Single-particle Schrödinger fluid. I. Formulation*†

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The problem of a single quantal particle moving in a time-dependent external potential well is formulated specifically to emphasize and develop the fluid dynamical aspects of the matter flow. This idealized problem, the single-particle Schrödinger fluid, is shown to exhibit already a remarkably rich variety of fluid dynamical features, including compressible flow and line vortices. It provides also a sufficient framework to encompass simultaneously various simplified fluidic models for nuclei which have earlier been postulated on an *ad hoc* basis, and to illuminate their underlying restrictions. Explicit solutions of the single-particle Schrödinger fluid problem are studied in the adiabatic limit for their mathematical and physical implications (especially regarding the collective kinetic energy). The basic generalizations for extension of the treatment to the manybody Schrödinger fluid are set forth.

NUCLEAR STRUCTURE Fluid dynamical formulation of quantum mechanics, singleparticle behavior in nuclear collective motion, fission and heavy-ion collision, inertial parameter, adiabatic approximation.

I. INTRODUCTION

The surge of interest in recent years in nuclear heavy-ion reactions is at one time the response to newly available experimental capacity and simultaneously the embodiment and the driving force for a shift of attention towards the dynamical physics of nuclear matter flow, rather than the "structural" properties of low-lying nuclear eigenstates.¹⁻³ The present work⁴⁻⁶ follows from this viewpoint: It is an attempt to begin again with the simplest of problems and systematically to seek out and emphasize those features of relevance to the matter-flow dynamics.

The choice of a single nucleon as a first object of study in such a dynamical context, is supported, we believe, by the central lesson of nuclear manybody physics: The Pauli principle implies the shell model.⁷⁻¹⁰ It follows that an adequate description of matter flow in nuclei must encompass also matter flow in the shell model limit, and that to build such a description one ought to understand the matter flow of the single quantal particle. This paper attempts such a beginning.

In Sec. II, the idealized single-particle Schrödinger fluid is defined by the time-dependent Schrödinger equation for a single particle moving in an externally driven time-dependent potential. The fluid-like properties of such a time-dependent Schrödinger problem are extracted by use of the ansatz that the solution Ψ is in polar form.¹¹⁻¹⁹ The unique (irrotational) velocity field \vec{v}_{∞} of the wave function and the fluid density ρ emerges as a natural consequence.

In Sec. III, alternative velocity fields are considered which conveniently summarize the continuity relation, and satisfy other specified conditions, but in contrast to \vec{v}_{\otimes} , are not fixed uniquely by the solution Ψ . In Sec. IV, the line vortex singularity structure of \vec{v}_{\otimes} is studied, and seen to be strikingly analogous to the classical irrotational, but compressible, fluid flow.

Section V utilizes the adiabatic approximation to exhibit a mathematical trap in the most straightforward direct iteration method of solving the Schrödinger equation in fluid dynamical form. An improved technique is developed to obviate the obvious immediate difficulties, but leaves still some basis for residual doubt about its own convergence. Section VI considers physical implications in the adiabatic approximation for collective momenta and energy. For the latter, the variety of forms which the alternative velocity fields of Sec. III allow, are explored. Section VII summarizes different special cases of single-particle Schrödinger fluids of interest; some relationships among them are discussed. Section VIII outlines the appropriate many-body generalizations of the fundamental quantities of the problem.

II. FLUID DYNAMICAL EQUATIONS

We employ the semiclassical approach, i.e., we assume that each nucleon in the nucleus is

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moving in a single-particle potential $V(\mathbf{x}; \alpha(t))$, which is deforming with time t, through its parametric dependence on a classical shape variable $\alpha(t)$. Here $\alpha(t)$ is assumed to be an externally prescribed function of t. Thus, the Hamiltonian for the present problem is given by

$$H(\mathbf{x},\mathbf{p};\alpha(t)) = \frac{p^2}{2m} + V(\mathbf{x};\alpha(t)). \qquad (2.1)$$

The single-particle wave function $\Psi(t)$, which describes the motion of a nucleon, satisfies the time-dependent Schrödinger equation

$$H(\mathbf{x}, \mathbf{p}; \alpha(t))\Psi(\mathbf{x}, \alpha(t), t) = i\hbar \frac{\partial}{\partial t} \Psi(\mathbf{x}, \alpha(t), t). \quad (2.2)$$

Wave function in the polar form

To obtain a fluid dynamical description of the wave function $\Psi(\vec{\mathbf{x}}, \alpha(t), t)$, we use the polar form of the wave function following Madelung.¹² We first isolate the explicit time dependence in $\Psi(\vec{\mathbf{x}}, \alpha(t), t)$ by an energy phase factor, i.e., we write

$$\Psi(\mathbf{x}, \alpha(t), t) = \psi(\mathbf{x}, \alpha(t)) \exp\left[-\frac{i}{\hbar} \int^{t} \epsilon(\alpha(t')) dt'\right],$$
(2.3)

where the intrinsic energy $\epsilon(\alpha(t))$ of the nucleon depends on time through α . Then we write the complex wave function $\psi(\mathbf{x}, \alpha(t))$ in the polar form

$$\psi(\mathbf{x}, \alpha(t)) = \phi(\mathbf{x}, \alpha(t)) \exp\left[-\frac{i}{\hbar} mS(\mathbf{x}, \alpha(t))\right], \quad (2.4)$$

where $\phi(\mathbf{x}, \alpha(t))$ and $S(\mathbf{x}, \alpha(t))$ are assumed, without loss of generality, to be real functions of \mathbf{x} and α . Finally, we assume ϕ to be positive definite, thereby making the definition (2.4) unique.

The substitution of Ψ in Eq. (2.2) gives the equation for ψ :

$$H(\mathbf{x}, \mathbf{p}; \alpha(t))\psi(\mathbf{x}, \alpha(t)) - i\hbar \frac{\partial}{\partial t}\psi(\mathbf{x}, \alpha(t))$$
$$= \epsilon(\alpha(t))\psi(\mathbf{x}, \alpha(t)). \quad (2.5)$$

The substitution of the polar form of ψ into this equation yields from its real and imaginary parts a pair of coupled equations for ϕ and S:

$$\frac{1}{2}\phi\nabla^2 S + \nabla\phi \cdot \nabla S = \frac{\partial\phi}{\partial t}$$
(2.6)

and

$$\left[H - m\left(\frac{\partial S}{\partial t} - \frac{1}{2}\nabla S \cdot \nabla S\right)\right]\phi = \epsilon\phi.$$
(2.7)

We may call Eq. (2.7) a modified Schrödinger equation because it differs from the usual time-independent Schrödinger equation by an added term which we refer to as the "dynamical modification potential"

$$V_{\rm dyn} = -m \left(\frac{\partial S}{\partial t} - \frac{1}{2} \nabla S \cdot \nabla S \right). \tag{2.8}$$

We call Eq. (2.6) the continuity equation because of the natural interpretation we now discuss.

Interpretation of the probability as a fluid: Continuity equation

The physical interpretation of Eq. (2.6) as the continuity equation becomes, when we identify the probability density of the single particle as the square of the amplitude $|\phi|^2$ and recognize that Eq. (2.6), when multiplied by 2ϕ , becomes the equation of continuity familiar from classical fluid dynamics,

$$\nabla \cdot (\rho \vec{\mathbf{v}}) = -\frac{\partial \rho}{\partial t} , \qquad (2.9)$$

if the velocity field \vec{v} is identified with the negative gradient of S:

$$\vec{\mathbf{v}} = \vec{\mathbf{v}}_{\otimes} \equiv -\nabla S \,. \tag{2.10}$$

(The notation \vec{v}_{\otimes} indicates that this field is irrotational by construction: $\nabla \times \vec{v}_{\otimes} \equiv 0.$)

Because of the continuity equation (2.9) we can interpret the changing probability distribution of the single particle as a fluid of density ρ whose motion is described by the velocity field \vec{v} of Eq. (2.10). We shall refer to this fluid as the *singleparticle Schrödinger fluid*.

Relationship of the velocity field and the current

Since the velocity potential *S* is defined as proportional to the phase of the wave function ψ as in Eq. (2.4), we can invert this equation to obtain an expression for *S* in terms of ψ :

$$S = \frac{i\hbar}{2m} \ln \frac{\psi}{\psi^*} \,. \tag{2.11}$$

From Eqs. (2.10) and (2.11), the velocity field can be expressed as

$$\vec{\nabla} = \frac{i\hbar}{2m} \left[(\nabla \psi^*) / \psi^* - (\nabla \psi) / \psi \right].$$
(2.12)

On the other hand, the current of the singleparticle state $|\psi\rangle$ is defined as

$$\vec{\mathbf{J}} = \frac{i\hbar}{2m} \left(\psi \nabla \psi^* - \psi^* \nabla \psi \right) \,. \tag{2.13}$$

It follows by comparing Eqs. (2.12) and (2.13) that

$$\vec{\mathbf{J}} = \rho \vec{\mathbf{v}} \tag{2.14}$$

which is exactly the relationship between current and velocity in classical fluid dynamics.

Euler's equation and the equation of state

Of course, the continuity equation contains only the kinematic part of any fluid dynamical system. To describe the dynamical behavior of the system completely, an equation of motion (which can, in various approximations, be the Euler's equation, the Navier-Stokes equation, or other equations involving higher order spatial derivatives, such as the Burnett equations,²⁰ or their analogs) and an equation of state have to be introduced.

For a nonviscid fluid which admits a pressure p, the equation of motion is Euler's equation

$$\frac{\partial \mathbf{\tilde{v}}}{\partial t} + (\mathbf{\tilde{v}} \cdot \nabla) \mathbf{\tilde{v}} = -\nabla p / \rho \,. \tag{2.15}$$

For ideal fluids (in which the conductivity and viscosity are negligible), the gradient of the pressure p is related to the enthalpy per unit mass w of the fluid as [see, e.g., Landau and Lifshitz²¹]

$$\nabla p / \rho = \nabla w \,. \tag{2.16}$$

Then Euler's equation, Eq. (2.15), can be written in the form

$$\frac{\partial \vec{\mathbf{v}}}{\partial t} + (\vec{\mathbf{v}} \cdot \nabla) \vec{\mathbf{v}} = -\nabla w .$$
 (2.17)

A first integral of Eq. (2.17) can be obtained as

$$\frac{\partial S}{\partial t} - \frac{1}{2} (\nabla S)^2 = w , \qquad (2.18)$$

where S is the velocity potential for \mathbf{v} ($\mathbf{v} = -\nabla S$). The integration constant in Eq. (2.18), chosen here to be zero, merely sets the zero of the scale of enthalpy, the absolute value of which has no physical significance. But the left-handed side of Eq. (2.18) is proportional to the extra term V_{dyn} in the modified Schrödinger equation. Hence, if we assume that Euler's equation in the form (2.17) holds for the single-particle Schrödinger fluid, then the modified Schrödinger equation takes the form

$$(H - mw)\phi = \epsilon \phi , \qquad (2.19)$$

where w is now the "enthalpy" of the single-particle Schrödinger fluid.

Equation (2.19) relates the density $|\phi|^2$ of the single-particle Schrödinger fluid with its internal properties H and ϵ , and its fluid dynamical state via w(S). Thus it fills the role of equation of state for the single-particle fluid, although of a type somewhat simpler than most equations of state since this particular fluid lacks any quantity analogous to the temperature.

Hence, we have a set of fluid dynamical equations completely analogous to those which describe a classical fluid. This set consists of the continuity equation [Eq. (2.6)], the Euler equation [Eq. (2.17)], and an equation of state [Eq. (2.19)]. By derivation, their content is precisely that of the original time-dependent Schrödinger equation.

Irrotational compressible flows

The velocity field $\vec{\mathbf{v}}$, as a gradient (2.10) of the scalar function $S(\mathbf{x}, \alpha)$, is irrotational ($\nabla \times \mathbf{v} = 0$) whenever $\vec{\mathbf{v}}$ is differentiable. We therefore signify this velocity field (as distinguished from other velocity fields to be defined later) by $\vec{\mathbf{v}}_{\otimes}$. The function $S(\mathbf{x}, \alpha)$ which gives the complex phase of the wave function Ψ in Eq. (2.4) serves as the velocity potential for this irrotational single-particle velocity field $\vec{\mathbf{v}}_{\otimes}$.

Since S is completely defined (up to at most an additive time-dependent spatial constant) by the wave function ψ , the divergence of the velocity field,

$$\nabla \cdot \mathbf{v}_{\otimes} = -\nabla^2 S , \qquad (2.20)$$

is also completely determined by the wave function, which is determined, in turn, by the Hamiltonian. Hence, the choice of the single-particle Hamiltonian and its time dependence will determine whether the velocity field \vec{v}_{\otimes} is incompressible $(\nabla \cdot \vec{v}_{\otimes} = 0)$.

This distinguishes the single-particle Schrödinger fluid from the fluid studied by Hill and Wheeler²² (see Appendix A) for which they assumed irrotational (and implicitly, incompressible) flow. By virtue of this assumption their study is applicable only to very limited kinds of collective motion. The present formulation is specifically not restricted to incompressible flows, but allows also irrotational, but compressible, velocity fields to be described if they should arise naturally out of the Schrödinger equation, as they do in some important specific cases²³ to be discussed in paper II.

Physical nonobservability of the velocity field

The description of the density $|\psi|^2$ as a classical fluid implies that we are assigning labels to each "mass element," $|\psi|^2 \Delta x \Delta y \Delta z$, and considering its motion in time, as described by the velocity field \mathbf{v}_{\otimes} . However, in quantum mechanics, the quantity $|\psi|^2 \Delta x \Delta y \Delta z$, is interpreted as the probability of finding the nucleon in the volume element $\Delta x \Delta y \Delta z$. It would violate the uncertainty principle to attempt to define measurably the motion of such a microscopic probability element of the state ψ , or to attribute to assertions about its motion in time the implication of measurability.

We therefore view the velocity field which describes the motion of the probability fluid as a mathematical object, rather than a physically observable quantity. (The nonobservability of the velocity field is discussed more rigorously in Appendix B.) It follows that the value of the field \vec{v}_{\otimes} and, indeed, of the whole fluid dynamical interpretation, must derive solely from the insight and convenience which they offer for handling and computing the physically observable quantities, such as momentum and energy, which are valid objects of experiment.

In addition, it follows that since the velocity field in this fluid dynamical description of the wave function is physically unobservable, we are free to consider other velocity fields which might prove convenient, and which are consistent with the continuity equation, i.e., which describe correctly the change of the probability $|\psi|^2$ in time. Thus we shall choose later to consider in addition to the irrotational velocity field \vec{v}_{\otimes} , other velocity fields which satisfy the continuity equation (2.9), in spite of the fact that only the irrotational velocity field \vec{v}_{\otimes} is uniquely related to the phase of the wave function, when such fields promise insight and simplicity for the description obtained. Some of these other velocity fields will be introduced and discussed in the next section.

III. ALTERNATIVE VELOCITY FIELDS

The irrotational velocity field \mathbf{v}_{\otimes} of (2.10) is uniquely prescribed at each time by the wave function ψ . The (scalar) continuity equation (2.9) for a prescribed time-dependent density function ρ underdetermines the (vector) velocity field \mathbf{v} . It follows that many velocity fields might exist which obey continuity.

In this section, we consider some of these velocity fields^{4d} other than the unique irrotational velocity field which follows from the wave function Ψ . These velocity fields satisfy the continuity equation (2.9) only and have no direct relationships with the dynamical part (2.7) of the Schrödinger equation. Nevertheless they prove useful in expressing some dynamical quantities such as the collective kinetic energy.

Nonuniqueness of solution to continuity equation. Between the velocity field \vec{v} and the density ρ the continuity equation (2.9) provides a relationship as

$$\rho \nabla \cdot \vec{\nabla} + \nabla \rho \cdot \vec{\nabla} = -\frac{\partial \rho}{\partial t}.$$
 (3.1)

Viewed as an equation for \vec{v} , this single scalar equation is insufficient to determine the three functions of position which define this vector field. Thus, the solution of (3.1) is uniquely prescribed only when additional conditions are imposed, as, for example, the irrotational assumption (2.10) which reduces (3.1) to a single equation for the (scalar) velocity potential S, which (together with Neumann boundary conditions) admits a unique solution.

Taken alone, however, (3.1) admits many solutions $\vec{v}(\vec{x})$ for a given set of boundary conditions, some of which prove to be mathematically convenient for the discussion of the time-dependent matter flow. Of these, the incompressible velocity field, the regular velocity field, and the geometric velocity field are of some special interest.

A. Incompressible velocity field

The "incompressible velocity field" \mathbf{v}_{0} is here defined²⁴ to be that solution of (3.1) which satisfies everywhere the condition that the density at any point moving with the flow be constant; i.e., that its total derivative vanish:

$$\frac{D\rho}{Dt} = \frac{\partial\rho}{\partial t} + \vec{\mathbf{v}}_{\odot} \cdot \nabla\rho = 0.$$
(3.2)

Note that, together with continuity equation (3.1), Eq. (3.2) implies that

$$\nabla \cdot \vec{v}_{0} = 0 \tag{3.3}$$

whenever $\rho \neq 0$. Equations (3.1) and (3.2), or equivalently, (3.2) and (3.3) serve as the defining equations for the incompressible velocity^{25, 26} field \vec{v}_{ρ} .

Nonuniqueness of the incompressible velocity field

The two equations (3.2) and (3.3) are still insufficient to define all three components of \vec{v}_{\odot} uniquely.

To specify the arbitrary part of \vec{v}_{\odot} , we note that \vec{v}_{\odot} is the solution of the inhomogeneous pair of differential equations, (3.2) and (3.3), with the inhomogeneous term $-\partial \rho / \partial t$. The general solution is the sum of a particular solution and the general homogeneous solution, which we denote by \vec{v}_N , of the problem defined by (3.2) and (3.3) with $-\partial \rho / \partial t$ replaced by zero.

Nonphysicality of homogeneous solution

The subscript N denotes the fact that the velocity field \mathbf{v}_N is "nonphysical" in the present context, as we now discuss. By (3.2), \mathbf{v}_N is incompressible and everywhere perpendicular to $\nabla \rho$. That is, \mathbf{v}_N is parallel everywhere to the equidensity surfaces of the fluid. Thus the flow described by such a velocity field cannot change the density distribution of the fluid.

But for the present problem of the single-particle Schrödinger fluid, the analogous fluid density is the quantum probability density of the single particle. It follows at once that the velocity field \vec{v}_{v} is nonphysical: it always carries the probability density identically into itself, effecting therefore on the quantum probability always an identity transformation, regardless of the magnitude of \vec{v}_N . It can therefore be added in arbitrary amounts to any homogeneous solution of the problem (3.2) and (3.3), without altering the physical content of the solution. It follows that the essential physics of the incompressible velocity field resides in the particular (incompressible) solution to the continuity equation; the arbitrariness in any such solution allows the addition of \vec{v}_N in any amount but can effect no change in the physical content of the solution. We can therefore say that the incompressible condition and the continuity equation define a "physically unique" velocity field \vec{v}_{\odot} .

B. Regular velocity field

Another interesting class of solution of the continuity equation (3.1) satisfies the requirement that the velocity field \vec{v}_R is regular, exhibiting no discontinuities and no singularities in the finite \vec{x} space. We call such a velocity field a "regular" velocity field.

The convenience of such a regular velocity field, when it exists (and it can be exhibited in some particular cases), will become clear in the discussions of collective kinetic energy in Sec. VI. There, the collective kinetic energy is expressed as a sum of one integral over a quadratic form of two velocity fields and another integral which involves the singularities of the velocity field. Therefore, in any case where the regular velocity field exists, its introduction allows the expression for the collective kinetic energy to be greatly simplified.

In contrast to the irrotational condition and the incompressible condition, the condition that \vec{v}_R be regular is not easily expressible as a mathematical equation, nor do we know at present under what conditions the regularity condition is sufficient to determine a velocity field, or compatible with a given collective motion. But when it exists (as in the case of rotational motion, where $\vec{v}_R = \vec{\Omega} \times \vec{r}$) it offers substantial simplification and (at least the promise of) an intuitive interpretation.

C. Geometric velocity field

There (sometimes) exists a special case of the incompressible velocity field which can be interpreted purely in terms of geometrical considerations. We refer to it as the geometric velocity field and denote it by \tilde{v}_{G} .

Definition of the geometric field

Consider a set of orthogonal curvilinear coordinates (ξ_1, ξ_2, ξ_3) which depends on the deformation parameter $\alpha(t)$. Suppose that *all* the single-particle wave functions ψ_i for a specified collective motion can be written as functions of α through these coordinates alone with no other α dependence.²⁷ I.e., assume that

$$\psi_i = \psi_i(\xi_1(\mathbf{x}, \alpha), \xi_2(\mathbf{x}, \alpha), \xi_3(\mathbf{x}, \alpha)).$$
(3.4)

In general, any point in space with fixed values of ξ_1 , ξ_2 , and ξ_3 will move in space as time advances. The instantaneous local velocities of all such points constitute the "geometric" velocity field \vec{v}_G :

$$\vec{\mathbf{v}}_{\mathbf{G}}(\xi_1,\xi_2,\xi_3) = \vec{\mathbf{x}}(\xi_1,\xi_2,\xi_3) .$$
(3.5)

At each point \mathbf{x} we can express the geometric field \mathbf{v}_{G} in terms of a set of orthogonal unit vectors \hat{e}_{n} and the scale functions h_{n} (n=1,2,3) as follows:

$$\dot{\mathbf{v}}_{\mathbf{G}} = -\sum_{n=1}^{3} h_n(\xi_1, \xi_2, \xi_3) \dot{\xi}_n \hat{e}_n .$$
 (3.6)

Thus, the geometrical velocity field $\bar{\mathbf{v}}_{\mathbf{G}}$ is a single velocity field, completely determined for all single-particle densities $|\phi_i|^2$ by the curvilinear coordinates ξ_n , and their time dependence. [Equation (3.6) is also a convenient way to obtain $\bar{\mathbf{v}}_{\mathbf{G}}$ when the curvilinear coordinates are known.]

Geometrical velocity field as both the regular and the incompressible velocity fields

We now show that this geometrical velocity field is a regular incompressible velocity field of the single-particle Schrödinger fluid; that is, \vec{v}_{g} is regular and satisfies the equations (3.2) and (3.3).

To prove Eq. (3.2), we need only to construct $\partial \psi_i / \partial t$ and $\nabla \psi_i$:

$$\frac{\partial \psi_i}{\partial t} = \sum_{n=1}^3 \dot{\xi}_n \frac{\partial \psi_i}{\partial \xi_n}$$
(3.7)

and

$$\nabla \psi_i = \sum_{n=1}^3 \frac{1}{h_n} \frac{\partial \psi_i}{\partial \xi_n} \, \hat{e}_n \,. \tag{3.8}$$

Then by Eqs. (3.6) - (3.8), we have

$$\frac{\partial \psi_i}{\partial t} + \vec{\mathbf{v}}_{\mathbf{G}} \cdot \nabla \psi_i = 0 \tag{3.9}$$

which in turn implies that \vec{v}_{g} obeys Eq. (3.2) identically. Thus \vec{v}_{g} is incompressible.

The proof that \dot{v}_G is regular and satisfies Eq. (3.3) is more elaborate. It is executed in detail in Appendix C.

$$\mathbf{\dot{v}}_{\odot i} = \mathbf{\ddot{v}}_{\mathbf{R}i} = \mathbf{\ddot{v}}_{\mathbf{G}} \,. \tag{3.10}$$

Necessary and sufficient condition for a geometric field

Indeed, we now show that the necessary and sufficient condition for a collective motion to have a geometric velocity field \vec{v}_G is that the incompressible velocity field for every single-particle state is identical,^{25,27} i.e., if and only if

$$\mathbf{v}_{\odot i} = \mathbf{v}_{\odot j} \equiv \mathbf{v}_{\odot}$$
 for all states $|i\rangle$ and $|j\rangle$. (3.11)

If the geometric velocity field \mathbf{v}_{G} exists, then Eq. (3.10) holds for all single-particle states. But Eq. (3.10) says that the incompressible velocity field for every single-particle state is equal to one and the same \mathbf{v}_{G} . Hence, condition (3.11) is necessary.

To prove sufficiency, assume that Eq. (3.11) holds, and consider the incompressible condition (3.2), as an equation (first order partial differential equation) to determine the functional form of ϕ_i , the norm of $\psi_i = \phi_i \exp(-imS_i/\hbar)$. The solution of such a first order partial differential equation is discussed in many textbooks.²⁸ The general solution of this equation is a functional which depends only on three independent integrals, $\xi_1(\bar{\mathbf{x}}, \alpha)$, $\xi_2(\bar{\mathbf{x}}, \alpha)$, and $\xi_3(\bar{\mathbf{x}}, \alpha)$, of the set of simultaneous ordinary differential equations:

$$\frac{dx}{(\bar{\mathfrak{v}}_{\odot})_{x}} = \frac{dy}{(\bar{\mathfrak{v}}_{\odot})_{y}} = \frac{dz}{(\bar{\mathfrak{v}}_{\odot})_{z}} = dt.$$
(3.12)

Then every ϕ_i which satisfies (3.2) must be of the form

$$\phi_i = \phi_i(\xi_1, \xi_2, \xi_3) . \tag{3.13}$$

Moreover, by the continuity equation (2.6) which ϕ_i and S_i have to satisfy everywhere in space, the form (3.13) of ϕ_i also implies a similar form for S_i , and hence

$$\psi_i = \psi_i(\xi_1, \xi_2, \xi_3) . \tag{3.14}$$

But this form of ψ_i is identical with Eq. (3.4). Therefore, the geometric velocity field exists.

Condition (3.11) is hence both the necessary and the sufficient condition for a collective motion to have a geometric velocity field.

IV. VORTEX SINGULARITIES IN THE IRROTATIONAL VELOCITY FIELD

By construction [(2.10)], the irrotational velocity field \vec{v}_{\otimes} has zero curl whenever it can be differen-

tiated. However, \mathbf{v}_{\otimes} may be singular when ϕ vanishes, without violating the Schrödinger equation (2.6) and (2.7). We now show that these singularities comprise line vortices, and occur along the nodes of ψ .^{29,30}

A. Singularities of the irrotational velocity field

We write the wave function ψ as

$$\psi = u + i\mu \quad (u, \mu, \text{real}) \tag{4.1a}$$

$$=\phi \exp(-imS/\hbar). \tag{4.1b}$$

From Eq. (4.1) the expression (2.11) for S can be written as

$$S = \frac{i\hbar}{2m} \left[\ln \frac{u+i\mu}{u-i\mu} + 2\pi\theta(-u) \right]$$
(4.2)

$$= -\frac{\hbar}{m} \left[\arctan \frac{\mu}{u} + \pi \theta(-u) \right], \qquad (4.3)$$

where the function $\theta(x)$ describes a unit jump discontinuity at x = 0.

The fact that an arbitrary addition of $2n\pi$ (*n* integer) to the phase of a wave function can have no physical significance, suggests that in general Smay be multivalued. This fact is evident also in Eq. (4.2), where multivalued functions ln and arctan arise. In order to make S single-valued, we have chosen in (4.2) and (4.3) the principal branch of ln and of arctan, i.e., $-\pi < \arg(\ln) \le +\pi$ and $-\frac{1}{2}\pi < \arg(\arctan) \leq +\frac{1}{2}\pi$. With this choice for ln and arctan, the terms involving the step function θ in Eq. (4.2) are introduced to honor the convention that ϕ in (4.1b) be positive. Then S is continuous everywhere except upon certain cuts in space, which comprise the portions of the nodal surfaces of u upon which μ is negative. Across one of these cuts, S has a discontinuity of $2\pi\hbar/m$.

Using Eq. (4.2) we write the velocity field \vec{v}_{\otimes} as³¹

$$\vec{\mathbf{v}}_{\otimes} = -\nabla S = \frac{\hbar}{m} \left(\frac{u \nabla \mu - \mu \nabla u}{\phi^2} \right) , \qquad (4.4)$$

where $\phi^2 = u^2 + \mu^2$.

From Eq. (4.4) we see that $\overline{\mathbf{v}}_{\otimes}$ can become singular only when ϕ (and hence ψ , or u and μ) go to zero. One can imagine two distinct ways in which both u and μ may vanish as follows.

(1) The nodal surfaces of u intersect the nodal surfaces of μ . Then ψ is zero on the lines of intersection. This leads to line singularities in \vec{v}_{\otimes} . (2) The functions u and μ may have a common nodal surface. Let f(x, y, z) = 0 be the equation for this common nodal surface. Then u and μ contain f as a common factor. We can write $u = f\vec{u}$ and $\mu = f\vec{\mu}$, so that

$$\phi = f\overline{\phi} = f(\overline{u}^2 + \overline{\mu}^2)^{1/2}. \tag{4.5}$$

With these factorizations, the expression (4.4)

of \vec{v}_{∞} becomes

$$\vec{\mathbf{v}}_{\otimes} = \frac{\hbar}{m} \frac{\vec{u} \nabla \overline{\mu} - \overline{\mu} \nabla \overline{u}}{\overline{\phi}^2} , \qquad (4.6)$$

whence we see that such common nodal surfaces do not result in singularities in \vec{v}_{\odot} .

Hence, we can remove the common nodes of uand μ , until \overline{u} and $\overline{\mu}$ contain no common nodes. Then the singularities of \overline{v}_{\otimes} are again determined by the intersection of nodal surfaces of \overline{u} and $\overline{\mu}$. Hence, case (2) is subsumed in the following discussion of case (1).

B. Line vortex of the irrotational field

Consider the line integral of \mathbf{v}_{\otimes} along a closed path Γ in space. Assume that on Γ , \mathbf{v}_{\otimes} has no singularity. Since \mathbf{v}_{\otimes} is equal to the negative gradient of *S*, such a closed line integral is equal to the sum of the discontinuities which *S* may possess along Γ . As noted above in Eq. (4.2), discontinuities of *S* must have value magnitude $2\pi\hbar/m$. This implies that any closed line integral of \mathbf{v}_{\otimes} is quantized and

$$\oint \vec{\mathbf{v}}_{\otimes} d\vec{\mathbf{I}} = 2n\pi\hbar/m , \qquad (4.7)$$

where n is an integer. This quantization condition for circulation was first obtained by Dirac.²⁹

When Γ encircles no singularities of \vec{v}_{\otimes} , we must have n = 0 in Eq. (4.7), because the lefthand side is evidently zero. [Use Stoke's theorem and the fact that \vec{v}_{\otimes} is irrotational wherever it is not singular.]

When Γ encircles a line of singularities of \vec{v}_{\otimes} , the line integral (4.7) is generally nonzero. Then, if we let the dimension of Γ go to zero, we conclude that \vec{v}_{\otimes} must have an unbounded curl (vorticity) on the line of singularity, which, as we have already noted, is also the nodal line of ψ . We follow the terminology of classical fluid dynamics to denote such a line singularity of vorticity distribution as a *line vortex*.³² Thus we conclude that the irrotational velocity field³³ \vec{v}_{\otimes} possesses line vortices on the nodal lines of ψ .

C. Irrotational velocity field near a vortex

Consider a region in which a nodal surface of u intersects a nodal surface of μ . (See Fig. 1.) Choose an arbitrary point P along such a nodal line of ψ and consider the irrotational velocity field $\vec{v}_{\otimes} = -\nabla S$ near this point. Let \vec{r} be the position vector measured with respect to this arbitrarily chosen point.

We divide the discussion into two parts. First, we consider in (a) the simplest situation where both u and μ vary linearly in space within a small

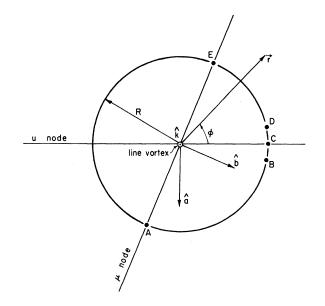


FIG. 1. Relationship between a line vortex and the nodal surfaces of the real part u and the imaginary part μ of the wave function. Unit vectors \hat{a} and \hat{b} are the normals to the u node and the μ node, respectively. The line vortex is along the polar axis \hat{k} , which is pointing perpendicular outwards from the page. The azimuthal angle ϕ is also shown. The velocity potential S on the path *ABCDEA* is schematically sketched in Fig. 3 and discussed in Appendix D.

neighborhood of *P*. Next, in (b), some of these results are generalized to cases where u and μ depend upon \mathbf{r} in higher degree.

(1) *u* and μ vary linearly. Suppose that everywhere within a small neighborhood of *P*, both *u* and μ vary linearly, i.e.,

$$u(\mathbf{r}) \simeq \mathbf{\ddot{a} \cdot \dot{r}}$$
 (4.8a)

and

$$\mu(\mathbf{r}) \simeq \mathbf{b} \cdot \mathbf{r} \,. \tag{4.8b}$$

Here

and

$$\vec{a} \equiv \nabla u \Big|_{\vec{r}=0} \tag{4.9a}$$

$$\vec{\mathbf{b}} \equiv \nabla \mu \Big|_{\vec{\mathbf{r}}=\mathbf{0}} \tag{4.9b}$$

are (constant) normals to the nodal surfaces of u and μ on the nodal line of ψ , respectively. (See Fig. 1.) From Eq. (4.3), we obtain \vec{v}_{\otimes} (to lowest order in \vec{r}) as

$$\vec{\mathbf{v}}_{\otimes} \simeq \frac{\hbar}{m} \frac{\vec{\mathbf{b}}(\vec{\mathbf{a}} \cdot \vec{\mathbf{r}}) - \vec{\mathbf{a}}(\vec{\mathbf{b}} \cdot \vec{\mathbf{r}})}{\phi^2} \\ = \frac{\hbar}{m} \frac{(\vec{\mathbf{a}} \times \vec{\mathbf{b}}) \times \vec{\mathbf{r}}}{(\vec{\mathbf{a}} \cdot \vec{\mathbf{r}})^2 + (\vec{\mathbf{b}} \cdot \vec{\mathbf{r}})^2} .$$
(4.10)

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Let the z direction \vec{k} be the direction of $\vec{a} \times \vec{b}$. The normals \vec{a} and \vec{b} then lie in the xy plane. Let the azimuthal angles of \vec{a} and \vec{b} be ϕ_a and ϕ_b , respectively. Equation (4.9) then becomes

$$\vec{\mathbf{v}}_{\otimes} \simeq \frac{\hbar}{m} g(\theta, \phi) \frac{\hat{k} \times \hat{r}}{r}$$
 (4.11)

with $g(\theta, \phi)$ dependent only upon angles, and given explicitly by the expression

$$g(\theta,\phi) = \frac{ab\sin(\phi_a - \phi_b)}{\sin^2\theta \left[a^2(\sin\phi_a \sin\phi + \cos\phi_a \cos\phi)^2 + b^2(\sin\phi_a \sin\phi + \cos\phi_a \cos\phi)^2\right]},$$
(4.12)

where a and b are the magnitudes of \overline{a} and \overline{b} , respectively.

From Eq. (4.11), we see that the irrotational velocity field v_{\otimes} has the following two properties: (a) \vec{v}_{\otimes} varies³⁴ as r^{-1} for $r \rightarrow 0$. Hence, the irrotational field is singular on the nodal line of ψ . (b) Since \mathbf{v}_{\otimes} is parallel to $\hat{k} \times \mathbf{r}$, the stream lines³⁵ of \vec{v}_{\otimes} are circles lying in the planes perpendicular to and centered upon the nodal line. Since the angles θ and ϕ cannot change the sign of the function $g(\theta, \phi)$ as can be seen from Eq. (4.12), the sense of circulation of \bar{v}_{\otimes} about the nodal line is unchanged throughout any part of a stream line. It follows that any closed line integral of \vec{v}_{\otimes} around the nodal line of ψ is nonzero. In accordance with the discussion following Eq. (4.3), we compute the value of such a closed line integral (circulation) to be $2\pi\hbar/m$, since there is only one cut for S extending out from the line vortex for the case when u and μ vary linearly in \mathbf{r} . (The circulation for a general vortex is discussed below.)

A familiar example of the velocity field³² created by a line vortex in a classical, incompressible, irrotational fluid is the velocity field

$$\vec{\mathbf{v}} = \lambda \frac{\hat{k} \times \vec{\mathbf{r}}}{\gamma^2} , \qquad (4.13)$$

where λ is the "strength" and *k* is the direction of the line vortex. Comparing this equation with Eq. (4.11), we see that the velocity field in the neighborhood of the line vortex in the present Schrödinger fluid differs from the velocity field in Eq. (4.13) by a factor $g(\theta, \phi)$, which depends on the angles. The deviation of this factor from unity distinguishes a vortex in compressible flow from a vortex in incompressible flow.

(2) u and μ vary in higher powers of \mathbf{r} . Suppose the first nonvanishing terms in the power series expansion of $u(\mathbf{r})$ and $\mu(\mathbf{r})$ about a point P on a nodal line of ψ are of powers p and q, respectively. We refer to such a case as a vortex of order (p,q). Then in a small neighborhood of P, u, and μ can be approximated by³⁶

$$u \simeq \frac{1}{p!} \sum_{i,j,\ldots,r} u_{ij,\ldots,r} (0) x_i x_j \cdots x_r$$
(4.14a)

 $\mu \simeq \frac{1}{q!} \sum_{i, j, \dots, s} \mu_{, ij, \dots, s}(0) x_i x_j \cdots x_s ,$ (4.14b)

where x_i , i=1,2,3, are the three Cartesian components of \mathbf{r} , and the sets of indices (i, j, \ldots, r) and (i, j, \ldots, s) contain p and q elements, respectively.

In this approximation, the gradients of u and μ can be found by direct operation of $\nabla \equiv \sum_i \hat{e}_i \partial / \partial x_i$ on Eq. (4.14). The results are

$$\nabla u \simeq \mathbf{\hat{a}} \equiv \frac{1}{(p-1)!} \sum_{i,j,\ldots,r} u_{i,j,\ldots,r}(0) \hat{e}_i x_j \cdots x_r \quad (4.15a)$$

and

$$\nabla \mu \simeq \mathbf{\vec{b}} \equiv \frac{1}{(q-1)!} \sum_{i, j, \dots, s} \mu_{i, j, \dots, s}(0) \hat{e}_i x_j \cdots x_s. \quad (4.15b)$$

Comparing Eq. (4.15) with (4.14), one can represent u and μ in analog with Eq. (4.8):

$$u(\mathbf{\dot{r}}) \simeq \frac{1}{p} \mathbf{\ddot{a}} \cdot \mathbf{\dot{r}}$$
 (4.16a)

and

$$\mu(\mathbf{\dot{r}}) \simeq \frac{1}{q} \, \mathbf{\ddot{b}} \cdot \mathbf{\dot{r}} \,, \tag{4.16b}$$

except that \overline{a} and \overline{b} are not constant here. The particular case (p = q = 1) of Eq. (4.16) reduces to Eq. (4.8). From Eq. (4.4), \tilde{v}_{∞} is equal to

$$\vec{\mathbf{v}}_{\otimes} = \frac{\hbar}{m} \frac{pq^2(\vec{\mathbf{a}} \cdot \vec{\mathbf{r}})\vec{\mathbf{b}} - qp^2(\vec{\mathbf{b}} \cdot \vec{\mathbf{r}})\vec{\mathbf{a}}}{q^2(\vec{\mathbf{a}} \cdot \vec{\mathbf{r}})^2 + p^2(\vec{\mathbf{b}} \cdot \vec{\mathbf{r}})^2} .$$
(4.17)

Some properties of \vec{v}_{\otimes} can be seen from this equation as follows. (a) Being the gradients of u and μ , \vec{a} and \vec{b} are vectors normal to the u node and the μ node, respectively. Hence \tilde{a} and \tilde{b} must lie on a plane perpendicular to the nodal line of ψ . Then Eq. (4.17) implies that \vec{v}_{\otimes} also lies on this perpendicular plane. (b) Since \overline{a} and \overline{b} vary as³⁴ r^{p-1} and r^{q-1} , respectively, the numerator in Eq. (4.17) varies as r^{p+q-1} . The denominator in Eq. (4.17) consists of two terms, one varying as r^{2p} and the other as r^{2q} . Thus, for any (positive integers) p and q, \mathbf{v}_{\otimes} exhibits various singular behaviors which we describe in the following.

If p = q, Eq. (4.17) reduces to

and

$$\mathbf{\tilde{v}}_{\otimes} = \frac{\hbar}{m} p \frac{(\mathbf{\tilde{a}} \times \mathbf{\tilde{b}}) \times \mathbf{\tilde{r}}}{(\mathbf{\tilde{a}} \cdot \mathbf{\tilde{r}})^2 + (\mathbf{\tilde{b}} \cdot \mathbf{\tilde{r}})^2} .$$
(4.18)

Similar to the velocity field for the linear case, case (1) [cf., Eq. (4.9)], \vec{v}_{\otimes} has circular stream lines and varies for small r as r^{-1} . However, unlike the linear case, \vec{a} and \vec{b} are not constants but vary in space.

When $p \neq q$, \vec{v}_{\otimes} has different limiting values when the vortex is approached from different directions. If p > q, then

$$2p > p + q - 1 \ge 2q . \tag{4.19}$$

The velocity \mathbf{v}_{\otimes} then tends to infinity as $r^{-p+q^{-1}}$ when $\mathbf{r} \to 0$ along the μ node. When $\mathbf{r} \to 0$ in other directions, \mathbf{v}_{\otimes} tends to zero or to finite constant values when the quantity p-q-1 is greater than or equal to zero, respectively.

For q > p, similar conclusions can be drawn with the roles of u and μ reversed.

D. Circulation of a line vortex

The circulation of \mathbf{v}_{\otimes} at the line vortex is of course given by the general formula (4.7). For a specific case, the number n in (4.7) can be determined by summing up the jump discontinuities of all the cuts which extend outwards from the line vortex. In general, the inequality

$$|n| \le \min(p, q) \tag{4.20}$$

applies, as we demonstrate in the following.

Consider again the small neighborhood of point P on the line vortex. We choose a coordinate system such that its origin is located at P and its z axis coincides with the line vortex. We calculate the circulation of \vec{v}_{\otimes} by utilizing a circular path Γ in the xy plane.

In the xy plane, the approximate expression (4.14a) for u becomes a pth order homogeneous polynomial in x and y. We can factorize this polynomial and represent u as

$$u \Big|_{z=0} = a_0 \prod_{i=1}^{p} (x - a_i y), \qquad (4.21)$$

where a_0 is real and a_i $(i=1,\ldots,p)$ can be complex. For a real a_i , the equation $x - a_i y = 0$ defines a straight line on the xy plane on which u vanishes. Since there are at most p real a_i 's, there can only be $\overline{p} \le p$ such straight lines. Since each straight line intersects the path Γ twice, u must have $2\overline{p}$ zeroes on Γ . (A degenerate zero of order m is counted as m zeroes.)

Similarly, by applying the same argument to μ , we conclude that μ has $2\overline{q} \leq 2q$ zeroes on Γ .

According to Eq. (4.2), S has a jump discontinuity of $\pm 2\pi\hbar/m$ across a cut, where the positive (nega-

tive) sign corresponds to the situation where u goes from negative (positive) to positive (negative) values in crossing the cut. Let there be n_1 and n_2 positive and negative jump discontinuities on the path Γ , respectively. Then according to Eq. (4.7) the circulation of \vec{v}_{\otimes} is $2n\pi\hbar/m$ and

$$n = n_1 - n_2 \,. \tag{4.22}$$

Since u has $2\overline{p}$ zeroes on Γ , it changes from negative to positive values at most \overline{p} times and from positive to negative values also at most \overline{p} times. This implies the inequalities,

$$\begin{cases} n_1 \leq \overline{p} \\ n_2 \leq \overline{p} \end{cases}. \tag{4.23}$$

From Eqs. (4.22) and (4.23), we conclude that

$$|n| \le \max(n_1, n_2) \le \overline{p} \le p.$$
(4.24)

On the other hand, since μ has $2\overline{q}$ zeroes on Γ , it is negative on at most \overline{q} segments of Γ . Since cuts of S lie in the regions where μ is negative, and since we have altogether $n_1 + n_2$ cuts, we have

$$n_1 + n_2 \le \overline{q} \ . \tag{4.25}$$

From Eqs. (4.22) and (4.25), we conclude that

$$|n| \le n_1 + n_2 \le \overline{q} \le q . \tag{4.26}$$

Combining this result with Eq. (4.24), we establish Eq. (4.20) which we promised to show.

V. ADIABATIC LIMIT

In this section, we consider the adiabatic limit $\dot{\alpha} \rightarrow 0$. We exhibit a natural, but false, expansion of ϕ and S in powers of $\dot{\alpha}$, and its more adequate replacement. We also discuss the behavior of the incompressible and regular velocity fields in this limit.

A. Irrotational velocity field

1. Simplest iterative approach is false

When $\dot{\alpha}$ is small it is natural to attempt an iterative solution of the fluid dynamical equations (2.6)-(2.7). On the other hand, our foreknowledge (from Sec. IV) that the velocity field exhibits singularities suggests that great care must be exercised in managing perturbative expansions. We here demonstrate this fact by considering a natural iterative procedure and showing that it leads to a false singularity structure and hence to qualitative erroneous results (in particular, nonphysical infinities in the values of certain physical quantities).

Direct iterative procedure. Consider a direct iterative approach to the solution of the fluid dy-

namical equations (2.6) and (2.7), by expansion of ϕ and S:

$$\phi = \sum_{n=0}^{\infty} (\dot{\alpha})^{2n} \hat{\phi}^{(2n)}$$
 (5.1a)

and

$$S = \sum_{n=0}^{\infty} (\dot{\alpha})^{2n+1} \hat{S}^{(2n+1)}.$$
 (5.1b)

(Here ϕ contains only even powers of $\dot{\alpha}$ because it is assumed to be positive, and *S* is odd in $\dot{\alpha}$ because the velocity field $\dot{v}_{\otimes} = -\nabla S$, which describes the collective motion, must be odd under time reversal.) Substitution of (5.1) into Eqs. (2.6) and (2.7) leads to obtain the infinite set of equations, one from the coefficient of each power of $\dot{\alpha}$:

$$(H - \epsilon^0)\hat{\phi}^{(0)} = 0 , \qquad (5.2)$$

$$\frac{1}{2}\hat{\phi}^{(0)}\nabla^{2}\hat{S}^{(1)} + \nabla\hat{\phi}^{(0)}\cdot\nabla\hat{S}^{(1)} = \dot{\alpha}\frac{\partial}{\partial\alpha}\hat{\phi}^{(0)}, \qquad (5.3)$$

$$(H - \epsilon^{0})\hat{\phi}^{(2)} = \left[\dot{\alpha} \frac{\partial \hat{S}^{(1)}}{\partial \alpha} - \frac{1}{2}\nabla \hat{S}^{(1)} \cdot \nabla \hat{S}^{(1)}\right]\hat{\phi}^{(0)},$$

.... (5.4)

The process of solving this set of equations [Eqs. (5.2)-(5.4)] successively defines the direct iterative procedure on the fluid dynamical equations.

Equation (5.2) is just the unperturbed Schrödinger equation whose solutions are the unperturbed wave functions $u^{(0)}$, chosen here real, except that our convention that ϕ is always positive implies that

$$\hat{\phi}^{(0)} = \left| u^{(0)} \right| \,. \tag{5.5}$$

Although $\hat{\phi}^{(0)}$ is continuous, its derivative is discontinuous at nodal surfaces under this convention, a sign, but not the cause, of difficulties to come. (The alternative choice $\hat{\phi}^{(0)} = u^{(0)}$ leads, for all finite $\dot{\alpha}$, to a discontinuity in the value of ϕ , and is therefore even more awkward.)

Singularities of the approximate velocity potential. The singularities of $\hat{S}^{(1)}$ can be exhibited by transforming Eq. (5.3), using (5.2) and the identity for the Laplacian of a product, into the form

$$(H - \epsilon^{0}) \left[-\frac{m}{\hbar} \hat{\phi}^{(0)} \hat{S}^{(0)} \right] = \hbar \dot{\alpha} \frac{\partial}{\partial \alpha} \hat{\phi}^{(0)}.$$
 (5.6)

This equation says that the product $-(m/\hbar)\hat{\phi}^{(0)}\hat{S}^{(1)}$ obeys the same equation,

$$(H-\epsilon^{0})\mu^{(1)} = \hbar\dot{\alpha}\frac{\partial}{\partial\alpha}u^{(0)}, \qquad (5.7)$$

as the first order correction to the wave function in the familiar cranking³⁷ model treatment of the problem. Hence one has

$$u^{(0)}\hat{S}^{(1)} = -\frac{\hbar}{m}\mu^{(1)} + \overset{\circ}{S}u^{(0)}, \qquad (5.8)$$

where \mathring{S} is an arbitrary constant and the velocity potential $S^{(1)}$ is obtained by dividing Eq. (5.8) by $u^{(0)}$. Thus,

$$\hat{S}^{(1)} = -\frac{\hbar}{m} \frac{\mu^{(1)}}{u^{(0)}} + \hat{S}^{(1)}$$
(5.9a)

$$= -\frac{\hbar}{m} \dot{\alpha} \sum_{j(\neq i)} \frac{\langle j | \partial/\partial \alpha | i \rangle}{\epsilon_j^0 - \epsilon_i^0} \frac{u_j^{(0)}}{u_i^{(0)}} + \overset{\circ}{S}, \qquad (5.9b)$$

where $\mu^{(1)}$ is written out explicitly.³⁸ (Here we write $u^{(0)} \equiv u_i^{(0)}$ and $\epsilon_i^0 \equiv \epsilon^0$.) From this result (first obtained by Gross¹⁶), one can draw some inferences about the singularity structure of $S^{(1)}$.

Each summand in Eq. (5.9b) is a ratio of an eigenfunction $u_j^{(0)}$ of the Hamiltonian *H* and the particular eigenfunction $u_i^{(0)}$. Thus, unless its eigenfunction vanishes everywhere on the nodal surface of $u_i^{(0)}$, each of these terms is singular. However, we are certain that not every eigenfunction can vanish everywhere that $u_i^{(0)}$ vanishes, since then the set of eigenfunctions $u_j^{(0)}$ ($j = 1, 2, \ldots, i, \ldots$) would not form a complete set, since every function expandable in them would have to vanish wherever $u_i^{(0)}$ vanishes. Hence some of the terms of the summation in Eq. (5.9b) must be infinitely large on the nodes of $u_i^{(0)}$.

In special cases (e.g., the case of quadrupole deformation with an harmonic oscillator potential, which will be discussed in paper II), the function $\mu^{(1)}$ may be proportional to $u^{(0)}$ so that no infinities occur. But such a cancellation depends explicitly upon interrelationships among the coefficients of $u_i^{(0)}$ for $j=1,2,\ldots$, and requires a special dependence of the eigenfunctions upon α . (These special cases possess interesting properties, e.g., the collective kinetic energy is equal to the irrotational value. Discussion of such properties can be found in the next section.) Therefore, apart from such special circumstances, which one has no reason to expect to occur in general, the expression (5.9b) is singular on the nodal surfaces of $u^{(0)}$.

Since we have seen in Sec. IV that the exact velocity potential can process singularities only on one-dimensional curves and never over two-dimensional surfaces, we must conclude that the approximation of the velocity potential by the function $\hat{S}^{(1)}$ defined in Eq. (5.9) is qualitatively erroneous. Morever, it would imply an infinitely large kinetic energy for the system as we next demonstrate.

Divergent kinetic energy implied by $\hat{S}^{(1)}$. One operational evidence of the inadequacy of the ve-

locity potential (5.9) is the fact that it implies a divergent value for the collective kinetic energy. We consider here one term of the collective kinetic energy (which itself will be discussed in more detail in the next section) of the single-particle Schrödinger fluid: the "classical fluid kinetic energy"³⁹

$$\hat{T} = \frac{1}{2} \int \hat{\rho}^{(0)} \left| \hat{\nabla}^{(1)}_{\otimes} \right|^2 d^3 x .$$
(5.10)

At a small distance ϵ from a node of $u^{(0)}$ (where $u^{(0)} \propto \epsilon, \rho^{(0)} = |u^{(0)}|^2 \propto \epsilon^2$), by Eqs. (5.9) the velocity field $\hat{\nabla}_{\otimes}^{(1)} = -\nabla \hat{S}^{(1)}$ has singularities which behave there as $1/\epsilon^2$. Thus, the collective kinetic energy density in (5.10) behaves as

$$\frac{1}{2}\hat{\rho}^{(0)} \left| \hat{\vec{\nabla}}_{\otimes}^{(1)} \right|^2 \sim \epsilon^2 \left(\frac{1}{\epsilon^2} \right)^2 \rightarrow \frac{1}{\epsilon^2} .$$
 (5.11)

Consequently, the integral (5.10) for the classical kinetic energy \hat{T} is divergent in this approximation.

However, we are certain that this same term in the kinetic energy is finite when calculated for the exact ρ and S, because then (as discussed in Sec. IV) ∇S behaves as $1/\epsilon$ near the singular line vortex while ρ behaves as ϵ^2 . Thus in the exact case, no singularity arises in $T = \frac{1}{2} \int \rho v_{\otimes}^2 d^3 x$, even though the velocity field $v_{\otimes} = -\nabla S$ is singular on its line vortices.

Since [see the next section, especially Eq. (6.20)] the collective kinetic energy of the single-particle Schrödinger fluid is the sum of this classical fluid kinetic energy and a certain additional integral, the false divergence in Eq. (5.10) would, at best, require a corresponding cancelling divergence to occur in the second integral, rendering both physically uninterpretable. At worst, there might occur no such cancellation; then this approximation would be simply wrong in its description of such a physically important quantity as the collective kinetic energy. We therefore consider $\hat{S}^{(0)}$, as given in Eq. (5.9), to be a qualitatively unacceptable approximation to the velocity potential.

2. Adiabatic cranking as a guide to improved approximation

We have seen that the naive direct iterative procedure yields an approximate velocity field with a false singularity structure in which nodal surfaces occur instead of nodal lines. We now discuss an alternative iterative procedure which corrects this deficiency in leading order by starting in "zeroth" order with a magnitude $\phi^{(0)}$, which already incorporates the (pure imaginary, in our phase convention) first order cranking correction $\mu^{(1)}$. Then, for any finite value of $\mathring{\alpha}$ this function vanishes not on the nodal surfaces of $u^{(0)}$, but only on the curves where nodes of $u^{(0)}$ cross nodes of $\mu^{(1)}$. The resulting velocity field is qualitatively better structured already in the first order.

The cue for executing this improved starting point thus lies in the cranking³⁷ model description of the adiabatic limit of the present problem. We insist that the zeroth order magnitude $\phi^{(0)}$ include the effects of cranking (or the deformation of the nuclear potential in general). Hence we write⁴⁰

$$\phi^{(0)} = \left| \left[(u^{(0)})^2 + (\mu^{(1)})^2 \right]^{1/2} \right| . \tag{5.12}$$

Then we use (5.12) and solve the continuity equation,

$$\frac{1}{2}\phi^{(0)}\nabla^2 S^{(1)} + \nabla\phi^{(0)} \cdot \nabla S^{(1)} = \dot{\alpha} \frac{\partial}{\partial \alpha} \phi^{(0)}, \qquad (5.13)$$

to obtain the first approximate $S^{(1)}$. This $S^{(1)}$ is then substituted into the modified Schrödinger equation,

$$\left[H - m\left(\dot{\alpha}\frac{\partial S^{(1)}}{\partial \alpha} - \frac{1}{2}\nabla S^{(1)} \cdot \nabla S^{(1)}\right)\right]\phi^{(2)} = \epsilon^{0}\phi^{(2)},$$
(5.14)

to obtain the second approximate $\phi^{(2)}$. In principle, the iteration would be continued by substituting back $\phi^{(2)}$ to the continuity equation to obtain a better $S^{(3)}$ and so on until the desired degree of accuracy is achieved. In practice, we have so far restricted our study to the determination of $S^{(1)}$, and to some general considerations which signal some further caution of the ensuing infinite sequence.

To execute the next iterative step, we must solve Eq. (5.13). Again the process is simplified by consideration of the cranking model solution. Since Eq. (5.12) is equivalent to approximating ψ by $u^{(0)} + i\mu^{(1)}$ except for a phase factor $\exp[i\hbar S^{(1)}/m]$, we can make use of the general expression for the velocity potential in Eq. (4.2) and assert that the solution to Eq. (5.12) is given to order $\dot{\alpha}^2$ by

$$S^{(1)} = \frac{i\hbar}{2m} \ln \frac{u^{(0)} + i\mu^{(1)}}{u^{(0)} - i\mu^{(1)}} + \mathring{S}^{(1)}.$$
 (5.15a)

[We here drop the additive term $2\pi\theta(-u)$ of Eq. (4.2) since it plays no role in the present discussion.] The first (ln) term of this equation is most important and will be denoted by the symbol $\tilde{S}^{(1)}$. Hence Eq. (5.15a) can be written simply as

$$S^{(1)} = \tilde{S}^{(1)} + \tilde{S}^{(1)}$$
. (5.15b)

The approximate velocity field derived from this velocity potential is

$$\vec{\nabla}_{\otimes}^{(1)} = -\nabla S^{(1)} = -\nabla \tilde{S}^{(1)}$$
$$= -\frac{\hbar}{m} \frac{1}{\rho^{(0)}} \left(\mu^{(1)} \nabla u^{(0)} - u^{(0)} \nabla \mu^{(1)} \right).$$
(5.16)

Since $S^{(1)}$ is defined by an expression of exactly the same (logarithmic) structure as the exact velocity potential, the entire discussion of the compressible line vortices in Sec. IV applies here. Then, $S^{(1)}$ has line vortices on the lines of intersections between the nodal surfaces of $u^{(0)}$ and $\mu^{(1)}$.

It remains to verify the assertion that $S^{(1)}$ of Eq. (5.15) satisfies the continuity equation to order of $\dot{\alpha}^2$. Substitute $S^{(1)}$ into the left-handed side of Eq. (5.13). Then use the equation $Hu^{(0)} = \epsilon u^{(0)}$ and Eq. (5.7) satisfied by $\mu^{(1)}$ to obtain

$$\rho^{(0)} \nabla^2 S^{(1)} + \nabla \rho^{(0)} \cdot \nabla S^{(1)} = 2 \dot{\alpha} u^{(0)} \frac{\partial u^{(0)}}{\partial \alpha} .$$
 (5.17)

But this equation is identical with the iterated continuity equation, Eq. (5.13), except for the term $2\dot{\alpha}\mu^{(1)}\partial\mu^{(1)}/\partial\alpha$, which is of the order $\dot{\alpha}^3$. This verifies the assertion.

It is interesting to note that the function $\phi^{(0)}$ which we have chosen by Eq. (5.12) satisfies the modified Schrödinger equation to order $\dot{\alpha}$. We can readily derive the identity

$$\begin{bmatrix} H - m \left(\dot{\alpha} \frac{\partial S^{(1)}}{\partial \alpha} - \frac{1}{2} \nabla S^{(1)} \cdot \nabla S^{(1)} \right) \end{bmatrix} \phi^{(0)}$$
$$= \epsilon^0 \phi^{(0)} + \dot{\alpha} \hbar \frac{u^{(0)}}{\phi^{(0)}} \frac{\partial \mu^{(1)}}{\partial \alpha} - m \dot{\alpha} \frac{\partial \overset{\circ}{S}^{(1)}}{\partial \alpha} \phi^{(0)}. \quad (5.18)$$

But this is precisely the modified Schrödinger equation for $S^{(1)}$ and $\phi^{(0)}$, except for the addition of the last two terms, both of which are of order $\dot{\alpha}^2$ or higher. This result is hardly surprising, because the choice of $\phi^{(0)}$ in Eq. (5.12) is equivalent to approximating ψ by the first order cranking perturbation, which in turn was constructed to satisfy the time-dependent Schrödinger equation to order $\dot{\alpha}$.

Singularities in higher order iterative velocity potentials. We have obtained so far only the first order iteration $S^{(1)}$ from the chosen $\phi^{(0)}$ in Eq. (5.12). One expects that if $\dot{\alpha}$ is too large, one may need to continue this iterative procedure to obtain contributions from higher powers of $\dot{\alpha}$.

However, the convergence of this process, as is so often true in physics, is not self-evident. Indeed, we wish to point out certain properties of the iterative scheme which open some doubt about its ability to converge to the exact solution.

Consider the singularity structure of the velocity potential. $S^{(1)}$ is singular on the nodal lines of $\phi^{(0)}$, tending to infinity as $1/\epsilon$ as the distance ϵ to a line vortex diminishes. In the next iteration for $\phi^{(2)}$, $S^{(1)}$ will be substituted into the modified Schrödinger equation, Eq. (5.14). Then the quantities $\nabla S^{(1)}$ and $\partial S^{(1)}/\partial \alpha$, which involved on differentiation (with respect to coordinates or α), exhibit singularities which behave like $1/\epsilon^2$ near nodal lines of $\phi^{(0)}$. Hence the "dynamical modification potential"

$$V_{\rm dyn} = -m \left(\dot{\alpha} \frac{\partial S^{(1)}}{\partial \alpha} - \frac{1}{2} \nabla S^{(1)} \cdot \nabla S^{(1)} \right), \qquad (5.19)$$

in the modified Schrödinger equation (5.14), acquires singularities $\sim \epsilon^{-4}$ through the term $+(\frac{1}{2}m)\nabla S^{(1)}\cdot\nabla S^{(1)}$, which behaves like an infinite repulsive potential on every node of $\phi^{(0)}$. One expects that in the next order $\phi^{(2)}$ also will be forced to have nodes precisely on the nodes of $\phi^{(0)}$. Extrapolating the above arguments to higher orders of iteration, we conclude that the magnitude of the wave function ϕ , obtained in all finite orders of iteration, will have nodes (and, correspondingly, the velocity fields will have line vortices) on the nodes of the zeroth order approximant $\phi^{(0)}$. This peculiar feature of the present iterative procedure supports the suspicion that in general the sequence of iterated solutions does not necessarily converge to the exact solution, since it can only reach solutions with the same spatial nodal structure as the starting function. Further investigation, therefore, might focus on any possible physical significance of such a nodal constraint, on the prospect of fashioning a zeroth order function which matches the exact solution in its nodal structure, and/or on the discovery of methods which allow the solution to escape this strong restriction.

We do not here offer answers to these questions. The further work reported here is based entirely on the first iteration which has been seen to be identical with the first order cranking model approximation. Hence, the validity of the present results rests upon the adequacy of the perturbation solution of the Schrödinger equation.

B. Incompressible velocity field and the regular velocity field

As has been emphasized in Sec. III. only the irrotational velocity field is uniquely determined by the wave function. All the other velocity fields which we consider (including the incompressible and the regular velocity fields) satisfy only the continuity condition (imaginary part) of the Schrödinger equation, Eq. (3.1). Since these velocity fields are not an integral part of any solution to the entire set of Schrödinger fluid equations, the question of consistent iterative approximation to them does not arise. Their structure is completely specified by the continuity equation (3.1) (in which ρ may be specified to any desired degree of accuracy), and the additional conditions which render them unique. Their adiabatic approximations, correspondingly, are simply the limits of these solutions to leading order in $\dot{\alpha}$.

Thus, the adiabatic approximation to the incompressible velocity field is defined by the solution of the first order approximation to the incompressible condition,

$$\frac{Du^{(0)}}{Dt} = \dot{\alpha} \frac{\partial u^{(0)}}{\partial \alpha} + \dot{\nabla}_{\otimes}^{(1)} \cdot \nabla u^{(0)} = 0 , \qquad (5.20)$$

and the condition from the continuity equation,

$$\nabla \cdot \overrightarrow{\mathbf{v}}_{\odot}^{(1)} = 0. \tag{5.21}$$

These two equations follow from Eqs. (3.2) and (3.3) when the density ρ is approximated by $|u^{(0)}|^2$. Thus, the discussions of the nonuniqueness of \vec{v}_{\odot} which occur in Sec. III are also here applicable to $\vec{v}_{\odot}^{(1)}$. It follows that $\vec{v}_{\odot}^{(1)}$ is unique up to additive incompressible velocity fields which are everywhere tangential to the constant density surfaces $|u^{(0)}| = \text{constant.}$

For the regular velocity field, we define its adiabatic approximation $\vec{v}_{R}^{(1)}$ as the regular solution to the analogous approximate continuity equation

$$\frac{1}{2}u^{(0)}\nabla \cdot \overrightarrow{\mathbf{v}}_{\mathbf{R}}^{(1)} + \overrightarrow{\mathbf{v}}_{\mathbf{R}}^{(1)} \cdot \nabla u^{(0)} = -\alpha \frac{\partial u^{(0)}}{\partial \alpha}.$$
 (5.22)

The two velocity fields $\vec{v}_{\otimes}^{(1)}$ and $\vec{v}_{R}^{(1)}$ defined here are particularly useful in studying the nature of the collective kinetic energy in the next section.

VI. COLLECTIVE ENERGY AND MOMENTA

Having discussed the kinematic aspects of the velocity fields in the previous sections, we are now in a position to examine the dynamical aspects of these velocity fields. Using these velocity fields, we shall study the collective kinetic energy, the collective momentum, and the collective angular momentum. The collective kinetic energy is further studied in the adiabatic limit, and is put into different forms with the help of the irrotational, the incompressible, and the regular velocity fields, respectively.^{4c,4d}

A. Relationship between the velocity field \vec{v}_{\otimes} and the collective motion

For collective motion, characterized by a finite velocity $\dot{\alpha}$, of some one (or more) collective coordinate, we now show that the velocity field $\bar{\mathbf{v}}_{\otimes}$ arises solely from the collective motion. Consider the current \mathbf{J} defined in Eq. (2.13) from which the velocity field $\bar{\mathbf{v}}_{\otimes} = \mathbf{J}/\rho$ is defined. Since $\bar{\mathbf{v}}_{\otimes}$ is zero only when \mathbf{J} is zero, it is only necessary to observe that \mathbf{J} is identically zero when the nucleus (as represented by the α -dependent nuclear potential) is not performing a collective motion. Indeed, if the nucleus is not performing a collective motion (i.e., the nuclear potential is independent

of time), then each nucleon is described by a stationary single-particle wave function, which can always be chosen to be real by adjusting the (arbitrary) constant phase. Hence the current \overline{J} vanishes⁴¹ identically when α is constant.

Conversely, if the nucleus is deforming with time (i.e., if the nuclear potential, and hence the Hamiltonian, are time-dependent), then no stationary solutions of the Schrödinger equation exist. The single-particle wave functions are "essentially" complex,⁴² and a finite matter flow exists in each single-particle state. Therefore, the velocity field \bar{v}_{\otimes} is nonzero if and only if the nucleus is in collective motion.

With the assumption that $\overline{\mathbf{v}}_{\otimes}$ is a regular function of α , this fact and the odd-time-reversal behavior of a velocity field imply that the velocity field $\overline{\mathbf{v}}_{\otimes}$ and its potential S will in general contain $\dot{\alpha}$ as a factor,⁴³ i.e.,

$$\vec{\mathbf{v}}_{\otimes}(\alpha, \dot{\alpha}) = \dot{\alpha} \vec{\mathbf{v}}_{\otimes}(\alpha, \dot{\alpha})$$
(6.1a)

and

$$S(\alpha, \dot{\alpha}) = \dot{\alpha}S'(\alpha, \dot{\alpha}) + \text{constant in space.}$$
 (6.1b)

This dependence of \overline{v}_{\otimes} and *S* on $\dot{\alpha}$ allows us to identify the physical quantities such as the collective kinetic energy and the collective momenta, which are discussed below.

We note that this dependence of S on $\dot{\alpha}$ also underlines the fact that the present formulation is especially constructed to handle problems with finite collective velocity $\dot{\alpha}$. When $\dot{\alpha} = 0$, the present formulation trivializes. (It also becomes awkward, because then the absolute magnitude ϕ of ψ has discontinuous derivatives at its nodes. However, we show (Appendix D) that these cause no inconsistencies.)

B. Collective kinetic energy for the exact single-particle state The total single-particle energy is given by the expectation value of H evaluated with the timedependent solution ψ . Writing ψ in the polar form [(2.4)] we obtain

$$\begin{aligned} \langle \psi \left| H \right| \psi \rangle &= \langle \psi \left| i\hbar \frac{\partial}{\partial t} \right| \psi \rangle \\ &= \epsilon + m \int \phi^2 \frac{\partial S}{\partial t} d^3 x + \int \phi i\hbar \frac{\partial}{\partial t} \phi d^3 x \,. \end{aligned} \tag{6.2}$$

Here the third term is identically zero (normalization of ψ).

We arrange, by construction, that ϵ be independent of $\dot{\alpha}$, as follows. Suppose that the eigenvalue $\hat{\epsilon}$ of the modified Schrödinger equation does depend upon $\dot{\alpha}$. Then separate it into two parts

$$\hat{\boldsymbol{\epsilon}} = \boldsymbol{\epsilon}^0 + \boldsymbol{\epsilon}' \,, \tag{6.3}$$

$$\overset{\circ}{S} = \frac{1}{m} \int^{t} \epsilon'(\alpha(t'), \dot{\alpha}(t')) dt'$$
(6.4)

and denote the velocity potentials before and after this definite choice of \mathring{S} by \hat{S} and S, respectively. That is

$$S = \hat{S} + \check{S} . \tag{6.5}$$

Since for \hat{S} , the modified Schrödinger equation (which involves a term proportional to $\partial S/\partial t$) was solved with eigenvalue $\hat{\epsilon}$, which we assumed to depend upon collective velocities, then for S, it is solved with eigenvalue ϵ^0 which is independent of $\dot{\alpha}, \dot{\alpha}^2$, etc., i.e.,

$$\left[H - m\left(\frac{\partial S}{\partial t} - \frac{1}{2}\nabla S \cdot \nabla S\right)\right]\phi = \epsilon^{0}\phi .$$
 (6.6)

Then by making this particular choice of \mathring{S} , we guarantee that the energy of the single-particle state in (6.2) takes the form

$$\langle \psi | H | \psi \rangle = \epsilon^{0} + m \int \rho \frac{\partial S}{\partial t} d^{3}x , \qquad (6.7)$$

where ϵ^{0} is independent of collective velocities.

The energy of the single-particle now separates into two distinct parts: a *collective potential energy* ϵ^0 which is the intrinsic quasistatic (as we see further below) energy of the single-particle state and is dependent only upon α but not upon $\dot{\alpha}$, and a *collective kinetic energy*, which may depend upon powers of the collective velocity $\dot{\alpha}$ (and higher time derivatives of α , if any). We denote the collective kinetic energy by T

$$T = m \int \rho \frac{\partial S}{\partial t} d^3 x .$$
 (6.8)

Since the modified Schrödinger equation Eq. (6.6) holds for all $\dot{\alpha}$, we can consider the limiting situation of no collective motion, i.e., $\dot{\alpha} = 0$. Then the velocity potential S must be a constant in space and time. But then (except for the δ functions discussed in Appendix D, which cause only some appropriate sign changes in the wave function to honor our convention that ϕ is positive)

$$\left[\frac{\partial S}{\partial t} - \frac{1}{2}\nabla S \cdot \nabla S\right]_{\dot{\sigma}=0} = 0.$$
(6.9)

Hence, the modified Schrödinger equation, Eq. (6.6), reduces to the quasistatic Schrödinger equation

$$Hu = \epsilon^0 u . (6.10)$$

From this equation, we see that $\varepsilon^{\rm 0}$ is the quasistatic energy of the single-particle state under consideration.

For a model nucleus of noninteracting particles, the total collective potential energy and the total collective kinetic energy can be obtained by summing up the occupied single-particle contributions.

C. Collective kinetic energy in the adiabatic approximation

In this section we consider specific aspects of the collective kinetic energy in the adiabatic cranking model approximation.

Determination of S in the adiabatic approximation. In the adiabatic approximation, we write the single-particle wave function as

$$\psi^{(1)} = \phi^{(0)} \exp\left(-\frac{im}{\hbar}S^{(1)}\right)$$
$$= (u^{(0)} + i\mu^{(1)}) \exp\left(\frac{im}{\hbar}\mathring{S}^{(1)}\right)$$
(6.11)

and determine $\mathring{S}^{(1)}$ so that the energy expectation value with $\psi^{(1)}$,

$$\begin{aligned} \langle E \rangle &= \langle \psi^{(1)} | H | \psi^{(1)} \rangle \\ &= \langle \phi^{(0)} | H | \phi^{(0)} \rangle + \frac{1}{2} m \int \rho^{(0)} \nabla S^{(1)} \cdot \nabla S^{(1)} d^3 x \end{aligned}$$
(6.12)

becomes a sum of one $\dot{\alpha}$ -independent and one $\dot{\alpha}$ dependent term, as in (6.7). Using Eq. (5.18) for $\phi^{(0)}$, we can rewrite Eq. (6.12) in terms of the quasistatic energy ϵ° as

$$\langle E \rangle = \epsilon^{\circ} + m \int \rho^{(0)} \dot{\alpha} \, \frac{\partial S^{(1)}}{\partial \alpha} \, d^3 x + \hbar \dot{\alpha} \, \left\langle u^{(0)} \right| \frac{\partial}{\partial \alpha} \left| \mu^{(1)} \right\rangle$$
$$- m \dot{\alpha} \, \frac{\partial \, \mathring{S}^{(1)}}{\partial \alpha} \, .$$
 (6.13)

Then the choice

$$\mathring{S}^{(1)} = \frac{\hbar}{m} \int \left\langle u^{(0)} \middle| \frac{\partial}{\partial \alpha} \middle| \mu^{(1)} \right\rangle d\alpha$$
(6.14)

puts $\langle E \rangle$ into the form (6.7):

$$\langle E \rangle = \epsilon^{\circ} + m \int \rho^{(0)} \dot{\alpha} \, \frac{\partial S^{(1)}}{\partial \alpha} \, d^3x \, . \tag{6.15}$$

Collective kinetic energy. The collective kinetic energy given by the second term of Eq. (6.15) can be put into a more convenient form by expressing it in terms of $\tilde{S}^{(1)}$ defined in Eq. (5.15). By Eq. (5.15), we have

$$\begin{split} m\dot{\alpha} \int \rho^{(0)} \frac{\partial S^{(1)}}{\partial \alpha} d^{3}x &= \hbar\dot{\alpha} \left\langle \mu^{(1)} \right| \frac{\partial}{\partial \alpha} \left| u^{(0)} \right\rangle \\ &- \hbar\dot{\alpha} \left\langle u^{(0)} \right| \frac{\partial}{\partial \alpha} \left| \mu^{(1)} \right\rangle \\ &= -2\hbar\dot{\alpha} \left\langle u^{(0)} \right| \frac{\partial}{\partial t} \left| \mu^{(1)} \right\rangle \\ &= -2\dot{\alpha} \frac{\partial S^{(1)}}{\partial \alpha} , \qquad (6.16) \end{split}$$

where Eq. (6.14) is used in obtaining the last line. Since $S^{(1)} = \tilde{S}^{(1)} + \tilde{S}^{(1)}$ [Eq. (5.15)], the collective kinetic energy is

$$T^{(1)} = m \int \rho^{(0)} \dot{\alpha} \, \frac{\partial S^{(1)}}{\partial \alpha} \, d^3 x$$
$$= \frac{m}{2} \int \rho^{(0)} \dot{\alpha} \, \frac{\partial \tilde{S}^{(1)}}{\partial \alpha} \, d^3 x \quad . \tag{6.17a}$$

This result is identical to that given by Inglis's cranking³⁷ model: By Eq. (6.16), we obtain from Eq. (6.17a)

$$T^{(1)} = \hbar \dot{\alpha} \int \mu^{(1)} \frac{\partial}{\partial \alpha} u^{(0)} d^3 x \qquad (6.17b)$$

which is exactly Inglis's formula for the collective kinetic energy.

D. Adiabatic collective kinetic energy in terms of various velocity fields

1. Irrotational velocity field \vec{v}_{∞}

We now write the collective kinetic energy (6.17) in terms of the irrotational velocity field $\vec{\mathbf{v}}_{\otimes}^{(1)} = -\nabla \tilde{S}^{(1)}$. In Eq. (6.17b), we make use of the continuity equation (5.17) to obtain

$$T^{(1)} = -\frac{\hbar}{2} \int \frac{1}{u^{(0)}} \vec{\nabla}^{(1)}_{\otimes} \cdot \left[\frac{1}{2} \mu^{(1)} \nabla \rho^{(0)} - \rho^{(0)} \nabla \mu^{(1)}\right] d^{3}x$$
$$-\frac{\hbar}{2} \int \frac{\phi^{(0)}}{u^{(0)}} \nabla \cdot (\mu^{(1)} \phi^{(0)} \vec{\nabla}^{(1)}_{\otimes}) d^{3}x \quad (6.18)$$

The quantity inside the square bracket in the first integral of this equation is related to the single-particle current $\overline{J}^{(1)} \equiv \rho^{(0)} \overline{V}^{(0)}_{\otimes}$, since

$$\frac{1}{u^{(0)}} \left[\frac{1}{2} \mu^{(1)} \nabla \rho^{(0)} - \rho^{(0)} \nabla \mu^{(1)} \right] = \mu^{(1)} \nabla u^{(0)} - u^{(0)} \nabla \mu^{(1)}$$
$$= -\frac{m}{\hbar} \rho^{(0)} \nabla_{\otimes}^{(1)} . \quad (6.19)$$

With this relationship, Eq. (6.18) can be written as

$$T^{(1)} = \frac{m}{2} \int \rho^{(0)} \vec{\mathbf{v}}_{\otimes}^{(1)} \cdot \vec{\mathbf{v}}_{\otimes}^{(1)} d^{3}x - \frac{\hbar}{2} \int \frac{\phi^{(0)}}{u^{(0)}} \nabla \cdot (\mu^{(1)} \phi^{(0)} \vec{\mathbf{v}}_{\otimes}^{(1)}) d^{3}x .$$
(6.20)

The first term of this equation is equal to the ki-

netic energy of a classical fluid with density $\rho^{(0)}$ moving with a velocity field $\vec{v}_{\otimes}^{(1)}$. We therefore call this part of the kinetic energy the "classical fluid kinetic energy" $T_{\rm cl}$. The second term of Eq. (6.20) is generally nonzero. It is because of this nonzero term that the single-particle Schrödinger fluid has a kinetic energy different from that of a classical fluid.

However, whenever the second term in Eq. (6.20) vanishes, the single-particle Schrödinger fluid has a kinetic energy equal to that of a classical fluid. Moreover, it is equal to an irrotational value⁴⁴ because the velocity field which appears in the classical fluid kinetic energy is the irrotational velocity field $\vec{v}_{\infty}^{(1)}$.

Kinetic energy of the single-particle Schrödinger fluid equals the classical fluid kinetic energy when $\vec{v}_{\otimes}^{(1)}$ has no singularity. We show in the following that when $\vec{v}_{\otimes}^{(1)}$ has no singularity the kinetic energy of the single-particle Schrödinger fluid is equal to the classical fluid kinetic energy. If $\vec{v}_{\otimes}^{(1)}$ has no singularity, then the continuity relation (5.17) can be approximated as

$$2\dot{\alpha}u^{(0)}\frac{\partial u^{(0)}}{\partial \alpha} \simeq -(u^{(0)})^2 \nabla \cdot \overrightarrow{\nabla}^{(1)}_{\otimes} - \overrightarrow{\nabla}^{(1)} \cdot \nabla(u^{(0)})^2 ,$$
(6.21)

neglecting only terms which go to zero everywhere in space as $\dot{\alpha} \rightarrow 0$. Substitute Eq. (6.21) into Eq. (6.17b) and follow the same steps outlined from Eq. (6.17b) through Eq. (6.20). We arrive at an equation exactly the same as Eq. (6.20), but with $\phi^{(0)}$ replaced by $u^{(0)}$, i.e., we have

$$T^{(1)} = T_{c1} - \frac{\hbar}{2} \int \nabla \cdot (\mu^{(1)} u^{(0)} \nabla^{(1)}_{\mathbb{V}_{\otimes}}) d^{3}x \quad (6.22)$$

Now the second term of this equation can be transformed to a surface integral. Since $\vec{\mathbf{v}}_{\otimes}^{(1)}$ has no singularity by assumption, the surface involved in this surface integral is only the boundary of the box of normalization. Since the wave function ψ = $u^{(0)} + i\mu^{(1)}$ vanishes on this boundary, this surface integral is zero. Hence Eq. (6.22) becomes

$$T^{(1)} = T_{c1}, \text{ for regular } \vec{\mathbf{v}}_{\otimes}^{(1)}.$$
 (6.23)

Therefore, the kinetic energy of the single-particle Schrödinger fluid is equal to the classical fluid kinetic energy when $\vec{v}_{\otimes}^{(1)}$ has no singularity.

2. Incompressible velocity field \vec{v}_{\odot}

As with the irrotational velocity field, other velocity fields, especially the incompressible velocity field and the regular velocity field introduced in Sec. III, can also be involved into the expression for the collective kinetic energy by utilizing

the continuity equation to replace the time derivative of the density (or density amplitude). Introduce the incompressible velocity field $\vec{v}_{0}^{(1)}$, defined by Eqs. (5.20) and (5.21). We obtain

$$T^{(1)} = -\hbar \int \mu^{(1)} \nabla^{(1)}_{\nabla_{\odot}} \cdot \nabla u^{(0)} d^{3}x$$

= $-\frac{\hbar}{2} \int \{ \nabla^{(1)}_{\odot} \cdot [\mu^{(1)} \nabla u^{(0)} - u^{(0)} \nabla \mu^{(1)}]$
+ $\nabla \cdot (\nabla^{(1)}_{\odot} u^{(0)} \mu^{(1)}) \} d^{3}x$ (6.24)

with the help of some vector identities. By Eq. (6.19) and the divergence theorem, Eq. (6.24) can be put into the form,

$$T^{(1)} = \frac{m}{2} \int \rho^{(0)} \vec{\mathbf{v}}^{(1)}_{\otimes} \cdot \vec{\mathbf{v}}^{(1)}_{\odot} d^{3}x$$
$$-\frac{\hbar}{2} \oint_{\sigma} u^{(0)} \mu^{(1)} \vec{\mathbf{v}}^{(1)}_{\odot} \cdot \hat{n} d\sigma , \qquad (6.25)$$

where σ is the totality of surfaces surrounding the singularities of $\vec{\mathbf{v}}_{\circ}$, if any, and \hat{n} is the unit normal on σ pointing towards the singularities.

3. Regular velocity field \vec{v}_R

Likewise, for the regular velocity field \overline{v}_{R} (when it exists) we convert the expression (6.17b) for the collective kinetic energy, by means of the continuity equation, Eq. (5.22), for the regular velocity field into the form

$$T^{(1)} = -\hbar \int \mu^{(1)} [\frac{1}{2} u^{(0)} \nabla \cdot \vec{\mathbf{v}}_{\mathbf{R}}^{(1)} + \vec{\mathbf{v}}_{\mathbf{R}}^{(1)} \cdot \nabla u^{(0)}] d^{3}x ,$$
(6.26)

and thence by similar algebraic manipulation, we obtain

$$T^{(1)} = \frac{m}{2} \int \rho^{(0)} \vec{\mathbf{v}}_{\otimes}^{(1)} \cdot \vec{\mathbf{v}}_{\mathbf{R}}^{(1)} d^{3}x - \frac{\hbar}{2} \int \nabla \cdot (u^{(0)} \mu^{(1)} \vec{\mathbf{v}}_{\mathbf{R}}^{(1)}) d^{3}x .$$
(6.27)

In this case, however, the integrand of the last integral is regular everywhere and is transformed to a surface integral over only the external boundary of the box of normalization, which vanishes since $u^{(0)}$ and $\mu^{(1)}$ are zero at the external boundary. Then we have simply,

$$T^{(1)} = \frac{m}{2} \int \rho^{(0)} \vec{\mathbf{v}}_{\otimes}^{(1)} \cdot \vec{\mathbf{v}}_{\mathbf{R}}^{(1)} d^{3}x . \qquad (6.28)$$

Comparing with the expressions for the collective kinetic energy, which we have in Eqs. (6.20)and (6.25), respectively, we see that the present expression, Eq. (6.28) is especially simple: No terms not expressible in the quadratic form of the velocity fields are involved. Therefore, for the collective motion in which a regular velocity field can be found, Eq. (6.28) is the most convenient expression for the collective kinetic energy.

It can also be noted that the second integral in Eq. (6.20) and the surface integral in Eq. (6.25) are all due to the presence of singularities in either the irrotational velocity field \vec{v}_{\odot} , or the incompressible velocity field \vec{v}_{\odot} . In the special cases where \vec{v}_{\odot} or \vec{v}_{\odot} are free from singularities (i.e., equal to the regular velocity field \vec{v}_{R}), Eqs. (6.20) and (6.25) go over to Eq. (6.28), as they must.

The result (6.28) is one remarkable product of the present attempt to redescribe Schrödinger processes in fluid dynamical terms, as we shall discuss further in paper II in connection with applications of the present theory.

E. Collective linear and angular momenta

Using again the polar form (2.4) for the exact wave function, we calculate the expectation values of the linear momentum operator \vec{p} and the angular momentum operator $\vec{l}=\vec{r}\times\vec{p}$, as

$$\langle \psi | \overrightarrow{\mathbf{p}} | \psi \rangle = \langle \phi | \overrightarrow{\mathbf{p}} | \phi \rangle + m \int \rho \overrightarrow{\mathbf{v}}_{\otimes} d^{3}x \qquad (6.29)$$

and

$$\langle \psi | \vec{\mathbf{I}} | \psi \rangle = \langle \phi | \vec{\mathbf{I}} | \phi \rangle + m \int \vec{\rho \mathbf{r}} \times \vec{\mathbf{v}}_{\otimes} d^{3}x \quad . \tag{6.30}$$

In the same spirit as in treating the energy, we can separate both of these equations into an $\dot{\alpha}$ -independent part and an $\dot{\alpha}$ -dependent part. The $\dot{\alpha}$ dependent parts in these two equations can then be defined as the collective linear and angular momenta.

The second term in either Eq. (6.29) or Eq. (6.30) depends on $\dot{\alpha}$ surely through its dependence on \dot{v}_{\odot} . However, the first term is not $\dot{\alpha}$ -independent because ϕ may also be $\dot{\alpha}$ -dependent. Therefore, Eqs. (6.29) and (6.30) are not appropriate separations for the collective momenta. In fact, no satisfactory separations for the exact solution have yet been found.

However, if we limit our considerations in the adiabatic limit, then Eqs. (6.29) and (6.30) are already in a form separating $\dot{\alpha}$ -independent and $\dot{\alpha}$ -dependent parts. Since ϕ is approximated by $\phi^{(0)}$ [Eq. (5.12)] in the adiabatic limit, we have

$$\langle \phi^{(0)} | \vec{\mathbf{p}} | \phi^{(0)} \rangle = \langle u^{(0)} | \vec{\mathbf{p}} | u^{(0)} \rangle + O(\dot{\alpha}^2)$$
 (6.31)

and

$$\langle \phi^{(0)} | 1 | \phi^{(0)} \rangle = \langle u^{(0)} | 1 | u^{(0)} \rangle + O(\dot{\alpha}^2) .$$
 (6.32)

The first term in either Eq. (6.31) or (6.32) is $\dot{\alpha}$ independent. Hence, to order $\dot{\alpha}$, the collective linear and angular momenta are, respectively,

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$$\vec{\mathbf{P}}^{(1)} = m \int \rho^{(0)} \vec{\mathbf{v}}_{\otimes}^{(1)} d^3 x$$
(6.33)

and

$$\vec{\mathbf{L}}^{(1)} = m \int \rho^{(0)} \vec{\mathbf{r}} \times \vec{\mathbf{v}}^{(1)}_{\otimes} d^3 x.$$
(6.34)

VII. MORPHOLOGY OF THE SINGLE-PARTICLE SCHRÖDINGER FLUID

In this section, we classify the single-particle Schrödinger fluids according to some general properties of these fluids. This can provide, we believe, an overview of several of the topics we discussed, such as vortex singularity, compressibility, and some relationships among the various kinds of velocity fields which can arise in the single-particle Schrödinger fluid.

In Fig. 2, we present our classification in the form of a set diagram. We denote by F the set of all single-particle Schrödinger fluids. Inside F we consider as subsets F_i those special cases of the single-particle Schrödinger fluids which possess a volume conserving \vec{v}_{\otimes} (subset F_c), a regular velocity field $\vec{v}_{\rm R}$ ($F_{\rm R}$), a vortex-free \vec{v}_{\otimes} ($F_{\rm VF}$), a geometric velocity field $\vec{v}_{\rm G}$ ($F_{\rm G}$), an incompressible \vec{v}_{\otimes} ($F_{\rm I}$), and/or a nodeless density distribution (F_0). We discuss the relationship among these subsets and summarize their special properties in the following.

Subsets characterized by properties of the irrotational field $\vec{v}_{\infty} = -\nabla S$

For every single-particle Schrödinger fluid, we can define the irrotational velocity field \vec{v}_{\otimes} [through Eqs. (2.9) and (2.10)] and the incompressible velocity field \vec{v}_{∞} [through Eqs. (3.2) and (3.3)], although in some cases, these fields may exhibit singularities. But the conditions for the existence of more restrictive velocity fields are not completely known. For example, as mentioned in Sec. III B, the conditions for the existence of the regular velocity field \vec{v}_{R} are not known at all; we can exhibit such a field in some cases, and in other cases we believe that no such field exists. Therefore, we view $F_{\rm R}$ as a proper subset of F to keep open the possibility that single-particle Schrödinger fluids possessing no $\vec{v}_{\rm R}$ exist. A similar conservation has been consistently employed in the conservative attitude of Fig. 2.

The vortex-free subset $F_{\rm VF}$ is a subset of $F_{\rm R}$, since the line vortex singularity is the only singularity of \vec{v}_{\otimes} (Sec. IV). A vortice-free \vec{v}_{\otimes} is therefore a regular velocity field. Hence, the corresponding single-particle Schrödinger fluid belongs to $F_{\rm R}$. We note also that in the adiabatic limit, the fluids in $F_{\rm VF}$ have the interesting property that its kinetic energy is equal to the class-

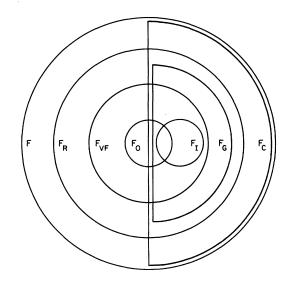


FIG. 2. Relationships of different kinds of single-particle Schrödinger fluid. F: the set of all single-particle Schrödinger fluids; $F_{\rm C}$: fluids conserving the nuclear volume; $F_{\rm R}$: fluids possessing a regular velocity field $\bar{\bf v}_{\rm R}$; $F_{\rm VF}$: fluids possessing a vortex-free $\bar{\bf v}_{\otimes}$; $F_{\rm G}$: fluids possessing a geometric velocity field $\bar{\bf v}_{\rm G}$; $F_{\rm I}$: irrotational incompressible fluids; $F_{\rm 0}$: fluids with a nodeless density distribution.

ical irrotational (not necessarily incompressible) value (Sec. VID1).

Fluids with nodeless density distribution (F_0) are very special cases of $F_{\rm VF}$, since only the lowest single-particle states have nodeless wave functions. The fact that these lowest single-particle states possess a (regular) irrotational velocity field was recognized by Wick⁴⁵ long ago. In the present context, this theorem is almost a triviality, following at once from the simple argument that, since the only singularity of the fluid, the vortex singularity, comes only from the zeroes of the wave function (Sec. IV), then the lowest single-particle states, being nodeless, must be singularity-free, i.e., they must have a \vec{v}_{\otimes} which is regular.

Subsets characterized by properties of the collective motion

We can generally divide the collective motions according to whether the motion involves a net expansion or contraction of the total nuclear volume (as, e.g., in the case of the breathing mode). Because the overall nuclear compressibility is very small,⁴⁶ a substantial energy is needed to excite such a collective motion. In contrast, one believes that the low-lying collective motions (as well as the processes of fission), preserve the nuclear volume to a good extent. There-

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fore, the subset $F_{\rm C}$ is of particular interest to us. The set of fluids $F_{\rm G}$ having a geometric velocity field is simultaneously a subset of $F_{\rm R}$ and $F_{\rm C}$, since the geometric velocity field $v_{\rm G}$ is regular and incompressible (Sec. III C and Appendix C), and hence volume conserving. The necessary and sufficient condition for the existence of $\vec{v}_{\rm G}$ is given in Eq. (3.11). However, $F_{\rm G}$ is not entirely included in the subset $F_{\rm VF}$ characterized by vortex-free \vec{v}_{\otimes} , since the case of collective rotation, where the geometric velocity field exists (and is known: $\vec{v}_{\rm G} = \vec{\Omega} \times \vec{r}$), provides a counterexample in which the irrotational velocity field \vec{v}_{\otimes} has line vortex singularity for wave functions with nodes. (The case of rotation will be discussed in detail in paper II.)

On the other hand, the set of irrotational incompressible fluids $F_{\rm I}$ is entirely a subset of $F_{\rm G}$ and $F_{\rm VF}$. These irrotational incompressible fluids have been first systematically considered in connection with nuclear collective motions by Hill and Wheeler.²² They are discussed further in Appendix A. The single-particle Schrödinger fluids in the Hill-Wheeler box or in a quadrupole deformed osciallator potential⁴⁷ provide specific examples of the fluids in $F_{\rm I}$.

VIII. GENERALIZATIONS TO THE MANY-BODY CASE

Although our discussions in the preceding sections are confined to single-particle wave functions in three spatial dimensions, the interest (at least ultimately) for applications to nuclei must lie in the generalization to the many-particle problem. Although the program of incorporating two nucleon forces into such a generalization has hardly begun, we execute in this section some of the most straightforward many-particle generalizations of the theory of the single-particle Schrödinger fluid, namely, we concentrate our discussions on the continuity equation.

In analogy with the single-particle case in three dimensions, we first obtain the continuity equation and the modified Schrödinger equation for the N-particle case in the 3N-dimensional space. Then we derive the continuity equation for the three-dimensional space from the continuity equation in the original 3N-dimensional space.

A. Continuity equation and the modified Schrödinger equation

1. In 3N-dimensional space

A Schrödinger equation for N interacting nucleons can be written in the following form⁴⁸

$$\underline{H}(\vec{\mathbf{x}}_{1}\cdots\vec{\mathbf{x}}_{N};\vec{\alpha})\underline{\Psi}(\vec{\mathbf{x}}_{1}\cdots\vec{\mathbf{x}}_{N};\vec{\alpha}) = i\hbar\frac{\partial}{\partial t}\underline{\Psi}(\vec{\mathbf{x}}_{1}\cdots\vec{\mathbf{x}}_{N};\vec{\alpha}) ,$$
(8.1)

where

$$\underline{H}(\mathbf{\bar{x}}_{1}\cdots\mathbf{\bar{x}}_{N};\mathbf{\bar{\alpha}}) \equiv \sum_{i=1}^{N} \frac{\mathbf{\bar{p}}_{i}^{2}}{2m} + \sum_{i=1}^{N} V(\mathbf{\bar{x}}_{i};\mathbf{\bar{\alpha}}) + \underline{\tilde{V}}(\mathbf{\bar{x}}_{1}\cdots\mathbf{\bar{x}}_{N};\mathbf{\bar{\alpha}}) . \quad (8.2)$$

Here we assume $V(\bar{\mathbf{x}}_i; \bar{\boldsymbol{\alpha}})$ to be an average potential felt by the ith nucleon due to the interactions with all other nucleons, and $\tilde{V}(\vec{x}_1 \cdots \vec{x}_N; \vec{\alpha})$, the residual interaction between the nucleons, which is not included in the average potential $V(\bar{\mathbf{x}}_i; \bar{\alpha})$. Because we are working within a description of collective motion which does not assume self-consistency, but instead assumes that certain collective variables, well described in a classical approximation, define the potential for the single-particle motion; the average field is here externally driven through its dependence on the classical collective parameters $\bar{\alpha}$. (The very deep and persistent problem arising from the redundancy between the collective degrees of freedom and the particle degrees of freedom are not considered in the present discussion.) Then the N-body wave function Ψ is a function of $\mathbf{x}_1, \ldots, \mathbf{x}_N$ and \mathbf{a} .

In analogy to the single-particle wave function, we obtain a "fluid dynamical" description of the N-body wave function by writing Ψ in the polar form:

$$\underline{\Psi}(\mathbf{\tilde{x}}_{1}\ldots;\mathbf{\tilde{\alpha}}) = \underline{\Phi}(\mathbf{\tilde{x}}_{1}\ldots;\mathbf{\tilde{\alpha}}) \exp\left[-\frac{i}{\hbar} m_{-}^{S}(\mathbf{\tilde{x}}_{1}\ldots;\mathbf{\tilde{\alpha}}) - \frac{i}{\hbar} \int^{t} E(\mathbf{\tilde{\alpha}}(t')) dt'\right].$$
(8.3)

Here the norm Φ and the phase S are assumed (without loss of generality) to be real functions of the particle coordinates and the collective parameters. The quantity $E(\bar{\alpha})$ is the intrinsic energy of the system.

The substitution of Eq. (8.3) into the *N*-body Schrödinger equation, Eq. (8.1), yields the continuity equation and the modified Schrödinger equation in the 3N-dimensional coordinate space:

$$\frac{1}{2} \underline{\Phi} \, \underline{\nabla}^2 \underline{S} + \underline{\nabla} \, \underline{\Phi} \, \cdot \, \underline{\nabla} \, \underline{S} = \frac{\partial}{\partial t} \underline{\Phi} \tag{8.4}$$

and

$$\left[\underline{H} - m\left(\frac{\partial}{\partial t}\underline{S} - \frac{1}{2}\nabla\underline{S}\cdot\nabla\underline{S}\right)\right]\underline{\Phi} = E\left(\overline{\alpha}\right)\underline{\Phi}, \qquad (8.5)$$

where $\underline{\nabla} \equiv \sum_{i=1}^{N} \nabla_i$. Equations (8.4) and (8.5) are the obvious generalizations of the continuity equation [Eq. (2.6)] and the modified Schrödinger equa-

tion [Eq. (2.7)] of the single-particle Schrödinger fluid.

2. Continuity equation in the 3-dimensional coordinate space

In terms of the N-body density $\underline{\rho}$ and the N-body current \mathbf{J} defined by

$$\underline{\rho}(\mathbf{\vec{x}}_{1}\cdots\mathbf{\vec{x}}_{N};\mathbf{\vec{\alpha}}) = \underline{\Phi}^{2} = \underline{\Psi}^{*} \underline{\Psi}$$
(8.6)

and

$$\underline{\mathbf{J}}(\mathbf{x}_{1}\cdots\mathbf{x}_{N};\mathbf{\tilde{\alpha}}) = -\underline{\rho}\nabla S = -\frac{i\hbar}{2m}\left(\underline{\Psi^{*}\nabla\Psi} - \underline{\Psi}\nabla\Psi^{*}\right),$$
(8.7)

the continuity equation [Eq. (8.4)] becomes simply

$$\nabla \cdot \vec{\mathbf{j}} = -\frac{\partial}{\partial t} \underline{\rho} \,. \tag{8.8}$$

The *N*-body density ρ is the probability of finding the particles $1, 2, \ldots, N$ in positions $\vec{x}_1, \vec{x}_2, \ldots, \vec{x}_n$, respectively. We relate this density to the *total matter density* $\rho_T(\vec{x}; \vec{\alpha})$ in three-dimensional space and the corresponding *total matter current* $\vec{J}_T(\vec{x}; \vec{\alpha})$, following the method of Landau in his study on liquid helium.⁴⁹ We first extract from the *N*-body wave function the one-particle density ρ_i and current \vec{J}_i , contributed by the *i*th particle, by averaging over the 3(N-1) dimensions which describe the rest of the particles, as follows⁵⁰

$$\rho_i(\vec{\mathbf{x}}_i) = \int dx \, {}^{3(N-1)}_{(i)} \underline{\Psi}^* \underline{\Psi}$$
(8.9)

and

$$\mathbf{\tilde{J}}_{i}(\mathbf{\tilde{x}}_{i}) = -\frac{i\hbar}{2m} \int dx \, {}^{3(N-1)}_{(i)} \{ \underline{\Psi}^{*} \nabla_{i} \underline{\Psi} - \underline{\Psi} \nabla_{i} \underline{\Psi}^{*} \} \,. \tag{8.10}$$

Then the total matter density $\rho_{\rm T}$ and the total current $\mathbf{J}_{\rm T}$ are obtained by summing these one-particle contributions; viz.,

$$\rho_{\rm T}(\vec{{\bf x}}) = \sum_{i=1}^{N} \rho_i(\vec{{\bf x}}) = \sum_{i=1}^{N} \int dx_{(i)}^{3(N-1)} \underline{\Psi}^* \underline{\Psi} \qquad (8.11)$$

and

$$J_{\mathrm{T}}(\mathbf{\bar{x}}) \equiv \sum_{i=1}^{N} J_{i}(\mathbf{\bar{x}})$$
$$= -\frac{i\hbar}{2m} \sum_{i=1}^{N} \int dx_{(i)}^{3(N-1)} \left\{ \underline{\Psi}^{*} \nabla_{i} \underline{\Psi} - \underline{\Psi} \nabla_{i} \underline{\Psi}^{*} \right\}.$$
(8.12)

It remains only to show that $\rho_{\rm T}$ and $J_{\rm T}$ obey a (three-dimensional) continuity equation analogous to Eq. (2.9). Rewrite the continuity equation (8.8), via (8.7):

$$-\frac{\partial}{\partial t} \underline{\rho} = -\frac{i\hbar}{2m} \sum_{i=1}^{N} (\underline{\Psi}^* \nabla_i^2 \underline{\Psi} - \underline{\Psi} \nabla_i^2 \underline{\Psi}^*); \quad (8.13)$$

integrate over all but the coordinates of the jth particle and summing over the index j we obtain

$$-\frac{\partial}{\partial t}\rho_{\mathrm{T}} = -\frac{i\hbar}{2m}\sum_{i,j}\int dx_{(j)}^{3(N-1)}(\underline{\Psi}^*\nabla_i^2\underline{\Psi} - \underline{\Psi}\nabla_i^2\underline{\Psi}^*).$$
(8.14)

The sum of the i=j terms in the right-hand side of this equation is just the divergence of the total current \mathbf{J}_{T} , as can be seen from Eq. (8.12). Hence, we have

$$-\frac{\partial \rho_T}{\partial t} = \nabla \cdot \vec{\mathbf{J}}_{\mathrm{T}} - \frac{i\hbar}{2m} \sum_{\substack{i,j \\ (i\neq j)}} \int dx^{3(N-1)}_{(j)} (\underline{\Psi}^* \nabla_i^2 \underline{\Psi} - \underline{\Psi} \nabla_i^2 \underline{\Psi}^*) .$$
(8.15)

It remains only to show that the summation on the right vanishes term by term. This can be done directly by expanding Ψ in any complete set of determinants based on an appropriate single-particle Hamiltonian. Then the fact that only one-body operators occur therein and the mutual orthogonality combined to make every term vanish identically. Therefore, the last term in Eq. (8.15) vanishes identically and we obtain the continuity equation for the total matter density and the total current of the nucleus:

$$\nabla \cdot \vec{\mathbf{J}}_{\mathrm{T}}(\vec{\mathbf{x}};\vec{\alpha}) = -\frac{\partial}{\partial t} \rho_{\mathrm{T}}(\vec{\mathbf{x}};\vec{\alpha}) . \qquad (8.16)$$

3. Total velocity field in N-particle case

From the total density distribution ρ_T and the total current \mathbf{J}_T it is natural to define the *total* velocity field $\mathbf{\tilde{v}}_T$ of the nucleus as

$$\vec{\mathbf{v}}_{\mathrm{T}}(\vec{\mathbf{x}}) = \frac{\dot{\mathbf{J}}_{\mathrm{T}}(\vec{\mathbf{x}})}{\rho_{\mathrm{T}}(\vec{\mathbf{x}})} \,. \tag{8.17}$$

In terms of $\vec{\nabla}_{T}$, the continuity equation, Eq. (8.16), takes the form

$$\rho_{\rm T} \nabla \cdot \vec{\nabla}_{\rm T} + \vec{\nabla}_{\rm T} \cdot \nabla \rho_{\rm T} = -\frac{\partial \rho_{\rm T}}{\partial t} \quad . \tag{8.18}$$

We note that the definition, Eq. (8.17), of the total velocity field gives, in the case of a one-particle system, the single-particle irrotational velocity field \vec{v}_{\otimes} .

In order to obtain a complete fluid dynamical description, some dynamical equation of motion [which, for example, might be (approximately) an Euler equation, a Navier-Stokes equation, or a Burnett equation, or any of the infinite series of higher order equations, were a hydrodynamic description to prevail] and an equation of state must be constructed out of the many-body Schrödinger equation, which here is presumed to comprise the complete description of the system. This is a should one say "the"—fundamental problem in the theory of quantum fluids, which we do not attack here.

We should note that Wong *et al.* have studied the possibility of obtaining a fluid dynamical equation of motion utilizing the time-dependent Hartree-Fock theory,¹⁵ which is certainly a first step to-wards this goal.

B. Nonobservability of the total velocity field

In Sec. II, we pointed out that the single-particle velocity field is not a physically observable quantity. We discuss here the nonobservability of tht total velocity field $\vec{\mathbf{v}}_{T}$ defined in Eq. (8.17). (The mathematical proof is given in Appendix B.)

According to the statistical interpretation of quantum mechanics,⁵² a physical observation is symbolized by the action of an operator O on a state vector Ψ of the system. The possible results of this observation are the eigenvalues of the operator in question, and each has a probability given by the square of the amplitude of the corresponding eigenfunction in the function $O\Psi$. Furthermore, the average result of a large number of observations of this physical observable is the expectation value $\langle \Psi | O | \Psi \rangle$. This statistical interpretation is the physical ground of the superposition principle of quantum mechanics.⁵² By the superposition principle the operator representing a physical observation is necessarily linear.

The total matter density $\rho_{\rm T}$ and the total current $\vec{J}_{\rm T}$ are physical observables. There exist linear (in fact, Hermitian) operators $p_{\rm op}$ and $\vec{J}_{\rm op}$ whose expectation values give, respectively, the average values of the total matter density and total current for a large number of observations on the system. These operators are, in coordinate representation,⁴⁹

$$\langle \mathbf{\vec{x}} \mid \rho_{op} \mid \mathbf{\vec{x}'} \rangle = \sum_{i=1}^{N} \delta(\mathbf{\vec{x}}_i - \mathbf{\vec{x}}) \delta(\mathbf{\vec{x}} - \mathbf{\vec{x}'})$$
 (8.19a)

and

$$\langle \vec{\mathbf{x}} \mid \vec{\mathbf{J}}_{op} \mid \vec{\mathbf{x}}' \rangle = \frac{\hbar}{i2m} \sum_{i=1}^{N} \left\{ \delta(\vec{\mathbf{x}}_{i} - \vec{\mathbf{x}}) \nabla \delta(\vec{\mathbf{x}} - \vec{\mathbf{x}}') + \left[\nabla \delta(\vec{\mathbf{x}} - \vec{\mathbf{x}}') \right] \delta(\vec{\mathbf{x}}_{i} - \vec{\mathbf{x}}') \right\}.$$

$$(8.19b)$$

Thse operators are linear, and their expectation values in any state $|\Psi\rangle$ are identical everywhere with $\rho_{\rm T}(\vec{\mathbf{x}})$ and $J_{\rm T}(\vec{\mathbf{x}})$, defined in Eqs. (8.11) and (8.12), i.e.,

$$\langle \underline{\Psi} \mid \rho_{op} \mid \underline{\Psi} \rangle = \rho_{T}(\mathbf{x})$$
(8.20a)

and

$$\langle \Psi \mid \vec{\mathbf{J}}_{op} \mid \Psi \rangle = \vec{\mathbf{J}}_{T}(\vec{\mathbf{x}}) .$$
 (8.20b)

The total velocity field $\bar{\mathbf{v}}_{\mathrm{T}}$ will be a physical observable, only if a linear operator exists whose expectation value in $|\Psi\rangle$ is everywhere equal to $\bar{\mathbf{v}}_{\mathrm{T}}(\mathbf{\vec{x}})$, defined in Eq. (8.17). In Appendix B, we show that any operator which has an expectation value equal everywhere to $\bar{\mathbf{v}}_{\mathrm{T}}(\mathbf{\vec{x}})$ cannot be linear, and therefore cannot be a physical observable in quantum mechanics.

In the study of liquid helium, Landau has defined an operator \vec{v}_{op} for the total velocity field as 49

$$\vec{\mathbf{v}}_{\rm op} = \frac{1}{2} \left(\frac{1}{\rho_{\rm op}} \cdot \vec{\mathbf{J}}_{\rm op} + \vec{\mathbf{J}}_{\rm op} \cdot \frac{1}{\rho_{\rm op}} \right) \,. \tag{8.21}$$

From the above discussion, Landau's operator (8.21), although linear must not give the correct $\vec{v}_{\rm T}$ as defined in Eq. (8.17).

In fact, as has been pointed out by London,⁵³ this operator, for a system consisting of one particle, is simply the momentum divided by the mass $(1/m)\vec{p}$. Its expectation value on a state of the system is in this case just a number independent of position, the average momentum over the coordinate space, which has no immediate relationship with the local velocity field. Therefore, Landau's suggestion that the operator (8.21) be utilized as the quantum theoretical velocity field operator is quantum mechanically inconsistent.

IX. SUMMARY AND CONCLUSIONS

We have presented a formalism suitable for use in constructing a theory of mass flow in nuclei based upon an independent-particle shell model and exhibiting substantial fluid dynamical content. Some mathematical features of this idealized single-particle Schrödinger fluid have been discussed and some general implications drawn for physical quantities. More specific physical applications will be discussed in paper II.

APPENDIX A. WHEELER-HILL DYNAMICS: INCOMPRESSIBLE SCHRÖDINGER FLUID FLOW

Wheeler-Hill dynamics

In their very comprehensive paper on the foundations of the collective model, Hill and Wheeler²² consider the effect of a time-dependent nuclear shape on the evolution in time of a single-particle wave function. We show here that this Wheeler-Hill^{54, 55, 47} irrotational nuclear fluid dynamics (which also, incidentally, provided one of the starting points of the present research) is a special case of the single-particle Schrödinger fluid dynamics studied here, which involves an additional assumption of incompressible flow, and as a result, describes only certain special cases of the Schrödinger dynamics.

The Wheeler-Hill discussion is based on the ansatz

$$\psi(t) = u(x, \alpha(t)) \exp\left\{-\frac{i}{\hbar} \int^{t} \epsilon(\alpha(t')) dt' - \frac{i}{\hbar} mS_{I}\right\}$$
(A1)

for the solution to the time-dependent Schrödinger equation (2.1), where $u(\vec{x}, \alpha(t))$ is an eigensolution of the Schrödinger equation with a potential of shape $\alpha(t)$, and S_{I} is the velocity potential which would describe an irrotational incompressible⁵⁶ liquid flowing in the nuclear volume specified by $\alpha(t)$. Thus S_{I} is defined by Laplace's equation

$$\nabla^2 S_{\mathbf{r}} = 0 , \qquad (A2)$$

and the (Neumann) boundary condition that its normal gradient at the surface is equal to the normal velocity of the nuclear potential, as prescribed by $\alpha(t)$.

Wheeler and Hill showed that the wave function (A1) is a solution to the time-dependent Schrödinger equation (approximately up to terms in $\dot{\alpha}$) if only the wave function $u(x, \alpha(t))$ is carried along by the change in α with the local classical fluid velocity

$$\vec{\mathbf{v}}_{\mathbf{I}} = -\nabla S_{\mathbf{I}} , \qquad (A3)$$

so that the relationship

$$\dot{\alpha} \quad \frac{\partial u}{\partial \alpha} = \nabla S_{I} \cdot \nabla u \tag{A4}$$

is obeyed.^{54, 57} Then the kinetic energy of such a particle takes the form

$$\left\langle \psi \left| \frac{p^2}{2m} \right| \psi \right\rangle = \left\langle u \left| \frac{p^2}{2m} \right| u \right\rangle + \frac{m}{2} \int |u|^2 (\nabla S)^2 d^3 x , \quad (A5)$$

where the second term, due to the finite collective velocity $\dot{\alpha}$, is the "collective kinetic energy" of this particle. It has a value equal to that of a classical incompressible irrotational fluid of density $\rho = |u|^2$. Its sum over all particles then yields the irrotational incompressible fluid value for the total collective energy, and correspondingly, the irrotational incompressible value for the inertial parameter.

Relationship to Schrödinger fluid

The assumption (A4) is the distinctive feature of the Wheeler-Hill dynamics, and the source of its simple and general prediction (A5) of irrotational incompressible physics.

We show here (a) that this assumption is equivalent in the broader framework of the Schrödinger fluid to the (additional) requirement that the flow is incompressible, and (b) that such an assumption is inconsistent with the dynamics of the Schrödinger fluid, except for those special potential shapes where an irrotational geometric velocity field exists²⁵ (which is also always an incompressible velocity field as discussed in Appendix C), among which, as we noted above, are the quadrupole deformed oscillator and the Hill-Wheeler box.⁵⁷

Incompressibility of Wheeler-Hill flow

We note that incompressible flow for a system whose density is not constant in space implies that the density of any material element remains unchanged as it moves through space. I.e., the total derivative (3.2) of the density must vanish. But for $\rho = |u(\vec{x}, \alpha(t))|^2$ and \vec{v}_I given by (A3), the incompressibility condition (3.2) is immediately *identical* with the Wheeler-Hill assumption (A4).

We further note that as implied by condition (A3) and Laplace's equation (A2), $S_{\rm I}$ satisfies the continuity equation of the single-particle Schrödinger fluid. Therefore the Wheeler-Hill dynamics is a special case of the single-particle Schrödinger dynamics, in which each single-particle velocity field \vec{v}_{\otimes} is equal to $\vec{v}_{\rm I}$.

Wheeler-Hill dynamics implies existence of the irrotational geometric velocity field

Since the *incompressible* velocity field \vec{v}_{I} is determined only by Laplace's equation (A2) and the time-dependent boundary of the nuclear volume, this velocity field must be identical for every single-particle wave function u. But then, according to the necessary and sufficient condition (3.11), the geometric velocity field \vec{v}_{G} exists for the Wheeler-Hill dynamics and is equal to \vec{v}_{I} .

Since the single-particle velocity field \vec{v}_{\otimes} (= \vec{v}_{I}) is necessarily irrotational, we have, in fact, a special kind of geometric velocity field, namely, an irrotational geometric field.

This result also implies that in the case where no irrotational geometric velocity field exists, neither can the assumption (A4) be valid, and neither can the Wheeler-Hill dynamics be a valid description.

APPENDIX B. PROOF OF NONOBSERVABILITY OF THE VELOCITY FIELD

To be a quantum mechanical observable, a physical quantity must correspond to a linear, Hermitian operator in the Hilbert space. As promised in Sec. VIIIB, we show in this appendix that the assumption that \vec{v}_{T} is a linear operator, together with the established fact that \vec{J}_{T} and ρ_{T} are physical observables, leads to the absurd conclusion

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that \vec{v}_{T} must be merely a constant number independent of the state of the system. We therefore conclude that \vec{v}_{T} cannot be a linear operator. (All of these arguments apply also to the irrotational velocity field \vec{v}_{\odot} for each single particle.)

Let us consider in general three nontrivial (i.e., not proportional to the identity operator) operators A, B, and C, in which A and B are assumed to be linear and satisfying the relationship

$$\langle \psi | A | \psi \rangle = \langle \psi | B | \psi \rangle \langle \psi | C | \psi \rangle \tag{B1}$$

for any state $|\psi\rangle$ in the Hilbert space. We prove in the following that under these assumptions, *C* cannot be a linear operator. For the problem of observability under our consideration, the operators *A*, *B*, and *C* stand, respectively, for \mathbf{J}_{T} , ρ_{T} , and $\mathbf{\bar{v}}_{T}$ (and for the single-particle case, \mathbf{J} , ρ , and $\mathbf{\bar{v}}_{\otimes}$). [Cf. Eq. (8.19).]

To prove the nonlinearity of C, we assume the contrary that C be linear, and reduce this assumption *ad absurdum*.

We pick an arbitrary complete set $\{|i\rangle\}$ of states in the Hilbert space. Since Eq. (B1) is assumed to hold for any state in the Hilbert space, it must hold for any state and any linear combination of the states in $\{|i\rangle\}$. Consider then the states $|i\rangle$, $|j\rangle$, and $|a\rangle \equiv (|i\rangle + a|j\rangle)/\sqrt{2}$, where a is an arbitrary complex number of unit magnitude. By the linearity of A, B, and C, and by the arbitrariness of a, Eq. (B1) for $|\psi\rangle = |i\rangle$, $|j\rangle$, and $|a\rangle$ leads to three equations:

$$(B_{ii} - B_{jj})(C_{ii} - C_{jj}) - B_{ij}C_{ji} - B_{ji}C_{ij} = 0, \qquad (B2a)$$

$$2A_{ij} - B_{ii}C_{ij} - B_{jj}C_{ij} - B_{ij}C_{ii} - B_{ij}C_{jj} = 0, \quad (B2b)$$

$$B_{ii}C_{ii}=0. (B2c)$$

Since *B* is assumed to be nontrivial and since the set $\{|i\rangle\}$ is arbitrary, we can pick it in such a way that $B_{ij} \neq 0$ and $B_{ii} \neq B_{ji}$ for every $i \neq j$. (For the operator ρ , we can choose, e.g., the set of simple harmonic oscillator states as $\{|i\rangle\}$.) Then Eqs. (B2a) and (B2c) imply that (a) *C* is diagonal:

$$C_{ii} = 0$$
, for $i \neq j$; (B3a)

and (b) all its diagonal elements are equal:

$$C_{ii} = C_{ii} . \tag{B3b}$$

Therefore C is a c number times the identity operator in the representation $\{|i\rangle\}$, and hence in any other representation.

This contradicts the assumption that C is nontrivial. Therefore, C cannot be a linear operator. This completes the proof.

APPENDIX C. EACH GEOMETRIC FIELD IS ALSO REGULAR AND INCOMPRESSIBLE

In Sec. III C we have shown that the geometric velocity field \vec{v}_{G} obeys the condition (3.2) of incompressible flow. Here we demonstrate, first, that \vec{v}_{G} is regular in the finite volume, and, second, that it obeys the alternative compressibility condition (3.3) and, therefore, (by addition) the continuity equation (3.1). Thus, the geometric velocity field, whenever it exists, is proven to be a velocity field of the single-particle Schrödinger fluid, which is simultaneously a regular velocity field and an incompressible velocity field.

In the following proofs, we assume that the wave functions ψ_i form a complete set and that every ψ_i has a continuous first derivative with respect to *t*.

Proof of regularity of \vec{v}_G

We assume the contrary property, that \vec{v}_{G} has a singularity at some point \vec{x}_{0} , such that $\vec{v}_{G} \rightarrow \infty$ as $\vec{x} \rightarrow \vec{x}_{0}$, and reduce that assumption *ad absurdum*.

We have already shown in Sec. III C that when the velocity field \vec{v}_G can be defined for every wave function ψ_i , Eq. (3.9) holds for each ψ_i , $i=1,2,\ldots$. Since every ψ_i has a continuous time derivative by assumption, the first term of Eq. (3.9) is finite for every $i=1,2,\ldots$. Then every ψ_i must have at $\vec{x}=\vec{x}_0$ zero gradient along the direction of \vec{v}_G . Otherwise the right-hand side of Eq. (3.9), which has already shown to be zero, would become infinite at \vec{x}_0 for that ψ_i . It follows that every linear combination of ψ_i has zero gradient along the direction \vec{v}_G at \vec{x}_0 . On the other hand, consider as a counterexample the function,

$$\psi(\vec{\mathbf{x}}) = \frac{1}{\sqrt{2}} \pi^{-1/4} \exp\left\{-\frac{1}{2}(\vec{\mathbf{x}} - \vec{\mathbf{x}}_1)^2\right\}$$
(C1)

which obviously does not vanish at $\vec{\mathbf{x}} = \vec{\mathbf{x}}_0 \neq \vec{\mathbf{x}}_1$. Then

$$\nabla \psi \cdot \vec{\mathbf{v}}_{\mathbf{G}} \propto (\vec{\mathbf{x}}_{\mathbf{0}} - \vec{\mathbf{x}}_{\mathbf{1}}) \cdot \vec{\mathbf{v}}_{\mathbf{G}} \neq \mathbf{0} .$$
 (C2)

That is, ψ is a function in the Hilbert space, but has nonzero gradient along the direction of \vec{v}_{G} at \vec{x}_{0} , and so it cannot be expressed as a linear combination of the ψ_{i} 's. But this would contradict the completeness of the set of ψ_{i} 's. Hence \vec{v}_{G} cannot be singular at \vec{x}_{0} . Since \vec{x}_{0} is arbitrary, we conclude that \vec{v}_{G} is regular at every point in finite space.

In a similar way, we can prove that $\vec{\mathbf{v}}_{G}$ has no discontinuity: If we assume that at $\vec{\mathbf{x}}_{0}$ the component of $\vec{\mathbf{v}}_{G}$ in a direction $\vec{\mathbf{a}}$ is discontinuous, then all the ψ_{i} , $i=1,2,\ldots$, must have zero gradient along the direction of $\vec{\mathbf{a}}$ in order to honor Eq. (3.9). This leads again to a contradiction with the completeness of the set of ψ_{i} 's.

Proof that $\nabla \cdot \vec{v}_G$ vanishes

To prove that \vec{v}_{G} satisfies (3.3), consider

$$I_{ij} \equiv \frac{d}{dt} \int \psi_i^* \psi_j d^3 x$$
$$= \int \left[\psi_j \frac{d\psi_i^*}{dt} + \psi_i^* \frac{d\psi_j}{dt} \right] d^3 x = 0$$
(C3)

for all i and j, where the zero is implied by the orthonormality of the eigenfunctions. Then use (3.9) to obtain

$$I_{ij} = -\int (\psi_j \vec{\nabla}_G \cdot \nabla \psi_i^* + \psi_i^* \vec{\nabla}_G \cdot \vec{\nabla} \psi_j) d^3 x$$
$$= -\int \vec{\nabla}_G \cdot \nabla (\psi_i^* \psi_j) d^3 x \qquad (C4)$$

or, by Green's theorem,

$$I_{ij} = -\int_{s} \psi_{i}^{*} \psi_{j} \vec{\nabla}_{G} \cdot \hat{n} \, d\sigma + \int \psi_{i}^{*} \psi_{j} \nabla \cdot \vec{\nabla}_{G} d^{3}x , \qquad (C5)$$

where the surface s encloses the relevant finite volume. (There are no singularities or discontinuities of \vec{v}_{G} , according to the preceding discussion.) Then every ψ_i vanishes, or can be made arbitrarily small, on the surface s so that the surface integral itself vanishes. Thus we arrive at the result

$$I_{ij} = \int \psi_i^* \psi_j (\nabla \cdot \vec{\mathbf{v}}_G) d^3 x = 0 , \qquad (C6)$$

for all *i* and *j*. But since the ψ_k 's form a complete set, the quantity itself must be identically zero:

$$\nabla \cdot \vec{v}_{\rm G} \equiv 0 \ . \tag{C7}$$

Thus \vec{v}_G obeys (3.3), and consequently (3.1). This completes the proof that the geometric velocity field is also a regular and an incompressible velocity field.

APPENDIX D. POLAR FORM OF THE WAVE FUNCTION IN THE STATIC LIMIT

Throughout this paper, the polar form (2.4) of the wave function is utilized with the collective velocity $\dot{\alpha}$ assumed to be nonzero. We here examine this polar form of the wave function in the static limit $\dot{\alpha} = 0$. Then a single-particle state is described by an eigensolution ψ of the time-independent Schrödinger equation

$$H\psi = \epsilon \psi , \tag{D1}$$

which in general can assume both positive and negative values, and passes through zero continuously and with continuous first derivatives.

However, in the polar form,

$$\psi = \phi \exp\left\{-\frac{im}{\hbar}S\right\},\tag{D2}$$

with the conventions we have adopted, the phase S (interpreted as the velocity potential in the singleparticle Schrödinger fluid) exhibits a discontinuity and the magnitude ϕ , a discontinuous first derivative at each zero of ψ . We discuss here the relationship between this discontinuous form implied by Eq. (D2) and the more familiar continuous eigensolution in Eq. (D1).

Singular behavior is well defined as $\dot{\alpha} \rightarrow 0$

We consider the limit $\dot{\alpha} \rightarrow 0$, at which ψ becomes a purely real function. For all $\dot{\alpha} > 0$, however, ψ is complex. Figure 3 shows schematically the function S, as a function of the distance along the path *ABCDE* shown in Fig. 1, for a sequence of diminishing $\dot{\alpha}$ values. At points A and E, the imaginary part μ of ψ vanishes. According to Eq. (4.2), the value of S is 0 and $\pi \hbar/m$ at the nodal points A and E, of μ , respectively. As $\dot{\alpha}$ diminishes, μ diminishes everywhere (while the real part u of ψ remains finite) and the change of the value of S from 0 to $\pi \hbar/m$ takes place in a smaller and smaller interval across the u node. As Fig. 3 shows, the function S for decreasing $\dot{\alpha}$ values approaches a step function as a limit.

Discontinuities are consistent with (modified) Schrödinger equation

In the modified Schrödinger equation (2.7) and (2.8), the dynamical modification potential V_{dyn} depends on the derivatives of the velocity potential S and hence may exhibit singular behavior as $\dot{\alpha} \rightarrow 0$.

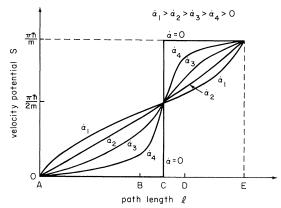


FIG. 3. Schematic representation of the velocity potential S across a nodal surface of the real part u of the wave function for different collective velocities. The velocity potential along the path ABCDE shown in Fig. 1 is shown here. Point C is on the nodal surface of u. The collective velocities $\dot{\alpha}_1$, $\dot{\alpha}_2$, $\dot{\alpha}_3$, and $\dot{\alpha}_4$ satisfies the inequalities $\dot{\alpha}_1 > \dot{\alpha}_2 > \dot{\alpha}_3 > \dot{\alpha}_4 > 0$.

As $\dot{\alpha} \rightarrow 0$, the first term $\partial S/\partial t$ of $V_{\rm dyn}$ can be approximated by $\dot{\alpha}(\partial S/\partial \alpha)$. By our assumption that the single-particle wave functions are smooth functions of α , we conclude that $\partial S/\partial t$ gives rise to no singularity as $\dot{\alpha} \rightarrow 0$.

However, as we show in the next section, the second term $(\nabla S)^2$ of $V_{\rm dyn}$ approaches a δ function of infinite strength on the *u* node as $\dot{\alpha} \rightarrow 0$. As a result, the dynamical modification potential $V_{\rm dyn}$ acts as an infinite repulsive [due to the positive sign of the $(\nabla S)^2$ term in $V_{\rm dyn}$] potential on the *u* node. Such a potential forces ϕ to have value zero and a discontinuous first spatial derivative at the *u* node.

Therefore, although S and the spatial derivatives of ϕ have the discontinuities mentioned above, they are nevertheless consistent with the Schrödinger equation, as modified by the singular dynamical modification potential. For $\dot{\alpha} = 0$, these singularities are purely the result of convention and could trivially be defined away. But, for $\dot{\alpha} \neq 0$ one would then have had to deal with discontinuous magnitudes ϕ in the polar forms, whereas our conventions give continuous positive ϕ .

Nature of the singularities

We now show that ∇S and $(\nabla S)^2$ approach δ functions of finite and infinite strength on the *u* node as $\dot{\alpha} \rightarrow 0$. We use the coordinate system of Fig. 1, as described in Sec. IV, and consider, along the path *ABCDE*, the functions $|\nabla S|$ and $(\nabla S)^2$ in the interval between two points *B* and *D* adjacent t o the *u* node at point *C*. On the path, ∇S is only a function of the azimuthal angle ϕ (since $\theta = \frac{1}{2}\pi$ and r=R), and therefore its behavior can be analyzed by the function $g(\theta, \phi)$ defined in Eq. (4.12). By our particular choice of the coordinate system in Fig. 1 ($\phi = 0$ at *C*, and hence $\phi_a = -\frac{1}{2}\pi$) we obtain by retaining only terms up to the second order of ϕ in Eq. (4.12),

$$g(\frac{1}{2}\pi,\phi)$$

$$=\frac{ab\sin\phi_{ab}}{b^2\sin^2\phi_{ab}+a^2\phi^2+b^2\phi^2\cos^2\phi_{ab}-b^2\phi\sin^2\phi_{ab}}$$
(D3)

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[†]Much of this research is reported in more detail in a dissertation submitted to the Graduate School, University of Maryland by K.-K. K. in partial fulfillment of the requirements of the Ph.D. degree.

‡ Present address.

§Alexander von Humboldt Foundation U.S. Senior Scientist at Universität, Giessen, and Hahn Meitner where $\phi_{ab} = \phi_a - \phi_b$. Since *b* is the magnitude of $\nabla \mu$ at the line vortex, it approaches zero as $\dot{\alpha} \rightarrow 0$. The last two terms in the denominator in Eq. (D3) are then negligible, and

$$g\left(\frac{1}{2}\pi,\phi\right) = \frac{\nu}{1+\nu^2\phi^2} \stackrel{\bullet}{\stackrel{\bullet}{\overleftarrow{\alpha}\to 0}} \pi\delta(\phi) , \qquad (D4)$$

where δ is the Dirac δ function, because the dimensionless quantity

$$\nu \equiv \frac{a}{b \sin \phi_{ab}} \tag{D5}$$

goes to infinity as $\dot{\alpha}$ goes to zero.⁵⁸ Introducing result (D4) in Eq. (4.11), we have, along the path *BCD*,

$$\lim_{\alpha \to 0} |\nabla S|_{BCD} = \frac{\pi \hbar}{mR^2} \,\delta(\phi) \,. \tag{D6}$$

For $(\nabla S)^2$, we consider the integral along the same path:

$$\lim_{t \to 0} \int_{-\epsilon}^{\epsilon} (\nabla S)^2 d\phi$$

$$= \left(\frac{\hbar}{mR}\right)^2 \int_{-\epsilon}^{\epsilon} \lim_{\nu \to \infty} g^2(\frac{1}{2}\pi, \phi) d\phi$$

$$= \left(\frac{\hbar}{mR}\right)^2 \lim_{\nu \to \infty} \nu \left\{\frac{\nu\epsilon}{1+\nu^2\epsilon^2} + \frac{1}{2} \int_{-\epsilon}^{\epsilon} g(\frac{1}{2}\pi, \phi) d\phi\right\},$$
(D7)

where ϵ is an arbitrarily small but fixed number. The first term in the parentheses tends to zero as $\nu \rightarrow \infty$ and is negligible compared with the second term, which integrates to $\frac{1}{2}\pi$. Hence, for any arbitrary fixed ϵ , we have

$$\lim_{\dot{\alpha}\to 0} \int_{-\epsilon}^{\epsilon} (\nabla S)^2 d\phi = \lim_{\nu\to\infty} \frac{1}{2} \pi \left(\frac{\hbar}{mR}\right)^2 \nu \tag{D8}$$

so that

...

 $\frac{1}{\alpha}$

$$\lim_{\hat{\alpha}\to 0} (\nabla S)^2 \Big|_{BCD} = \lim_{\nu\to\infty} \frac{1}{2} \pi \left(\frac{\hbar}{mR}\right)^2 \nu \delta(\phi) . \tag{D9}$$

Equations (D6) and (D9) show that the functions $|\nabla S|$ and $(\nabla S)^2$ tend to δ functions of finite and infinite strength as we have set out to prove.

Institute, Berlin, during 1975–76. The support of the foundation during the final stages of this work is greatly acknowledged.

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- ³J. J. Griffin and K.-K. Kan, Rev. Mod. Phys. <u>48</u>, 467

(1976).

- ⁴Part of the present work has been reported earlier in (a) K.-K. Kan and J. J. Griffin, Bull. Am. Phys. Soc. 18, 647 (1973); (b) J. J. Griffin and K.-K. Kan, in Proceedings of the Third International Conference on the Physics and Chemistry of Fission, Rochester, New York, 1973 (IAEA, Vienna, 1974), Vol. 1, p. 533; (c) K.-K. Kan and J. J. Griffin, Bull. Am. Phys. Soc. 19, 526 (1974); (d) K.-K. Kan and J. J. Griffin, *ibid*. 19, 996 (1974); (e) K.-K. Kan and J. J. Griffin, *ibid*. 20, 581 (1975); (f) J. J. Griffin and K.-K. Kan, in Proceedings of the Third International Workshop on Gross Properties of Nuclei and Nuclear Excitations, Hirschegg, Kleinwalsertal, Austria, 1975, edited by W. J. Myers [Institute für Kernphysik, Technische Hochschule Darmstadt, Germany, Report No. AED-Conf-75-009-000 (unpublished)], p. 56.
- ⁵K.-K. Kan, Ph.D. dissertation, University of Maryland, June 1975 (unpublished), provides a more detailed discussion of much of this research.
- ⁶K.-K. Kan and J. J. Griffin (unpublished) reports further results of Refs. 4 and 5 involving specific applications to rotations, dilatations, and shape distortions in nuclei. This reference is referred to as paper II.
- ⁷Precisely this same basis justifies the great interest in the time-dependent Hartree-Fock formalism (see Ref. 8), and [especially since the demonstration (see Ref. 9) that such studies could be executed with current available computers] its application to nuclear modelling by numerical computation (see Ref. 10). In the present work, the omission of the requirement of selfconsistency might allow perhaps a broader range of phenomena to be analyzed. E.g., see Ref. 26.
- ⁸S. T. Belyaev, Nucl. Phys. <u>64</u>, 17 (1965); M. Baranger and K. Kumar, *ibid*. <u>A122</u>, 241 (1968); F. M. H. Villars, in *Dynamic Structure of Nuclear States*, edited by D. J. Rowe *et al.* (Univ. of Toronto Press, Toronto, 1971), p. 3; D. J. Rowe and R. Bassermann, Can. J. Phys. 54, 1941 (1976).
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- ¹⁰S. E. Koonin, Phys. Lett. <u>61B</u>, 227 (1976); R. Y. Cusson and J. A. Maruhn, Phys. Lett. <u>62B</u>, 134 (1976); R. Y. Cusson, R. K. Smith, and J. A. Maruhn, Phys. Rev. Lett. <u>36</u>, 1166 (1976); S. E. Koonin, K. T. R. Davies, V. Maruhn-Rezwani, and J. W. Negele (unpublished).
- ¹¹This use of the polar form to obtain a modified form of the Schrödinger equation was first discussed by Madelung (Ref. 12). With different emphases and from different viewpoints the separation of the magnitude and phase of the wave function is a technique which (perhaps not surprisingly) seems repeatedly to be rediscovered and reapplied, and which therefore touches on a host of questions, ranging from the technical to the philosophical aspects in quantum physics (Refs. 13–19).

¹²E. Madelung, Z. Phys. 40, 322 (1926).

- ¹³The fluid dynamical equations of Madelung (Ref. 12) were rediscovered and further developed by T. Takabayasi, Prog. Theo. Phys. <u>8</u>, 143 (1952).
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- ¹⁸Wave functions in polar form were utilized to construct a Schrödinger equation with friction by K.-K. Kan and J. J. Griffin, Phys. Lett. <u>50B</u>, 241 (1974); in Proceedings of the International Conference on Reactions Between Complex Nuclei, Nashville, Tennessee, 1974, edited by R. L. Robinson et al. (North-Holland, Amsterdam, 1974), Vol. 1, p. 127.
- ¹⁹Dr. J. O. Hirschfelder has kindly pointed out to us that he and his collaborators have also reported recent studies of the Schrödinger fluid, with applications to atomic collisions. Their articles are cited here: J. O. Hirschfelder, A. C. Christoph, and W. E. Palke, J. Chem. Phys. <u>61</u>, 5435 (1974); J. O. Hirschfelder, C. J. Goebel, and L. W. Bruch, *ibid.* <u>61</u>, 5456 (1974); J. O. Hirschfelder and K. T. Tang, *ibid.* <u>64</u>, 760 (1976); <u>65</u>, 470 (1976).
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- ²¹L. Landau and E. M. Lifshitz, *Fluid Mechanics*, translated by J. B. Sykes and W. H. Reid (Addison-Wesley, Reading, 1959), p. 5.
- ²²D. L. Hill and J. A. Wheeler, Phys. Rev. <u>89</u>, 1102 (1953). See especially in this reference p. 1105 and Figs. 7 and 8 (pp. 1123–1124) for discussions on irrotational dynamics; p. 1106 for the first discussion of the wave function whose analysis was later to become known as the method of generator coordinates; and p. 1109 and Figs. 10–12 (pp. 1124–1125) for discussions on wave functions in an infinite square well, rectangular parallelpiped box. See also Secs. III C and VII and Appendixes A and C.
- ²³One important case which gives rise to compressible flow is the case of adiabatic adjustment of the singleparticle wave function so that it remains in the lowest energy state as it passes near a level crossing [Ref. 4(b)]. A detailed discussion of the level crossing case can be found in paper II.
- $^{24} The subscript <math display="inline">\odot$ denotes that \bar{v}_{\odot} has zero divergence wherever it is differentiable.
- ²⁵The assumption that the matter flow is incompressible (i.e., that $\nabla \cdot \hat{\nabla}_{\odot} = 0$) effects such a simplification in the analysis (e.g., of Ref. 22) as to seem most attractive and natural. We see here, especially in Sec. III C and in Appendix A, that this assumption involves substantial physical simplification, perhaps to the point of trivializing the content of the subsequent theoretical development. Sometimes the assumption may enter disguised as mathematics, as in a "locality" assumption in time-dependent Hartree-Fock theory, or, in other cases, as some other mathematical ansatz. See Ref. 26 and references cited therein.
- ²⁶Y. M. Engel, D. M. Brink, K. Goeke, S. J. Krieger, and D. Vautherin, Nucl. Phys. <u>A249</u>, 215 (1975);
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- ²⁷We make explicit the (otherwise suppressed) singleparticle state subscript *i* of single-particle quantities, such as ψ , ρ , ϕ , *S*, etc. only when we are considering more than one single particle at a time.
- ²⁸See, e.g., E. Sneddon, *Elements of Partial Differental Equations* (McGraw-Hill, New York, 1957), pp. 44-59.
- ²⁹P. A. M. Dirac, Proc. of Roy. Soc. Lond. <u>133</u>, 60 (1933), discovered that these singularities comprise line vortices. The present discussion emphasizes the behavior of the velocity field near the vortex, and particularly its compressibility.
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- ³¹Since S is discontinuous on its cuts its gradient is not defined there. However, when the cut is approached from either side, gradS is well defined, and has the same value on both sides of the cut. We therefore define gradS on the cut to be the limiting value of gradS as the point approaches the cut. The result is equivalent to the definition of gradS on the cut which follows from letting S continue onto its next branch. This definition conforms to the fact that any arbitrary change of phase of the wave function by $2n\pi$ (*n* integral) is of no physical consequence.
- ³²See, e.g., G. K. Batchelor, An Introduction to Fluid Dynamics (Cambridge U.P., London, 1967), pp. 72, 93.
- ³³Although the velocity field $\overline{\mathbf{v}}_{\otimes}$ possesses line vortices, we again follow the precedent of classical fluid dynamics (Ref. 32) and refer to it as an irrotational velocity field, since it is derived from the velocity potential S, everywhere except on these vortices.
- ³⁴We use the terminology "varies as r^{p} " in place of the more precise statement "is a homogeneous polynomial of degree p in the components x, y, z of the distance from the line vortex". One should keep in mind this notation suppresses a factor dependent upon the angle, which is essential for describing the actual behavior as the line vortex is approached along a specific direction.
- ³⁵We define stream lines, in analogy to classical fluid dynamics (Ref. 32), as lines in the fluid whose tangent is everywhere in the direction of the velocity field of the fluid.
- ³⁶We use the comma to denote differentiation. Thus, $f_{ij}(\mathbf{x})$ is the second partial derivative $\partial^2 f(\mathbf{x}) / \partial x_i \partial x_j$, etc.
- ³⁷D. R. Inglis, Phys. Rev. <u>96</u>, 1059 (1954).
- ³⁸The ket $|j\rangle$ denotes the state corresponding to the wave function $u_{j}^{(0)}$.
- ³⁹The terminology "classical fluid kinetic energy" of no special interest to the present discussion, is discussed further in Sec. VID.
- ⁴⁰Clearly $\phi^{(0)}$ in Eq. (5.12) is no longer of zeroth order in $\dot{\alpha}$. The superscript now signifies the order of iteration. Then $\phi^{(0)}$ denotes the starting quantity for an iterating procedure, $S^{(1)}$ is a quantity obtained from the first order iteration, and so on. We drop the carets from the symbols used earlier to distinguish

these quantities from $\hat{\phi}^{(0)}$, $\hat{S}^{(1)}$, etc.

- ⁴¹We are here implicitly excluding transitions among states of the nucleus, which occur as a result of effects other than the collective motion of the nuclear potential. Indeed, such time-dependent transitioning states describe other dynamical aspects of the nuclear system (e.g., the processes of nuclear excitation and deexcitation via coupling to the electromagnetic field) which are physically distinct from the collective motion and are therefore omitted here. For such transitioning states, the wave function is also essentially complex (Ref. 42).
- ⁴²A function is said to be "essentially complex" if it cannot be made real by a choice of its arbitrary phase.
- $^{43} This$ does not exclude the possibility that \bar{v}_{\otimes} may depend on $\dot{\alpha}^3,~\dot{\alpha}^5,~etc.$
- ⁴⁴But not necessarily the irrotational *incompressible* value so often referred to as "the" irrotational value. See also Ref. 56.
- ⁴⁵G. C. Wick, Phys. Rev. <u>73</u>, 51 (1948).
- ⁴⁶See, e.g., L. Wilets, *Theory of Nuclear Fission* (Clarendon, London, 1964), p. 43.
- ⁴⁷J. J. Griffin, in Proceedings of the Second International Conference on the Physics and Chemistry of Fission, Vienna, 1969 (IAEA, Vienna, 1969), p. 3.
- 48 We underline a quantity to signify that the quantity is defined in the 3N-dimensional coordinate space.
- ⁴⁹L. Landau, J. Phys. <u>5</u>, 71 (1941).
- ⁵⁰The symbol $dx_{(i)}^{3(N-1)}$ denotes $d^{3}x_{1} \cdots d^{3}x_{i-1} d^{3}x_{i+1} \cdots d^{3}x_{N}$.
- ⁵¹C. Y. Wong, J. A. Maruhn, and T. A. Welton, Nucl. Phys. <u>A253</u>, 469 (1975); C. Y. Wong and J. A. Mc-Donald (unpublished).
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 P. A. M. Dirac, Proc. Roy. Soc. London <u>113</u>, 621 (1926);
 P. Jordan, Z. Phys. <u>40</u>, 809 (1926); also see
 P. A. M. Dirac, *The Principles of Quantum Mechanics* (Clarendon, London, 1967), 4th ed. revised, p. 46.
- ⁵³F. London, Rev. Mod. Phys. <u>17</u>, 312 (1945).
- ⁵⁴The name ordering, "Wheeler-Hill," is chosen here purposely to minimize possible confusion with a separate and distinct topic, The Method of generator coordinates (Ref. 55), which is based on the "Hill-Wheeler" wave function, first proposed in this same paper (Ref. 22).
- ⁵⁵J. J. Griffin and J. A. Wheeler, Phys. Rev. <u>108</u>, 311 (1957); J. J. Griffin, *ibid.* <u>108</u>, 328 (1957).
- ⁵⁶Such a flow has usually been referred to in the nuclear physics literature simply as the "irrotational" flow, an impression which allows one more easily to overlook the possibilities which adhere to compressible flow in nuclei, some of which are discussed in more detail in Refs. 3 and 4(b).
- ⁵⁷The relationship (A4) is explicitly obeyed (Refs. 47) by particles moving in a quadrupole deformed oscillator potential, or in the Hill-Wheeler (infinite square well, rectangular parallelpiped) box (Ref. 22).
- ⁵⁸See, e.g., F. W. Byron, Jr., and R. W. Fuller, *Mathematics of Classical and Quantum Physics* (Addison-Wesley, Reading, 1969), Vol. 1, p. 224.