - K_{00}\hat{1})\,\Psi_0$ and the term $L^2\Psi_0$ contains two-body additive terms. Thus if we use a one-body additive trial function for G_2, we go beyond the limits of one-body theory. There is, however, little point in carrying out such a calculation since we have already done most of the work in Section 4. After eliminating the one-body part we need only take a trial constructed from $L^2\Psi_0$ and made orthogonal to all one-body functions.

Naturally, the trial functions discussed thus far are all inferior to a trial with general functional veriation of a two-body additive function. This yields Eq. (40) of Ref. 1 which will be discussed in more detail in the next paper in this series. However, it is impossible to solve the integrodifferential equations of the two-body additive approximation exactly. The variational framework of this and the preceding paper allows one to examine a variety of approximations intermediate between the one-body theory and the full two-body theory.

When one proceeds to the level of the functional J_3 even a zero value for the trial G_3 implies a trial F that contains three-body additive terms. This is a stage in the ordinary continued-fraction variation. We can easily do better. Thus we can take the trial $G_3 = -(\sigma^2 - L_0{}^2)^{-1}(L\rho(\mathbf{k})/\sigma)$, $L_0 = \sum p_\alpha/m\, \partial/\partial q_\alpha$. This is a free-streaming trial and the density autocorrelation function becomes exact in the limit of zero interaction, in contrast to the ordinary moment method. This choice for G_3 is one-body additive. While it leads to a straightforward estimate of the density autocorrelation function in terms of simple known integrals, it is possible to make a better theory. We merely use the theory of Section 4 and choose for the trial function a series of powers of $\hat{K}$ applied to Ψ_0. This function is then made orthogonal to the space of one-body additive functions.

For completeness we now set down the continued-fraction variation principles for the ordinary Liouville equation. This is slightly different since L is an anti-Hermitian operator. We start with

$$J = -\langle F_-{}^*, F_0\rangle\langle F_{-0}^*, F\rangle/\langle F_-{}^*(\sigma + L)\, F\rangle \tag{104}$$

If $\langle F_{0-}^*, F_0\rangle = 1, F_0 \equiv \Psi_0$, we find a functional

$$J_1 = -[\sigma + L_{00} - (\langle G_-{}^* L\Psi_0\rangle\langle L\Psi_0^{-*}, G\rangle/\langle G_-{}^*(\sigma + L)\, G\rangle)]^{-1} \tag{105}$$

where

$$G = F_T - \Psi_0\langle\Psi_{0-}^*, F_T\rangle, \qquad L_{00} = \langle\Psi_0^{-*}, \hat{L}\Psi_0\rangle \tag{106}$$

At the next step we introduce

$$\Psi_1 = (\hat{L} - L_{00}\hat{1})\,\Psi_0/\|(\hat{L} - L_{00}\hat{1})\,\Psi_0\| \tag{107}$$

The last structure in J_1 may be replaced by

$$(\langle G_-{}^*, \Psi_1\rangle\langle\Psi_1^{-*}, G\rangle/\langle G_-{}^*, (\sigma + L)\, G\rangle)\|(\hat{L} - L_{00}\hat{1})\,\Psi_0\|^2 \tag{108}$$

Thus the next functional is

$$-\frac{1}{J_2} = \sigma + L_{00} - \frac{\|(\hat{L} - L_{00}\hat{1})\,\Psi_0\|^2}{\sigma + L_{11} - \{\langle H_-{}^*, L\Psi_1\rangle\langle L\Psi_1^{-*}, H\rangle/\langle H_-{}^*, (\sigma + L)\, H\rangle\}} \tag{109}$$

where

$$H = F_T - \Psi_0\langle\Psi_0^{-*}, F_T\rangle - \Psi_1\langle\Psi_1^{-*}, F_T\rangle, \qquad L_{11} = \langle\Psi_1^{-*}, L\Psi_1\rangle \quad (110)$$

This continues in a self-evident manner.

6. SUMMARY

In this paper we have extended the considerations of Ref. 2. There we illustrated the utility of stationary variational principles for the Laplace transform of the Liouville equation. One obtains theories geared to the estimate of particular autocorrelation functions. For the ordinary Liouville equation one has a straightforward method of obtaining renormalized theories. The technical step of integrating by parts in the variational functional is a very efficient way of using the exact equilibrium hierarchy connecting the bare potential and the equilibirum correlation functions. We also showed in Ref. 2 that the parity-even and parity-odd parts of the distribution obeyed an equation governed by the square of the Liouville operator. In the variational formulation this is equivalent to always having the optimal odd-parity part of the distribution for an approximation even-parity part and vice versa. This formulation, however, involves the bare potential as well as equilibrium correlation functions.

In the present paper we have extended this projection technique. By projecting out a limited number of basis vectors in phase space we can find new stationary variational principles which guarantee results in accord with exact properties of the system. Thus in Section 2 we found variational principles for which the differential conservation laws must be obeyed. One operates in the vector space orthogonal to the space spanned by the vectors that enter into the conservation laws. In Section 4 we projected out the entire space of one-body additive functions for the L^2 formulation. In Section 5 we found functionals that apply to the space orthogonal to a given number of vectors used in a moment expansion. This led us to continued-fraction variational principles.

All of these techniques are conservative in the sense that they aim at consolidating known exact results and procedures. They aim at formulating the theory so that the starting point for approximations already incorporates significant knowledge. It is analogous to eliminating exact constants of the motion in classical mechanics. Thus far the approximations envisaged have been based on a division into one-body additive, two-body additive functions, etc. This is because our starting point was the development of theories based on approximations to the Liouville distribution that fit the exact microscopic initial conditions and short-time evolution. It is clear, however, that the variational formulation of Ref. 2 and the projection techniques of the present paper are not tied intrinsically to that approach. For example, one can develop hydrodynamic approximation schemes in which general functions of coordinates are admitted, and the restriction is to functions involving a few powers of particle momenta. Alternatively, the analysis may be based on divisions of L^2 into diagonal and off-diagonal parts. These matters remain to be investigated.

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