

Equations of motion for superfluids

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To the principles of least action and minimum error, for determining the time evolution of the parameters in a variational wave function, we add a third: continuous collapse dynamics. In this formulation, exact time evolution is applied for an infinitesimal time and is followed by projection of the state back into the variational manifold ("collapse"). All three principles lead to the same equations of motion when applied to complex parameters but take two distinct forms when the parameters are real. As an application of these principles, we study the time evolution of two variational wave functions for superfluids. The first wave function, containing real parameters, was considered by Kerman and Koonin [Ann. Phys. (N.Y.) **100**, 332 (1976)] and leads to the Euler equation in the hydrodynamic limit. The equation for our second wave function, a coherent state of Feynman excitations with complex parameters, has essentially the same hydrodynamic limit. The latter wave function, however, has a significant advantage in that the equation it generates is useful and meaningful on a microscopic scale as well.

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I. INTRODUCTION

Certain phenomena call for a description of fluid motion that goes beyond the hydrodynamical equations. One example, indeed the problem that motivated the present work, is the process whereby microscopic excitations in a superfluid are *created* [1]. A description of excitations as riding on a background of fluid flow is insufficient since one is ultimately interested in how the former evolve continuously from the latter. Aside from phonons, excitations defy a hydrodynamical description and a new approach is needed. Excitations of arbitrary wavelength as well as fluid flow can both be represented using the superfluid wave functions introduced by Feynman [2]. These wave functions are variational in character and up to now have served to model stationary states. The aim of the present paper is to derive the time evolution of these wave functions. Since the intent is to remain within the class of Feynman wave functions, there arises the problem of how to evolve the variational parameters so as to give the best approximation of the exact Schrödinger time evolution. This is the subject of the first half of the paper.

Although the general "time-dependent variational principle" has been addressed by several authors [3–8], there has been some confusion about different formulations yielding somewhat different equations of motion. We therefore begin by demonstrating the complete equivalence of Frenkel's [3] least action principle and the minimum error principle of McLachlan [4] for the case of complex parameters. By adding a refinement to these formulations, we show their equivalence to yet a third principle we refer to as "continuous collapse dynamics" [9]. We also show in detail how a difference among these formulations arises when the parameters are real [5].

In the second half of the paper we apply the time-

dependent variational principle to two super-fluid wave functions. We first consider a wave function introduced by Kerman and Koonin [6] where the density and phase are the variational parameters and by construction are conjugate variables in the equations of motion. Our second wave function is a coherent state formed from Feynman's excitation wave function [9]. Both wave functions lead to essentially the same hydrodynamic equations, although the Feynman wave function, in being more explicit in its construction, can be applied to microscopic phenomena as well.

II. THE TIME-DEPENDENT VARIATIONAL PRINCIPLE

In this section we consider a general time-independent Hamiltonian H and a state vector $|\alpha\rangle$ which depends parametrically on a set of complex parameters $\alpha_1, \alpha_2, \dots$. Our goal is to find the best approximation to the time evolution of $|\alpha\rangle$ by appropriately evolving the parameters in time. In approximating the time derivative of $|\alpha\rangle$ we have available the states

$$|\alpha_m\rangle \equiv \frac{\partial}{\partial \alpha_m} |\alpha\rangle, \quad (1)$$

as well as the state $|\alpha\rangle$ itself. The evolving state should thus be written in the form

$$\lambda(t)|\alpha(t)\rangle, \quad (2)$$

where λ is a complex number. In the following, the time dependence of λ and the parameters α_m will be understood and not always indicated explicitly.

In order to streamline our comparisons between the different principles for deriving equations of motion, we have found it useful to introduce the operator

$$\varepsilon = i\partial_t - H. \quad (3)$$

Since an exact time evolved state $|\Psi\rangle$ satisfies the equation $\varepsilon|\Psi\rangle=0$, we expect that matrix elements of ε are small in approximately evolved states.

A. Three formulations

1. Least action

Frenkel's least action principle [3] requires that the expression

$$\begin{aligned} S &= \int dt \langle \alpha | \lambda^* \varepsilon \lambda | \alpha \rangle \\ &= \int dt \langle \alpha | \lambda^* \varepsilon^\dagger \lambda | \alpha \rangle, \end{aligned} \quad (4)$$

is stationary with respect to arbitrary variations of the functions $\lambda(t)$ and $\alpha_m(t)$. Integration by parts leads to the second expression, where the time derivative in ε^\dagger acts to the left. Under the combined variation of both λ and the parameters α_m , we have

$$\begin{aligned} \delta S &= \int dt \{ \delta \lambda^* \langle \alpha | \varepsilon \lambda | \alpha \rangle + \delta \lambda \langle \alpha | \lambda^* \varepsilon^\dagger | \alpha \rangle \\ &\quad + \lambda^* \langle \delta \alpha | \varepsilon \lambda | \alpha \rangle + \lambda \langle \alpha | \lambda^* \varepsilon^\dagger | \delta \alpha \rangle \}. \end{aligned} \quad (5)$$

Since λ is complex, $\delta \lambda$ and $\delta \lambda^*$ represent independent variations and we conclude,

$$\begin{aligned} 0 &= \langle \alpha | \varepsilon \lambda | \alpha \rangle \\ &= i \dot{\lambda} \langle \alpha | \alpha \rangle + \lambda \langle \alpha | \varepsilon | \alpha \rangle. \end{aligned} \quad (6)$$

Using (6), we can solve for the time derivative of λ ($\dot{\lambda}$). We can then eliminate $\dot{\lambda}$ wherever it appears, in particular,

$$\begin{aligned} \varepsilon \lambda | \alpha \rangle &= \lambda \varepsilon | \alpha \rangle - \lambda \frac{\langle \alpha | \varepsilon | \alpha \rangle}{\langle \alpha | \alpha \rangle} | \alpha \rangle \\ &= \lambda P \varepsilon | \alpha \rangle. \end{aligned} \quad (7)$$

Here P is the projection operator

$$P = 1 - \frac{|\alpha\rangle\langle\alpha|}{\langle\alpha|\alpha\rangle}. \quad (8)$$

Using (6) and substituting (7) and its adjoint into (5), we have

$$\delta S = \int dt |\lambda|^2 \{ \langle \delta \alpha | P \varepsilon | \alpha \rangle + \langle \alpha | \varepsilon^\dagger P | \delta \alpha \rangle \}. \quad (9)$$

Recalling (1) to express the variation of the state vector,

$$|\delta \alpha\rangle = \sum_m \delta \alpha_m(t) |\alpha_m\rangle, \quad (10)$$

and again taking advantage of the fact that for complex α_m the variations $\delta \alpha_m$ and $\delta \alpha_m^*$ may be treated as independent, we arrive at the equations of motion

$$\langle \alpha_m | P \varepsilon | \alpha \rangle = 0, \quad m = 1, 2, \dots \quad (11)$$

Equations (11) reduce to the usual equations of the time-dependent variational principle when P is replaced by the identity operator. From the point of view that P affects at most a one dimensional subspace in the span of

the vectors $|\alpha_m\rangle$, the inclusion of P is a relatively minor refinement. The appearance of P is a direct result of expanding the freedom of the state vector's time evolution by means of the function $\lambda(t)$. As such, Eqs. (11) represent an improvement.

2. Minimum error

An alternative formulation, proposed by McLachlan [4], seeks to minimize the error in the approximation of the state vector's time derivative. Again using the form (2) for the state vector, the object now is to minimize

$$\Delta = \langle \alpha | \lambda^* \varepsilon^\dagger \varepsilon \lambda | \alpha \rangle. \quad (12)$$

The quantity Δ is now to be viewed as a function of the various time derivatives $\dot{\lambda}$ and $\dot{\alpha}_m$. The dependence on $\dot{\lambda}$ can be made explicit with the help of the identity

$$\varepsilon \lambda | \alpha \rangle = i \dot{\lambda} | \alpha \rangle + \lambda \varepsilon | \alpha \rangle. \quad (13)$$

Substituting (13) and its adjoint into (12), we have

$$\begin{aligned} \Delta &= \dot{\lambda}^* \dot{\lambda} \langle \alpha | \alpha \rangle - i \dot{\lambda}^* \lambda \langle \alpha | \varepsilon | \alpha \rangle + i \lambda^* \dot{\lambda} \langle \alpha | \varepsilon^\dagger | \alpha \rangle \\ &\quad + |\lambda|^2 \langle \alpha | \varepsilon^\dagger \varepsilon | \alpha \rangle. \end{aligned} \quad (14)$$

Minimizing this with respect to the complex number $\dot{\lambda}$ leads to the equation

$$\begin{aligned} 0 &= \frac{\partial \Delta}{\partial \dot{\lambda}^*} \\ &= \dot{\lambda} \langle \alpha | \alpha \rangle - i \lambda \langle \alpha | \varepsilon | \alpha \rangle. \end{aligned} \quad (15)$$

Solving for $\dot{\lambda}$ in (15) and using (13) we obtain

$$\Delta = |\lambda|^2 \langle \alpha | \varepsilon^\dagger P \varepsilon | \alpha \rangle. \quad (16)$$

This corresponds to McLachlan's original formulation when P is replaced by the identity operator. In order to further minimize with respect to the $\dot{\alpha}_m$, we recall the definition of ε ,

$$\varepsilon | \alpha \rangle = i \sum_m \dot{\alpha}_m |\alpha_m\rangle - H | \alpha \rangle, \quad (17)$$

where we have made use of (1). Substituting (17) into (16) we obtain

$$\begin{aligned} \Delta &= |\lambda|^2 \left\{ \sum_{m,n} \dot{\alpha}_m^* \langle \alpha_m | P | \alpha_n \rangle \dot{\alpha}_n + i \sum_m \dot{\alpha}_m^* \langle \alpha_m | P H | \alpha \rangle \right. \\ &\quad \left. - i \sum_n \langle \alpha | H P | \alpha_n \rangle \dot{\alpha}_n + \langle \alpha | H P H | \alpha \rangle \right\}, \end{aligned} \quad (18)$$

and the equations of motion are given by

$$\begin{aligned} 0 &= \frac{\partial \Delta}{\partial \dot{\alpha}_m^*} \\ &= \sum_n \langle \alpha_m | P | \alpha_n \rangle \dot{\alpha}_n + i \langle \alpha_m | P H | \alpha \rangle. \end{aligned} \quad (19)$$

These are in fact identical with Eqs. (11) obtained from the least action principle.

3. Continuous collapse

Our third formulation of the time-dependent variational principle [9] begins with the state vector at time zero, $|\alpha(0)\rangle$, and applies the exact Schrödinger time evolution for a short time Δt . Since the resulting state is generally outside our variational manifold of states, it must be “collapsed” back into this manifold. Our criterion for the “best” collapsed state $|\alpha(\Delta t)\rangle$ is that it have the largest possible overlap with the correctly evolved state. As shown below, this determines a unique state (up to overall phase) and the process can be repeated. In the limit $\Delta t \rightarrow 0$, an ever decreasing amount of collapse is being applied continuously as the state vector describes a curve on the variational manifold.

The overlap between the exactly evolved state and the collapsed state $|\alpha(\Delta t)\rangle$ is given by the dimensionless ratio

$$R = \frac{|\langle \alpha(\Delta t) | \exp(-i\Delta t H) | \alpha(0) \rangle|^2}{\langle \alpha(\Delta t) | \alpha(\Delta t) \rangle \langle \alpha(0) | \alpha(0) \rangle}. \quad (20)$$

We note that the inclusion of a time-dependent scale factor $\lambda(t)$ in the state vector would add nothing to this expression. Anticipating the fact that the collapsed state vector describes a smooth curve in parameter space, we write

$$|\alpha(\Delta t)\rangle = |\alpha(0)\rangle + \Delta t |\dot{\alpha}(0)\rangle + \frac{1}{2}(\Delta t)^2 |\ddot{\alpha}(0)\rangle + \dots \quad (21)$$

Substituting (21) into (20) and expanding to second order in Δt (and dropping explicit reference to $t=0$), we find

$$R = 1 - \frac{(\Delta t)^2}{\langle \alpha | \alpha \rangle} \{ \langle \alpha | \epsilon^\dagger P \epsilon | \alpha \rangle + \langle \alpha | H^2 | \alpha \rangle - \langle \alpha | H P H | \alpha \rangle \} + \dots \quad (22)$$

To this order in Δt , only first derivatives of the parameters appear. Maximizing R with respect to these first derivatives corresponds to minimizing the same quantity that appears in the minimum error formulation [Eq. (16)]. The “continuous collapse” equations of motion are therefore no different from those derived from the previous formulations.

B. Real parameters

When the parameters α_m are real, the equations of motion take on a slightly different form. In deriving these equations we nevertheless consider the prefactor λ in (2) to be complex. In the least action formulation the first point of departure follows Eq. (9):

$$\delta S = \int dt |\lambda|^2 \left\{ \sum_m \delta \alpha_m \left[\langle \alpha_m | P \epsilon | \alpha \rangle + \langle \alpha | \epsilon^\dagger P | \alpha_m \rangle \right] \right\}. \quad (23)$$

Stationarity of the action now implies

$$\text{Re}[\langle \alpha_m | P \epsilon | \alpha \rangle] = 0, \quad m = 1, 2, \dots, \quad (24)$$

or,

$$i \sum_n \left[\langle \alpha_m | P | \alpha_n \rangle - \langle \alpha_n | P | \alpha_m \rangle \right] \dot{\alpha}_n = \langle \alpha_m | P H | \alpha \rangle + \langle \alpha | H P | \alpha_m \rangle, \quad m = 1, 2, \dots \quad (25)$$

Kerman and Koonin [6] observed that Eqs. (25) can be written in a form that resembles Hamilton’s equations. Adopting their notation, we define

$$\langle H \rangle \equiv \frac{\langle \alpha | H | \alpha \rangle}{\langle \alpha | \alpha \rangle}, \quad (26)$$

$$\{ \alpha_m, \alpha_n \} \equiv i \frac{\langle \alpha_m | P | \alpha_n \rangle - \langle \alpha_n | P | \alpha_m \rangle}{\langle \alpha | \alpha \rangle}. \quad (27)$$

Equations (25) may now be rewritten as

$$\sum_n \{ \alpha_m, \alpha_n \} \dot{\alpha}_n = \frac{\partial}{\partial \alpha_m} \langle H \rangle, \quad m = 1, 2, \dots \quad (28)$$

In the minimum error formulation, Eq. (18) is replaced by

$$\Delta = |\lambda|^2 \left\{ \frac{1}{2} \sum_{m,n} \dot{\alpha}_m \text{Re}[\langle \alpha_m | P | \alpha_n \rangle] \dot{\alpha}_n + \sum_m \dot{\alpha}_m \text{Re}[i \langle \alpha_m | P H | \alpha \rangle] + \langle \alpha | H P H | \alpha \rangle \right\}, \quad (29)$$

and the corresponding equations of motion take the form

$$\sum_n \left[\langle \alpha_m | P | \alpha_n \rangle + \langle \alpha_n | P | \alpha_m \rangle \right] \dot{\alpha}_n = i \langle \alpha_m | P H | \alpha \rangle - i \langle \alpha | H P | \alpha_m \rangle, \quad m = 1, 2, \dots, \quad (30)$$

or

$$\text{Im}[\langle \alpha_m | P \epsilon | \alpha \rangle] = 0, \quad m = 1, 2, \dots \quad (31)$$

As already noticed by Kay [5], these equations are in general distinct from the least action equations (24) for real parameters. The continuous collapse formulation also leads to these equations since an intermediate step of the derivation [see (16) and (22)] implies the minimization of Δ .

C. Conservation of energy

The time independence of the energy expectation value, already noticed by several authors, is a simple consequence of the equations of motion. Taking the time derivative of both sides of (26), we find

$$\frac{d}{dt} \langle H \rangle = \frac{\langle \dot{\alpha} | P H | \alpha \rangle + \langle \alpha | H^\dagger P | \dot{\alpha} \rangle}{\langle \alpha | \alpha \rangle}. \quad (32)$$

Using (3) to replace H (and its adjoint) in terms of ϵ , this becomes

$$\frac{d}{dt} \langle H \rangle = - \frac{\langle \dot{\alpha} | P \epsilon | \alpha \rangle + \langle \alpha | \epsilon^\dagger P | \dot{\alpha} \rangle}{\langle \alpha | \alpha \rangle}. \quad (33)$$

Since

$$|\dot{\alpha}\rangle = \sum_m \dot{\alpha}_m |\alpha_m\rangle, \quad (34)$$

the equations of motion for complex parameters (11) imply that each term on the right-hand side of (33) vanishes. When the parameters are real, though, the right-hand side vanishes only in the least action formulation [see (24)]. Real parameters thus present the following dilemma [5]; either Δ is minimized and the energy is not conserved, or we choose the alternative formulation which conserves the energy but does not minimize Δ to the full extent possible.

III. EQUATIONS OF MOTION FOR SUPERFLUIDS

In contrast to the by now classical approach for deriving equations of motion for condensed systems wherein symmetries and conservation laws play a major role, the equations of motion being discussed here are simply the consequences of particular wave functions. To the extent that these wave functions exploit the relevant symmetries, the hydrodynamic limit of their corresponding equations of motion should reproduce the equations given by the classical approach [10]. If the wave functions that produced them are also meaningful on microscopic scales, we might even expect their usefulness to go beyond the description of hydrodynamic behavior.

In the following we consider two wave functions that describe superfluids. Both apply to a system of N identical particles described by the Hamiltonian

$$H = -\frac{1}{2M} \sum_{i=1}^N (\nabla_i^2) + V(\mathbf{r}_1, \dots, \mathbf{r}_N), \quad (35)$$

where the potential V is symmetric in all its arguments, and $\hbar=1$. In this and all subsequent expressions we use the position representation. A particularly important role will be played by the density operator:

$$\hat{\rho}(\mathbf{r}) = \sum_{i=1}^N \delta^3(\mathbf{r} - \mathbf{r}_i). \quad (36)$$

Its expectation value in the state under consideration defines the local density:

$$\rho(\mathbf{r}) = \langle \hat{\rho}(\mathbf{r}) \rangle. \quad (37)$$

This already represents one important degree of freedom in a fluid. The other hydrodynamic degree of freedom, the phase, is expressed by the wave functions themselves.

A. Superfluid wave functions

Kerman and Koonin [6] proposed the following wave function for a superfluid:

$$\Psi[\rho, \phi] = \exp \left\{ i \int d^3\mathbf{r} \hat{\rho}(\mathbf{r}) \phi(\mathbf{r}) \right\} \Psi_0[\rho]. \quad (38)$$

Rather than forming a discrete set, the parameters in this wave function are a pair of real numbers $\rho(\mathbf{r})$ and $\phi(\mathbf{r})$ at each point in space. The dependence on the density parameters $\rho(\mathbf{r})$ is defined implicitly through the properties

of the wave function $\Psi_0[\rho]$. The latter should be viewed as the lowest energy wave function having the prescribed density $\rho(\mathbf{r})$. A "ground state" energy that is itself a functional of the density is thus defined by

$$E_0[\rho] \equiv \langle H \rangle_{\phi=0}. \quad (39)$$

As shown below, the explicit construction of $\Psi_0[\rho]$ is not necessary in order to derive the hydrodynamic limit of the equations of motion. We pause, however, to contemplate such a construction because it bears upon an important property of $\Psi_0[\rho]$ that the derivation assumes. In one approach, an external potential

$$\int d^3\mathbf{r} \hat{\rho}(\mathbf{r}) U(\mathbf{r}) \quad (40)$$

is added to the Hamiltonian and the corresponding ground state and density are computed. This determines $\rho[U]$, the density as a functional of U . Inverting this functional (perturbatively, in practice) gives $U[\rho]$ and finally, $\Psi_0[\rho]$. Thus $\Psi_0[\rho]$ emerges as the ground state of some Hamiltonian and the question of degeneracy or near degeneracy arises. This is where bosonic and fermionic systems differ. While the bosonic ground state is in general nondegenerate, this is true of fermionic systems only in the closed-shell configurations. Moreover, in very large fermionic systems which possess a Fermi surface, the very high near degeneracy of the ground state makes the choice of a particular $\Psi_0[\rho]$ very questionable. We thus confine our attention in what follows to systems (bosonic or fermionic) which possess a clearly nondegenerate ground state. Because our Hamiltonian (35) is real, we can assume that $\Psi_0[\rho]$ is real as well.

Turning to the $\phi(\mathbf{r})$ dependent prefactor in (38), we observe that when the phase $\phi(\mathbf{r})$ is constant this merely counts the number of particles, a conserved quantity. Since adding an overall phase does not really change the state, a slowly varying $\phi(\mathbf{r})$ represents a hydrodynamic variable. We note that this phase does not affect the density expectation value so that $\rho(\mathbf{r})$ is also the density of the full wave function $\Psi[\rho, \phi]$.

The second wave function we consider has the form [9]

$$\Psi[\alpha] = \exp \left\{ \int d^3\mathbf{r} \hat{\rho}(\mathbf{r}) \alpha(\mathbf{r}) \right\} \Psi_0, \quad (41)$$

where the parameters $\alpha(\mathbf{r})$ form a complex function in space and Ψ_0 is simply the ground state wave function with energy

$$E_0 = \langle H \rangle_{\alpha=0}. \quad (42)$$

Although (41) has the same phase degree of freedom as (38) and therefore contains the same hydrodynamical variable, its main inspiration is Feynman's wave function for excitations [2]

$$\left\{ \int d^3\mathbf{r} \hat{\rho}(\mathbf{r}) \alpha(\mathbf{r}) \right\} \Psi_0. \quad (43)$$

Our second wave function is thus a coherent state of excitations.

The coherent-state wave function possesses the same number of degrees of freedom as the Kerman-Koonin

wave function. Also, the remarks concerning the real valuedness of $\Psi_0[\rho]$ apply to Ψ_0 as well. The latter property is exploited in the calculation of matrix elements, in particular,

$$\begin{aligned} & \int d\Omega \Psi^*[\alpha] \nabla_i^2 \Psi[\alpha] \\ &= \int d\Omega \{ \Psi_0 \nabla_i^2 \Psi_0 + 2i \Psi_0 \nabla \alpha(\mathbf{r}_i) \cdot \nabla_i \Psi_0 + i \Psi_0^2 \nabla^2 \alpha(\mathbf{r}_i) \\ & \quad - \Psi_0^2 |\nabla \alpha(\mathbf{r}_i)|^2 \} \\ &= \int d\Omega \{ \Psi_0 \nabla_i^2 \Psi_0 - \Psi_0^2 |\nabla \alpha(\mathbf{r}_i)|^2 \} , \end{aligned} \quad (44)$$

where the cancellation of the second and third terms in the second line required an integration by parts and the identity

$$2\Psi_0 \nabla_i \Psi_0 = \nabla_i \Psi_0^2 . \quad (45)$$

B. Conserved energy

The energy expectation values take the following forms for the two wave functions:

$$\langle H \rangle_{\rho, \phi} = E_0[\rho] + \frac{1}{2M} \int d^3\mathbf{r} \rho(\mathbf{r}) |\nabla \phi(\mathbf{r})|^2 , \quad (46)$$

$$\langle H \rangle_{\alpha} = E_0 + \frac{1}{2M} \int d^3\mathbf{r} \rho_{\alpha}(\mathbf{r}) |\nabla \alpha(\mathbf{r})|^2 . \quad (47)$$

Here subscripts ρ , ϕ , and α have been appended to the

$$\begin{aligned} \{ \phi(\mathbf{r}), \rho(\mathbf{r}') \} &= i \frac{\int d\Omega \{ -i \hat{\rho}(\mathbf{r}) \Psi_0^*[\rho] \} \left[\frac{\delta}{\delta \rho(\mathbf{r}')} \Psi_0[\rho] \right]}{\int d\Omega |\Psi_0[\rho]|^2} \\ & \quad - i \frac{\left[\int d\Omega \{ -i \hat{\rho}(\mathbf{r}) \Psi_0^*[\rho] \} \Psi_0[\rho] \right] \left[\int d\Omega \Psi_0^*[\rho] \left[\frac{\delta}{\delta \rho(\mathbf{r}')} \Psi_0[\rho] \right] \right]}{\left[\int d\Omega |\Psi_0[\rho]|^2 \right]^2} + \text{c.c.} \end{aligned} \quad (48)$$

Taking advantage of the real valuedness of $\Psi_0[\rho]$ and the identity

$$\Psi_0^*[\rho] \frac{\delta}{\delta \rho(\mathbf{r}')} \Psi_0[\rho] = \frac{1}{2} \frac{\delta}{\delta \rho(\mathbf{r}')} \Psi_0^2[\rho] , \quad (49)$$

we see that (48) simplifies greatly:

$$\begin{aligned} \{ \phi(\mathbf{r}), \rho(\mathbf{r}') \} &= \frac{1}{2} \frac{\delta}{\delta \rho(\mathbf{r}')} \langle \hat{\rho}(\mathbf{r}) \rangle + \text{c.c.} \\ &= \delta^3(\mathbf{r} - \mathbf{r}') . \end{aligned} \quad (50)$$

By similar manipulations, one finds

$$\begin{aligned} \{ \phi(\mathbf{r}), \phi(\mathbf{r}') \} &= 0 , \\ \{ \rho(\mathbf{r}), \rho(\mathbf{r}') \} &= 0 . \end{aligned} \quad (51)$$

These together with (50) show that the parameter functions ϕ and ρ have a conjugate relationship so that the equations of motion (28) take on the canonical Hamil-

tonian form to identify the Kerman-Koonin and coherent-state wave functions, respectively. In (47) the density has been given the subscript α to emphasize the fact that in the coherent-state wave function the density is not a variational parameter, but an expectation value determined by the parameter function α .

The energy of the coherent-state wave function is conserved by the equations for its complex parameter function. The energy of the Kerman-Koonin wave function, on the other hand, is a constant of the motion only if we apply the least action principle to its real parameters.

C. Equations of motion

1. Kerman-Koonin wave function

The Kerman-Koonin wave function was constructed to take advantage of the Hamiltonian form of the least action equations of motion for real parameters. As already mentioned, this choice of real-parameter equations also has the advantage of conserving the energy. Although the corresponding approximation of the time derivative of the wave function is not optimized in this formulation, we make this choice in what follows.

The parameters α_m in the general formalism become values of the functions $\phi(\mathbf{r})$ and $\rho(\mathbf{r}')$ at particular points in space, while partial derivatives are replaced by functional derivatives. As an example, we give some details in the calculation of one of the antisymmetric symbols (27):

tonian form:

$$\dot{\rho}(\mathbf{r}) = \frac{\delta}{\delta \phi(\mathbf{r})} \langle H \rangle_{\rho, \phi} , \quad (52)$$

$$-\dot{\phi}(\mathbf{r}) = \frac{\delta}{\delta \rho(\mathbf{r})} \langle H \rangle_{\rho, \phi} . \quad (53)$$

Taking the indicated functional derivative of (46) and defining the flow velocity by

$$M \mathbf{v}(\mathbf{r}) = \nabla \phi(\mathbf{r}) , \quad (54)$$

Eq. (52) is recognized as the equation of continuity:

$$\dot{\rho} + \nabla \cdot (\rho \mathbf{v}) = 0 . \quad (55)$$

Taking the gradient of (53) and dividing through by M , the second equation of motion takes the form

$$\dot{\mathbf{v}} + (\mathbf{v} \cdot \nabla) \mathbf{v} = -\frac{1}{M} \nabla \mu , \quad (56)$$

where μ represents a nonlocal chemical potential:

$$\mu[\rho](\mathbf{r}) \equiv \frac{\delta E_0[\rho]}{\delta \rho(\mathbf{r})}. \quad (57)$$

In order to be able to call (56) the Euler equation, we need to make the hydrodynamic approximation where μ is only a function of the local density:

$$\mu[\rho](\mathbf{r}) \approx \mu_h[\rho(\mathbf{r})]. \quad (58)$$

In fact, this is the only instance in the derivation where we use the fact that our wave function describes a liquid as opposed to a solid. Clearly, approximation (58) only makes sense if the density remains a relatively slowly varying function of space over the course of time. The local chemical potential function μ_h is obtained by taking the density derivative of the ground state energy of a uniform system characterized by a constant density (and external potential, if present).

2. Coherent-state wave function

In deriving equations of motion for the coherent-state wave function (41) we use the general formula (19) appropriate for complex parameters. The functional derivative of the state vector with respect to $\alpha(\mathbf{r})$, denoted $|\alpha(\mathbf{r})\rangle$, has the position space representation

$$\frac{\delta}{\delta \alpha(\mathbf{r})} \Psi[\alpha] = \hat{\rho}(\mathbf{r}) \Psi[\alpha]. \quad (59)$$

Using this, the two terms in (19) are easily expressed as expectation values:

$$\frac{\langle \alpha(\mathbf{r}) | P | \alpha(\mathbf{r}') \rangle}{\langle \alpha | \alpha \rangle} = \langle \hat{\rho}(\mathbf{r}) \hat{\rho}(\mathbf{r}') \rangle_\alpha - \langle \hat{\rho}(\mathbf{r}) \rangle_\alpha \langle \hat{\rho}(\mathbf{r}') \rangle_\alpha \\ = \sigma_\alpha(\mathbf{r}, \mathbf{r}'), \quad (60)$$

$$\frac{\langle \alpha(\mathbf{r}) | PH | \alpha \rangle}{\langle \alpha | \alpha \rangle} = \langle \hat{\rho}(\mathbf{r}) H \rangle_\alpha - \langle \hat{\rho}(\mathbf{r}) \rangle_\alpha \langle H \rangle_\alpha. \quad (61)$$

In (60) we have introduced the pair correlation function σ_α . The subscript α reminds us that, like ρ_α , we are again dealing with a functional of the parameter function $\alpha(\mathbf{r})$. Using the properties of the ground state wave function [as illustrated in (44)] to evaluate the expectation values in (61) and combining with (60) in the equation of motion (19), we obtain [9],

$$i[\sigma_\alpha \circ \dot{\alpha}](\mathbf{r}) = \frac{1}{2M} \{ -\nabla \cdot [\rho_\alpha(\mathbf{r}) \nabla \alpha(\mathbf{r})] + [\sigma_\alpha \circ |\nabla \alpha|^2](\mathbf{r}) \}, \quad (62)$$

where the symbol \circ denotes the convolution operator:

$$[\sigma_\alpha \circ f](\mathbf{r}) \equiv \int d^3 r' \sigma_\alpha(\mathbf{r}, \mathbf{r}') f(\mathbf{r}'). \quad (63)$$

The time evolution equation (62) for the complex-valued field $\alpha(\mathbf{r})$ is our principal result. Being nonlocal, both explicitly through the appearance of convolution terms and implicitly through the functionals ρ_α and σ_α , it expresses information at microscopic length scales. By linearizing the latter functionals about the state $\alpha(\mathbf{r})=0$ it has been possible to [11,12] (1) reproduce the Bijl-

Feynman spectrum of elementary excitations, (2) describe the propagation of excitations in a nonuniform flow field, and (3) obtain a detailed understanding of Landau's superflow instability as a quasiparticle pair-creation process.

Hydrodynamics can be recovered from (62) by decomposing $\alpha(\mathbf{r})$ into its real and imaginary parts:

$$\alpha(\mathbf{r}) = \chi(\mathbf{r}) + i\phi(\mathbf{r}). \quad (64)$$

The imaginary part of (62),

$$[\sigma_\alpha \circ \dot{\chi}](\mathbf{r}) = -\frac{1}{2M} \nabla \cdot [\rho_\alpha(\mathbf{r}) \nabla \phi(\mathbf{r})], \quad (65)$$

is recognized as the equation of continuity with the help of (54) and the identity

$$\dot{\rho}_\alpha(\mathbf{r}) = 2[\sigma_\alpha \circ \dot{\chi}](\mathbf{r}). \quad (66)$$

Perhaps a more direct approach is to rewrite the original wave function (41) in the form

$$\Psi[\alpha] = \exp \left\{ i \int d^3 \mathbf{r} \hat{\rho}(\mathbf{r}) \phi(\mathbf{r}) \right\} \tilde{\Psi}_0[\rho], \quad (67)$$

where

$$\tilde{\Psi}_0[\rho] = \exp \left\{ \int d^3 \mathbf{r} \hat{\rho}(\mathbf{r}) \chi(\mathbf{r}) \right\} \Psi_0 \quad (68)$$

is the counterpart of the Kerman-Koonin ground state having prescribed density, $\Psi_0[\rho]$. As written, (68) is a functional of χ that in turn determines the density ρ , also as a functional of χ . Since ρ and χ have the same number of degrees of freedom, the functional $\rho[\chi]$ (previously written as ρ_α) can formally be inverted, yielding χ , and consequently $\tilde{\Psi}_0$, as functionals of ρ . The difference that remains, between the coherent-state wave function $\Psi[\alpha]$ and the Kerman-Koonin wave function, is the fact that $\tilde{\Psi}_0[\rho]$ is not necessarily the *lowest* energy wave function having the prescribed density. But this is the only difference and implies the equations of motion in the ρ, \mathbf{v} variables are the same as before, but with $E_0[\rho]$ in the expression for the chemical potential (57) replaced by

$$\tilde{E}_0[\rho] \equiv \langle H \rangle_{\chi[\rho], \phi=0}. \quad (69)$$

D. Discussion

Although the functionals E_0 and \tilde{E}_0 are indeed different, we expect them to be nearly equal when the density is close to the density of the ground state, Ψ_0 . By definition,

$$E_0[\rho] \leq \tilde{E}_0[\rho], \quad (70)$$

and, moreover,

$$E_0[\rho_0] = \tilde{E}_0[\rho_0], \quad (71)$$

where $\rho_0(\mathbf{r})$ is the density of the ground state. Together, (70) and (71) imply

$$\left. \frac{\delta E_0[\rho]}{\delta \rho(\mathbf{r})} \right|_{\rho_0} = \left. \frac{\delta \tilde{E}_0[\rho]}{\delta \rho(\mathbf{r})} \right|_{\rho_0}. \quad (72)$$

Finally, since the energy of the ground state satisfies

$$\left. \frac{\delta E_0[\rho]}{\delta \rho(\mathbf{r})} \right|_{\rho_0} = 0, \quad (73)$$

it follows that

$$\mu[\rho_0](\mathbf{r}) = \bar{\mu}[\rho_0](\mathbf{r}) = 0. \quad (74)$$

Beyond the simple fact expressed by Eq. (74), the two chemical potentials are generally different. In the hydro-

dynamic approximation, where the chemical potential is an ordinary function of the local density, an expansion about the ground state density begins

$$\mu_h(\rho) = \frac{Mc^2}{\rho_0}(\rho - \rho_0) + \dots, \quad (75)$$

where c defines the velocity of sound waves. To see that the two wave functions lead to different sound velocities, consider the following more explicit representation of $\Psi_0[\rho]$:

$$\Psi_0[\rho] = \exp \left\{ \int d^3\mathbf{r} \hat{\rho}(\mathbf{r}) \chi_1(\mathbf{r}) + \frac{1}{2} \int d^3\mathbf{r} \int d^3\mathbf{r}' \hat{\rho}(\mathbf{r}) \hat{\rho}(\mathbf{r}') \chi_2(\mathbf{r}, \mathbf{r}') + \dots \right\} \Psi_0. \quad (76)$$

As was the case with $\tilde{\Psi}_0$ [Eq. (68)], the functions χ_1, χ_2, \dots are not independent degrees of freedom but really functionals of the density. On the other hand, Ψ_0 has more flexibility than $\tilde{\Psi}_0$ in being able to fine tune the two-body, three-body, etc., correlations at each density. By this mechanism, (70) becomes a strict inequality and the first nontrivial term in the hydrodynamic approximation (75) yields different values for the sound velocity—the Kerman-Koonin wave function having the lower value.

Because of its greater “structure” (76), it should not be concluded that the Kerman-Koonin wave function is superior to the coherent-state wave function. The requirement that the functions χ_2, χ_3, \dots be fine tuned to minimize the energy (for a given density) is not necessarily better and certainly no less rigid than simply setting them to zero. More in line with the original intent of the time-dependent variational approach is to improve the approximation of the wave function’s time derivative by giving it more freedom. A natural choice in this direction is an extension of the coherent-state wave function

$$\Psi[\alpha_1, \alpha_2, \dots] = \exp \left\{ \int d^3\mathbf{r} \hat{\rho}(\mathbf{r}) \alpha_1(\mathbf{r}) + \frac{1}{2} \int d^3\mathbf{r} \int d^3\mathbf{r}' \hat{\rho}(\mathbf{r}) \hat{\rho}(\mathbf{r}') \alpha_2(\mathbf{r}, \mathbf{r}') + \dots \right\} \Psi_0. \quad (77)$$

Here $\alpha_1, \alpha_2, \dots$ are time dependent and complex, the latter being necessary to achieve an optimized approximation of the time derivative without sacrificing energy conservation. The function of a single spatial variable, α_1 , having a natural quasiparticle interpretation [11], would thus be augmented by “multiparticle” degrees of freedom represented by the functions α_2, \dots .

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- [1] P. V. E. McClintock and R. M. Bowley, in *Progress in Low Temperature Physics*, edited by R. Halperin (Elsevier, Amsterdam, 1995), Vol. XIV, Chap. 1.
- [2] R. P. Feynman, *Phys. Rev.* **94**, 262 (1954).
- [3] J. Frenkel, *Wave Mechanics: Advanced General Theory* (Clarendon, Oxford, 1934), pp. 253 and 254.
- [4] A. D. McLachlan, *Mol. Phys.* **8**, 39 (1964).
- [5] K. G. Kay, *J. Chem. Phys.* **91**, 170 (1989).
- [6] A. K. Kerman and A. D. Koonin, *Ann. Phys. (N.Y.)* **100**, 332 (1976).
- [7] E. J. Heller, *J. Chem. Phys.* **64**, 63 (1976).
- [8] F. Arickx, J. Broeckhove, E. Kesteloot, L. Lathouwers, and P. Vanleuven, *Chem. Phys. Lett.* **128**, 310 (1986).
- [9] A. G. Basile, Ph.D. thesis, Cornell University, 1992.
- [10] I. M. Khalatnikov, *Introduction to the Theory of Superfluidity* (Benjamin, New York, 1965).
- [11] V. Elser, following paper, *Phys. Rev. E* **51**, 5695 (1995).
- [12] T. J. Lenosky and V. Elser, *Phys. Rev. B* **51**, 12 857 (1995).