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Nonlocal Nonlinear Schrödinger Equations as Models of Superfluidity

N. G. Berloff

Department of Mathematics, University of California, Los Angeles, California 90095-1555

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Condensate models for superfluid helium II with nonlocal potentials are considered. The potentials are chosen so that the models give a good fit to the Landau dispersion curve; i.e., the plot of quasi-particle energy E versus momentum p has the correct slope at the origin (giving the correct sound velocity) and the roton minimum is close to that experimentally observed. It is shown that for any such potential the condensate model has non-physical features, specifically the development of catastrophic singularities and unphysical mass concentrations. Two numerical examples are considered: the evolution of a radially symmetric mass disturbance and the flow around a solid sphere moving with constant velocity, both using the nonlocal Ginsburg-Pitaevskii model. During the evolution of the solution in time, mass concentrations develop at the origin in the radially symmetric case and along the axis of symmetry for the motion of the sphere.

1. INTRODUCTION

One of the most useful ways of describing superfluid helium at zero temperature begins with Schrödinger's equation for the one-particle wave function ψ. Since liquid helium is a strongly correlated system dominated by collective effects, the form of the Hamiltonian in Schrödinger's equation cannot be derived starting from the first principles. At zero temperature ^{4}He has large interatomic spacing and low density, which suggests a description in terms of a weakly interacting Bose gas for which such a derivation can be made rigorous. Continuum mechanical equations for ^{4}He are usually built on the assumption that a Bose condensate gives the exact description at zero temperature.

The imperfect Bose condensate in the Hartree approximation is governed by equations that were derived by Gross and by Ginsburg and Pitaevskii.

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In terms of the single-particle wavefunction $\psi(\mathbf{x},t)$ for the N bosons of mass m the time-dependent self-consistent field equation is

$$i\hbar\psi_t = -\frac{\hbar^2}{2m}\nabla^2\psi + \psi\int|\psi(\mathbf{x}',t)|^2U(|\mathbf{x}-\mathbf{x}'|)\,d\mathbf{x}', \tag{1}$$

where $U(|\mathbf{x}-\mathbf{x}'|)$ is the potential of the two-body interactions between bosons. The normalization condition is

$$\int\limits_V|\psi|^2\,d\mathbf{x} = N. \tag{2}$$

For a weakly interacting Bose system this 'nonlocal model' (as we shall call it) is simplified by replacing $U(|\mathbf{x}-\mathbf{x}'|)$ with a δ - function repulsive potential of strength W_0. This does not alter the nature of the results since the characteristic length of the weakly interacting Bose gas is larger than the range of the force [Gross (1963)]. Equation (1) for the "local model" is

$$i\hbar\psi_t = -\frac{\hbar^2}{2m}\nabla^2\psi + W_0|\psi|^2\psi. \tag{3}$$

If E_v is the average energy level per unit mass of a boson, we write

$$\Psi = \exp(imE_vt/\hbar)\psi, \tag{4}$$

so that (3) becomes

$$i\hbar\Psi_t = -\frac{\hbar^2}{2m}\nabla^2\Psi + W_0|\psi|^2\Psi - mE_v\Psi. \tag{5}$$

This model enjoys not only the advantage of comparative simplicity but also describes qualitatively correct superfluid behaviors. We may mention the annihilation of vortex rings [Jones and Roberts (1982)], the nucleation of vortices [Frisch *et al.* (1992)], vortex line reconnection [Koplik and Levine (1993, 1996)], and studies of superfluid turbulence [Nore *et al.* (1997)]. At the same time several aspects of the local model (5) are qualitatively or quantitatively unrealistic for superfluid helium. The dispersion relation between the frequency, ω, and wave number, k, of sound waves according to (5) is

$$\omega^2 = c^2k^2 + \left(\frac{\hbar}{2m}\right)^2k^4, \tag{6}$$

where

$$c = (W_0\rho_\infty)^{\frac{1}{2}}/m, \qquad \rho_\infty = mE_v/W_0. \tag{7}$$

This shows that the velocity, c, of long wavelength sound waves is proportional to $\rho^{\frac{1}{2}}$ (here we have replaced the bulk density, ρ_∞, by the total density, ρ). That this is unrealistic is seen from the experiments on Grüneisen constant $U_G = (\rho\partial c/c\partial\rho)_T$, which shows that, in the bulk (i.e., on length-scales long compared with the healing length, κ/c), the fluid behaves as a barotropic fluid ($p \propto \rho^\gamma$) with $\gamma = 2.8$ [see Brooks and Donnelly (1977) and references therein]. Also, the dispersion curve (6) has no roton minimum. At best, (6) describes the phonon branch of the excitation spectrum. The healing length and correlation length in real helium are known to be quite different, so making the local model (5) quantitatively inaccurate, and less satisfactory than its counterpart for superconductivity, the Ginsburg-Landau equation.

For some time there has been a belief that, as soon as the nonlocal model (1) with a realistic two-particle potential, U, that leads to phonon-roton-like spectra is solved, the properties of superfluid helium will be well represented [see, for example, Bogoliubov (1947), Gross (1963), Pomeau and Rica (1993), Lifshits and Pitaevskii (1978)]. The minimum requirements on such a potential would be the correct position of the roton minimum and the correct bulk normalization, $\int U(|\mathbf{x} - \mathbf{x}'|)\, d\mathbf{x}' = mE_v/\rho_\infty$. Actually such a fit can be obtained with a variety of potentials, and in Sec. 2 we describe some general properties of these.

Our goal is to investigate the applicability of (1) with a potential that adequately represents the dispersion curve. We shall show that, for liquid helium having the correct Landau dispersion curve, solutions of equation (1) develop non-physical mass concentrations. This indicates that the assumptions underlying the derivation of the equation break down and that higher order nonlinearities must be introduced. A new equation that lacks this shortcoming of model (1) will be considered in a subsequent paper [Berloff and Roberts (1999)].

2. NONLOCAL POTENTIALS

Equation (1) transformed by (4) and the scaling

$$\mathbf{x} \to \frac{\hbar}{(2m^2E_v)^{1/2}}\mathbf{x}, \qquad t \to \frac{\hbar}{2mE_v}t, \tag{8}$$

has the dimensionless form

$$-2i\frac{\partial\Psi}{\partial t} = \nabla^2\Psi + \Psi\Big(1 - \int |\Psi(\mathbf{x}')|^2 U(|\mathbf{x}-\mathbf{x}'|)\,d\mathbf{x}'\Big). \tag{9}$$

The bulk normalization condition is

$$\int U(|\mathbf{x}-\mathbf{x}'|)\,d\mathbf{x}' = 1, \tag{10}$$

or

$$4\pi\int_0^\infty U(r)r^2\,dr = 1, \tag{11}$$

because $U(|\mathbf{x}-\mathbf{x}'|) = U(r)$. We get the dispersion curve by linearizing about the uniform state. We write $\Psi = 1 + \Psi'$ and consider the plane waves of the form $\Psi' = \exp i(\omega t - kx)$. Then the dispersion relation can be written as

$$\omega^2 = \frac{1}{4}k^4 + \frac{1}{2}kF(k), \tag{12}$$

where

$$F(k) = 4\pi\int_0^\infty \sin(kr)U(r)r\,dr. \tag{13}$$

We require

$$\omega'(k_{rot}) = 0, \qquad \omega(k_{rot}) = \omega_{rot}, \tag{14}$$

where (k_{rot}, ω_{rot}) is the position of the roton minimum on the $k-\omega$ dispersion curve, which in dimensional units is found from experiments [Donnelly *et al.*, 1981] to be $k_{rot} = 1.926\mathring{A}^{-1}$, and $\omega = 8.62K^\circ k_B/\hbar$. By taking the limit of (12) for $k \to 0$ and using the normalization condition (11) the sound speed is found to be $1/\sqrt{2}$ as in the local model. By relating the known value of the sound speed at low k in He II, 238 m/s, to its nondimensional value the healing length of the model (9) is fixed as $[L] = 0.471\mathring{A}$, and therefore $k_{rot} = 0.907$ and $\omega_{rot} = 0.158$.

Jones (1993) considered the potential of the form

$$U(|\mathbf{x}-\bar{\mathbf{x}}|) = U(r) = (\alpha + \beta A^2r^2 + \gamma A^4r^4)\exp(-A^2r^2), \tag{15}$$

where A, α, β, and γ are parameters that could be chosen to give excellent agreement with the experimentally determined dispersion curve. The structure and dynamics of the vortices of such a nonlocal model differ considerably from those predicted by the local model (5). The approach of the fluid density [see (20) below] for a rectilinear vortex to the uniform state is oscillatory rather than monotonic, similar to the observations of Sadd *et al.* (1997). The energy per unit length is considerably reduced compared with that of the local model, and is in better agreement with the results of experiments [Jones (1993)]. Less satisfactory is the behavior at small k. The controversy in the literature [see Brooks and Donnelly (1977) and references therein] about the form of the dispersion curve at low momenta has by now been settled, and it is generally accepted that the dispersion relation has a positive k^3 term (the curve at the origin is concave up) until the pressure reaches some threshold at which the second derivative of ω at the origin changes sign. The potential (15) implies a negative k^3 term. This can be remedied if the term $\eta \exp(-B^2 r^2)$ is added to the expression (15) for U. The coefficients η and B can be chosen so that the resulting dispersion relation has, for instance, the same k^3 term as the Bogoliubov spectrum (6). At the same time, to obtain the roton minimum, B must be much smaller than A, and this makes the potential more nonlocal and less amenable for numerical work.

The undoubted advantage of nonlocal models such as (9) over the local model of liquid helium is their ability to achieve a good fit to the measured dispersion curve. But a serious question arises: "Can such nonlocal model be used for practical purposes?" For example, can it model flow created by a positive ion (modeled as a solid sphere) moving in superfluid at zero temperature? Unfortunately the answer is, "No," as will be demonstrated below.

By examining (12), (13), and (14) it is straightforward to see that $F(k)$ increases from zero with the slope 1 and becomes negative after reaching a zero at the point where the dispersion curve crosses the free particle spectrum $\omega = \frac{1}{2}k^2$. Note, that from (12), (13), and (14), $F(k_{rot}) < 0$ and $F'(k_{rot}) < 0$. This means that it is possible to find nonnegative functions $f(r)$, such that $\int_0^\infty f(r)U(r)r^2\,dr < 0$, and others for which this integral is positive. For example, consider $f(r,k) = 1 + \cos kr$. Then by (11) and (13)

$$4\pi \int_0^\infty f(r,k)U(r)r^2\,dr = 1 + F'(k). \tag{16}$$

Obviously $F'(k) > 0$, for sufficiently small k, and by differentiating (12) we can show that

$$F'(k_{rot}) = -(3k_{rot}^4 + 4\omega_{rot}^2)/2k_{rot}^2 < -1. \tag{17}$$

More generally, there exists a continuous nonnegative function $f(\mathbf{x}')$, such that

$$\int f(\mathbf{x}')U(|\mathbf{x}-\mathbf{x}'|)\,d\mathbf{x}' < 0 \tag{18}$$

in some finite volume for any nonlocal potential that produces a dispersion relationship that has a roton minimum close to that experimentally observed. Also notice (18) implies that $U(r)$ must take negative values on some interval. Therefore, for some separations particles are attracted to each other. The conditions we imposed on the potential do not guarantee that for small distances r $U(r)$ is positive (particles repel each other) as is observed in experiments. For example, the family of potentials given by (15) is repulsive at small distances if $A > 0.58$ and is attractive otherwise. In what follows we consider only realistic potentials with repulsion at small distances.

3. MASS CONCENTRATIONS

The nonlocal model (9) can be cast into hydrodynamic form through the Madelung transformation [e.g. Donnelly 1991, Jones and Roberts 1982]

$$\Psi(\mathbf{x},t) = R(\mathbf{x},t)e^{i\phi(\mathbf{x},t)}. \tag{19}$$

If we introduce the fluid density ρ and velocity $\mathbf{u}$ by

$$\rho = R^2(\mathbf{x},t), \qquad \mathbf{u} = \nabla\phi(\mathbf{x},t), \tag{20}$$

the transformation (19) in (9) gives the continuity equation

$$\frac{\partial\rho}{\partial t} + \nabla\cdot(\rho\mathbf{u}) = 0 \tag{21}$$

and the Bernoulli equation

$$\frac{\partial\phi}{\partial t} + \frac{1}{2}\mathbf{u}^2 + \mu(\rho) = 0, \tag{22}$$

where the chemical potential $\mu(\rho)$ is given by

$$\mu(\rho) = \frac{1}{2}\left[\int \rho(\mathbf{x}',t)U(|\mathbf{x}-\mathbf{x}'|)\,d\mathbf{x}' - 1\right] - \frac{1}{2}\frac{\nabla^2\sqrt{\rho}}{\sqrt{\rho}}. \tag{23}$$

The first term on the right hand side corresponds to the "mechanical chemical potential" and the second term to the "quantum chemical potential" that has no analog in standard fluid mechanics. Notice that the expression for the chemical potential (23) can be determined as a variational derivative of the internal energy per unit volume

$$w(\rho) = \frac{(\nabla\rho)^2}{2\rho} + \frac{1}{2}\left[\int \rho(\mathbf{x}', t)U(|\mathbf{x} - \mathbf{x}'|)\, d\mathbf{x}' - 1\right]\rho, \tag{24}$$

from the total energy W of the system,

$$W = \int w\, d\mathbf{x}, \qquad \delta W = \int \mu\delta\rho\, d\mathbf{x},$$

so that

$$\mu = \delta w/\delta\rho. \tag{25}$$

Using (23), (24), and (25) we can find the variational derivative of the mechanical pressure in the "semiclassical limit" ($\hbar \to 0$) as

$$\frac{\delta p}{\delta\rho} = \rho\frac{\delta\mu}{\delta\rho} = \frac{1}{2}\int \rho(\mathbf{x}')U(|\mathbf{x} - \mathbf{x}'|)\, d\mathbf{x}'. \tag{26}$$

This means that if integral on the right hand side of (26) is negative the pressure p decreases when the mass density increases, this phenomenon leads to the development of mass concentrations.

If, as it should, the Bernoulli equation (22) is a genuine momentum equation, then it will imply

$$\rho\Big(\frac{\partial u_i}{\partial t} + u_j\frac{\partial u_i}{\partial x_j}\Big) = -\frac{\partial p}{\partial x_i} + \frac{\partial \Pi_{ij}}{\partial x_j}. \tag{27}$$

Although it seems hard to achieve this for (23), we show in the appendix that (27) is true for a nonlocal potential that is a sum of $\delta-$functions and their derivatives. In (27), p is the thermodynamic pressure and Π_{ij} are the remaining stresses. Notice that for (27) to be hyperbolic the pressure p must be a strictly increasing function of ρ, which is not the case if (18) can hold true in some volume.

The virial theorem proved to be useful in establishing the blow-up of the solutions of the focusing nonlinear Schrödinger equation with zero boundary conditions [Zakharov, 1976]. Next we demonstrate that the virial theorem is illuminating in analyzing the nonlocal model. Equation (9) is a Hamiltonian

system with the following integrals being conserved: mass excess

$$M = \int (|\Psi|^2 - 1)\, d\mathbf{x}, \tag{28}$$

momentum

$$\mathbf{P} = \frac{1}{2i} \int [(\Psi^* - 1)\nabla\Psi - (\Psi - 1)\nabla\Psi^*]\, d\mathbf{x}, \tag{29}$$

and energy

$$E = \frac{1}{2} \int |\nabla\Psi|^2\, d\mathbf{x} + \frac{1}{4} \int (1 - |\Psi|^2) \left[1 - \int |\Psi|^2 U(|\mathbf{x} - \mathbf{x}'|)\, d\mathbf{x}'\right] d\mathbf{x}. \tag{30}$$

The derivation of (29) and (30) for the local model is given in [Jones and Roberts, 1982]. The expression for the energy depends on the normalization condition (10). For unbounded volume the first two integrals although convergent are improper integrals meaning that their values depend on the shape of the volume of integration even as that volume tends to infinity. Without loss of generality we shall assume that the initial disturbance only displaces mass so that $M = 0$, otherwise we can make an adjustment in the transformation to dimensionless variables to make the change in mass zero.

We consider the virial tensor

$$I(t) = \int \mathbf{x}^2 (|\Psi|^2 - 1)\, d\mathbf{x}, \tag{31}$$

in D dimensions. It can be shown using the original equation (9) and $M = 0$ that

$$\frac{\partial^2 I}{\partial t^2} = 4E + \frac{1}{2}(D - 2) \int (1 - |\Psi(\mathbf{x})|^2) \left[1 - \int |\Psi(\mathbf{x}')|^2 U(|\mathbf{x} - \mathbf{x}'|)\, d\mathbf{x}'\right] d\mathbf{x}. \tag{32}$$

We integrate this equation twice to obtain:

$$I = 2Et^2 + Bt + A + \int_0^t dt' \int_0^{t'} \xi(t'')\, dt'', \tag{33}$$

where we have written

$$\xi(t) = \frac{1}{2}(D-2)\int (1-|\Psi(\mathbf{x})|^2)\left[1-\int |\Psi(\mathbf{x}')|^2 U(|\mathbf{x}-\mathbf{x}'|)\,d\mathbf{x}'\right] d\mathbf{x},$$

$$A = I(0), \qquad B = I'(0). \tag{34}$$

In the case $D = 2$,

$$I = A + Bt + 2Et^2. \tag{35}$$

If the energy is negative then the right-hand side of (35) will become arbitrarily large and negative in a finite time. But if we consider the solution of (9) in a finite container of volume V with specified boundary conditions then I is bounded from below by $-\int_V \mathbf{x}^2\,d\mathbf{x}$. This contradiction establishes the possibility of collapse of the solution of (9) in two dimensions. For $D \neq 2$ collapse in the finite container can only be assured if $\xi(t) \leq 0$ and in addition one of the following conditions is satisfied:

$$\begin{aligned} &(1) \quad E < 0, \\ &(2) \quad E = 0 \quad \text{and} \quad B < 0, \\ &(3) \quad E > 0 \quad \text{and} \quad B \leq -4\sqrt{E}(A + \int_V \mathbf{x}^2\,d\mathbf{x}). \end{aligned} \tag{36}$$

The virial theorem does not establish that catastrophic singularities must occur, but it explains why, in the course of numerical calculations, persistent mass concentrations develop in regions where (9) loses its hyperbolicity in accordance with (18).

4. NUMERICAL EVIDENCE

To illustrate the development of mass concentrations, we solved (9) numerically in two cases. The first is the propagation of a spherically symmetric disturbance in density; the second is the flow round a moving sphere. The potential was taken in the form (15) with $A = 0.9, \alpha \approx 3.9762, \beta \approx -6.2501, \gamma \approx 1.4746$, so that the potential gives a good fit to the dispersion curve and at the same time is strongly repulsive at small particle separations. One of the main considerations in choosing the integration scheme was that outgoing sound waves should escape from the integration box. We used finite differences and the Raymond-Kuo radiation boundary condition [Raymond and Kuo (1986)]. In time stepping the leap-frog

scheme was implemented with a backward Euler step every 100 steps to prevent the even-odd instability. In space we used a 4th order finite difference scheme together with a 2nd order scheme close to the boundary. The Raymond - Kuo method uses the three previous time steps near the boundary to predict the direction of wave propagation. In two dimensions the value of ψ on the boundary depends on the phase velocity $\mathbf{C} = (C_x, C_y)$ through

$$\frac{\partial \psi}{\partial t} + C_x \frac{\partial \psi}{\partial x} + C_y \frac{\partial \psi}{\partial y} = 0. \tag{37}$$

Assuming that the phase velocity does not change rapidly in $\Delta t, C_x$ and C_y are approximated by using the earlier interior values of ψ:

$$C_x = -\frac{\partial \Psi}{\partial t}\frac{\partial \Psi}{\partial x} \Big/ \left[\left(\frac{\partial \Psi}{\partial x}\right)^2 + \left(\frac{\partial \Psi}{\partial y}\right)^2\right], \tag{38}$$

$$C_y = -\frac{\partial \Psi}{\partial t}\frac{\partial \Psi}{\partial y} \Big/ \left[\left(\frac{\partial \Psi}{\partial x}\right)^2 + \left(\frac{\partial \Psi}{\partial y}\right)^2\right]. \tag{39}$$

All derivatives are approximated by leap-frog differences unless points on the boundary must be included, in which case the scheme must be changed [Kreiss, 1966]. On the right boundary (say) we have

$$\frac{\partial \Psi}{\partial x} \approx \frac{1}{2\Delta x}(\Psi^{\tau}_{N,j} + \Psi^{\tau-2}_{N,j} - 2\Psi^{\tau-1}_{N-1,j}). \tag{40}$$

After the phase velocity is calculated we exclude the inwardly moving waves by setting the corresponding component of phase velocity equal to zero. Then we predict the value on the boundary from (38). On the right boundary (38) becomes

$$\Psi^{\tau+1}_{N+1,j} = \frac{1 - C_x\Delta t/\Delta x}{1 + C_x\Delta t/\Delta x}\Psi^{\tau-1}_{N+1,j} + \frac{2C_x\Delta t/\Delta x}{1 - C_x\Delta t/\Delta x}\Psi^{\tau}_{N,j} - \frac{\Delta t/\Delta y C_y}{1 - C_x\Delta t/\Delta x}(\Psi^{\tau-1}_{N+1,j+1} - \Psi^{\tau-1}_{N+1,j-1}). \tag{41}$$

The numerical scheme used does not conserve energy but the induced dissipation of energy is very small. When the reflective boundary conditions were used instead of the radiative ones, the energy loss due to the dissipative character of the scheme did not exceed $10^{-5}\%$ per 1000 time steps.

Nore *et al.* (1993) studied the acoustic behavior of the local model and demonstrated that the dispersive effects due to the quantum stress tensor become noticeable for some range of the width-to-height ratio of the traveling pulse. Similar dispersion takes place in the nonlocal model (9). To minimize such a dispersion we introduce a small dissipation into equation (9). The most physically relevant way of doing this for the local model was suggested by Carlson (1996). In real helium, even in the low temperature range, normal fluid is present that is coupled to the superfluid and, through its viscosity, provides a high wavenumber sink. When modified to include mutual friction with the normal fluid, the superfluid Euler equation becomes (e.g., Khalatnikov, 1965)

$$\dot{\mathbf{v}}_s + \nabla \frac{v_s^2}{2} = -\nabla\Big(\mu - \zeta_3 \nabla \cdot (\mathbf{j} - \rho \mathbf{v}_n) - \zeta_4 \nabla \cdot \mathbf{v}_n\Big), \tag{42}$$

where $\mathbf{j} = \rho \mathbf{v}$ is the mass current, μ is the chemical potential, $\mathbf{v}_n$ is the velocity of the normal fluid, and ζ_3 and ζ_4 are the coefficients of bulk viscosity. When the first dissipative term of (42) is introduced into the model (9) via the Madelung transform the nonlocal model with dissipation becomes

$$\begin{aligned} -2i\frac{\partial \Psi}{\partial t} = \nabla^2 \Psi + \Psi\left(1 - \int |\Psi(\mathbf{x}')|^2 U(|\mathbf{x} - \mathbf{x}'|)\, d\mathbf{x}'\right) \\ - 2\zeta_3 \psi \left(\frac{\partial}{\partial t} + \mathbf{v}_n \cdot \nabla\right) |\psi|^2. \end{aligned} \tag{43}$$

We will assume that the normal fluid is at rest, $\mathbf{v}_n = 0$. The kinetic coefficients of the nonideal degenerate Bose-system at low temperature were calculated by Tserkovnikov (1995) using method of collective variables and by Kirkpatrick and Dorfman (1985) using the Chapman-Engskog expansion. In the nondimensional units of our model, the dissipative parameter ζ_3 is about $2.6 \times 10^{-6} T^3$, where T is temperature. In our calculations ζ_3 was taken to be of order 10^{-3}. First, the initial field was evolved according to the dissipative model (43) which sufficiently minimizes the dispersive effects. After that, ζ_3 was set zero and the calculations were continued using the nondissipative model (9). We emphasize that the solution we present below satisfy the non-dissipative Hamiltonian system.

The code was tested towards the vortex solutions of the local model found in [Jones and Roberts (1982)] and towards the large vortex rings of the nonlocal model [Jones (1993)].

Spherically symmetric solutions of (9) obey

$$2i\frac{\partial\Psi}{\partial t}+\frac{\partial^2\Psi}{\partial r^2}+\frac{2}{r}\frac{\partial\Psi}{\partial r}+\Psi\left[1-\int\limits_0^\infty|\Psi(s)|^2U_2(r,s)\,ds\right]=0, \tag{44}$$

$$\Psi_r(0,t)=0, \qquad |\Psi|^2(\infty,t)=1,$$

where (r,θ,ϕ) are spherical coordinates. We performed the integration of the nonlocal potential over θ and ϕ, so that

$$\begin{aligned}U_2(r,s)&=2\pi\int\limits_{-1}^{1}U(\sqrt{r^2+s^2-2rs\mu})s^2\,d\mu\\&=\frac{\pi s}{A^2r}\Big(e^{-A^2(r-s)^2}\left[\alpha+\beta+\gamma+\beta A^2(r-s)^2+\gamma(1+A^2(r-s)^2)^2\right]\\&-e^{-A^2(r+s)^2}\left[\alpha+\beta+\gamma+\beta A^2(r+s)^2+\gamma(1+A^2(r+s)^2)^2\right]\Big).\end{aligned} \tag{45}$$

To approximate the integral in (44) we notice the rapid decay of the integrand to zero as s departs from r. In the calculations we took $A=0.9$ and it was sufficient to set

$$\int\limits_0^\infty|\Psi(s)|^2U_2(r,s)\,ds=\int\limits_{\max\{0,r-6\}}^{r+6}|\Psi(s)|^2U_2(r,s)\,ds. \tag{46}$$

The integral on the right-hand side of (46) is approximated using the four-point linear quadrature rule for $|\Psi(s)|^2$ on a uniform mesh (that coincides with the mesh of the equation) with weight $U_2(r,s)$. The general scheme for deriving such a quadrature rule is to write down the four linear equations that must be satisfied so that the quadrature is exact for polynomials of degree ≤ 3, and then to solve these equations for the coefficients. To do that we need to know the moments of the weight function

$$W_n(r)=\frac{1}{h^n}\int\limits_{kh}^{(k+3)h}s^nU_2(r,s)\,ds, \qquad n=0,...,3. \tag{47}$$

Such moments can be calculated very accurately on a highly refined grid since it needs to be done just once. For each r on the grid we calculate the corresponding weights of the integration scheme once and for all. During the numerical iteration of (44) the integral (46) is calculated as the sum of weights multiplied by the function $|\Psi|^2$.

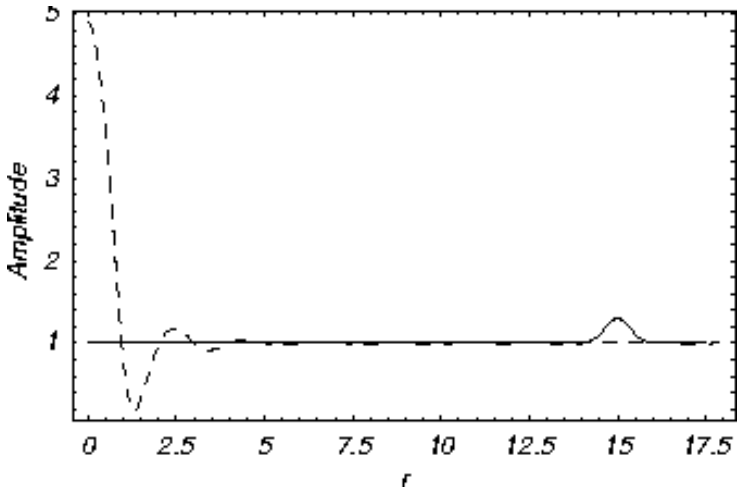

Fig. 1. The result of numerical integration of (44). The amplitude of the solution $|\Psi|$ as a function of r, the distance from the center of symmetry. At $t = 0$, $\Psi(r) = 1 + 0.3\exp\left[-4(r-15)^2\right]$ (solid line), at $t = 200$ (dashed line) the mass excess is concentrated at $r = 0$.

Figure 1 displays the results of the numerical integration of (44) from an initial perturbation of the form

$$\Psi(r, t = 0) = 1 + 0.3\exp\left[-4(r-15)^2\right] \tag{48}$$

on the interval $[0, 60]$ with 601 grid points. The right boundary is open according to the one-dimensional version of (37). The excess mass of this system,

$$\mathcal{M}(r,t) = 4\pi \int_0^r \left[|\Psi|^2 - 1\right] s^2\, ds \tag{49}$$

contained in a sphere of radius r is conserved for $r = \infty$ [see (28)] but, for small r it initially increases with t, corresponding to a concentration of mass at the origin. At time $t \approx 35$ the density, $|\Psi|^2$, at the origin is about 20 times larger than the density of the far field. Figure 2 shows how the amplitude, $|\Psi| = \sqrt{\rho}$, of the solution at the origin changes with time. After initial saturation, the amplitude at $r = 0$ starts to vary periodically between 4.45 and 5.03. The integral (26) at $r = 0$ becomes negative as the periodic solution is reached. Figure 3 is a plot of the pressure variation (26) at $r = 0$. The oscillations in the pressure variation, $\delta p/\delta\rho$, are in antiphase with the oscillations in the density, ρ. Since at small distances particles repel each other the mass concentrations that form do not lead to wave collapse.

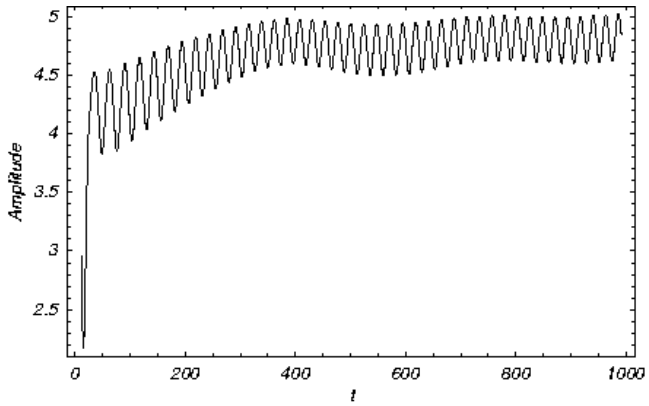

Fig. 2. The amplitude of the solution of (44) at the origin $r = 0$ as a function of time, t, from $t = 30$ to $t = 1000$.

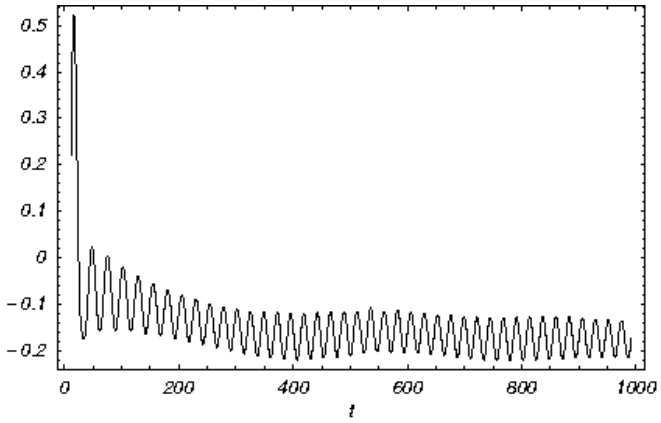

Fig. 3. The pressure variation, $\delta p/\delta\rho$ at the origin as defined by (26) as function of time, t.

At the same time the presence of the attractive region does not allow the mass concentrations to disperse.

In our calculations we took ζ_3 to be much larger than the calculated kinetic value (0.001 and 0.005). Even for such large values of the dissipation parameter no significant damping of the oscillations was observed, so

we may conclude, that those mass concentrations cannot be destroyed by coupling to normal fluid.

Mass concentrations appear in the regions where the density distribution leads to negativity of the integral (26). Not every initial configuration will evolve into persistent mass concentrations. It is easy to construct an example of an initial density profile, so that (26) is negative and the equation of motion is not hyperbolic in some parts of computational box. For example, $\rho(r) = 1 + 0.17\exp(-4(r-3/2)^2)$, that represents a sound wave with density up to 17% larger than the mean condensate density. Then integral (26) is negative at the center of symmetry. It is realistic to have deviations in density of the condensate as large as this. For example, the density of the straight line vortex calculated by Jones(1993) and observed experimentally can be as high as 120% of the density of the far field. As vortices interact, waves of even higher amplitude will be generated.

The next example is the flow around a sphere moving with a constant speed along the z-axis. We solve (8) in axisymmetric 3D case

$$\begin{aligned} &-2i\Psi_t + 2iU_S\Psi_z \\ &\quad = \Psi_{rr} + \frac{1}{r}\Psi_r + \Psi_{zz} + \Psi\Big(1 - \int_0^{\infty}\int_{-\infty}^{\infty}\int_0^{2\pi} |\Psi(r',z')|^2 \\ &\qquad \times U(\sqrt{r^2 + r'^2 - 2rr'\cos(\theta-\theta') + (z-z')^2})r'\,d\theta' dz' dr'\Big), \end{aligned} \tag{50}$$

where U_S is the velocity of the sphere. The coordinate frame moves with the sphere, so that the center of the sphere remains at the center of the computational box. The integral over θ' in the nonlinear term can be evaluated exactly for the potential (15) in terms of the modified Bessel functions, I_0 and I_1, of order 0 and 1

$$\begin{aligned} \int_0^{2\pi} U r'\,d\theta' &= U_s(r,z;r',z') \\ &= 2\pi r'\exp(-A^2 s)((\alpha + A^2\beta s + A^4\gamma(s^2 + 4r^2r'^2))I_0(\sigma) \\ &\quad - \sigma(\beta + \gamma(1 + 2A^2 s))I_1(\sigma)), \end{aligned} \tag{51}$$

where $\sigma = 2A^2 rr'$ and $s = r^2 + r'^2 + (z-z')^2$. Again $A = 0.9$ in (15) was taken in the calculations, so that

$$\begin{aligned} &\int_0^{\infty}\int_{-\infty}^{\infty} |\Psi(r',z')|^2 U_s(r,z;r',z')\,dz'\,dr' \\ &\quad = \int_{\max\{0,r-6\}}^{r+6}\int_{z-6}^{z+6} |\Psi(r',z')|^2 U_s(r,z;r',z')\,dz'\,dr'. \end{aligned} \tag{52}$$

We now write

$$U_s(r,z;r',z') = Z_1(z-z')R_1(r,r') + Z_2(z-z')R_2(r,r') + Z_3(z-z')R_3(r,r'), \tag{53}$$

where

$$Z_k(\xi) = 2\pi\xi^{2(k-1)}\exp[-A^2\xi^2], \qquad k=1,2,3, \tag{54}$$

$$\begin{aligned} R_1(r,r') &= r'\exp[-A^2(r^2+r'^2)]\Big(I_0(\sigma)(\alpha + A^2\beta(r^2+r'^2) \\ &\quad + A^4\gamma((r^2+r'^2)^2+4r^2r'^2)) - I_1(\sigma)\sigma((\beta+\gamma) \\ &\quad + 2A^2\gamma(r^2+r'^2))\Big), \end{aligned} \tag{55}$$

$$\begin{aligned} R_2(r,r') &= r'\exp[-A^2(r^2+r'^2)](I_0(\sigma)(A^2\beta + 2A^4\gamma(r^2+r'^2)) \\ &\quad - 2I_1(\sigma)A^2\gamma\sigma), \end{aligned} \tag{56}$$

$$R_3(r,r') = r'\exp[-A^2(r^2+r'^2)]I_0(\sigma)A^4\gamma. \tag{57}$$

Next we develop six four-point linear quadrature rules with weights $Z_k(z-z')$ and $R_k(r,r')$ $(k=1,2,3)$ so that

$$\int f(z')Z_k(z-z')\,dz' \approx \sum_j A_j^k(z)f(z_j'), \tag{58}$$

and

$$\int g(r')R_k(r,r')\,dz' \approx \sum_i B_i^k(r)g(r_i'). \tag{59}$$

For each point (r,z) of our computational grid we calculate a matrix ℓ with elements

$$\ell_{ij}(r,z) = \sum_{k=1}^{3} B_i^k(r)A_j^k(z) \tag{60}$$

just once. During the numerical iteration of (50) the integral on the right-hand side of (52) is calculated as

$$\iint |\Psi(r',z')|^2 \sum_{k=1}^{3} Z_k R_k \, dz' \, dr' = \int \sum_{k=1}^{3} R_k \Big(\int |\Psi|^2 Z_k \, dz' \Big) \, dr'$$
$$\approx \int \sum_{k=1}^{3} R_k \Big(\sum_j A_j(z) |\Psi(r', z'_j)|^2 \Big) \, dr'$$
$$\approx \sum_{k=1}^{3} \sum_i \sum_j B_i^k(r) A_j^k(z) |\Psi(r'_i, z'_j)|^2$$
$$= \sum_i \sum_j \ell_{ij}(r,z) |\Psi(r'_i, z'_j)|^2. \qquad (61)$$

Three sides of the computational box $[-80, 80] \times [0, 40]$ were taken to be open and the $r = 0$ side was reflective. We also took $\Delta r = \Delta z = 0.4$ and compared the results with the calculations for $\Delta r = \Delta z = 0.2$. The corresponding time step was chosen as $\Delta t = 0.1/(\Delta r^{-2} + \Delta z^{-2})$. Figure 4 presents the results of the calculation for the flow around a sphere of radius 10 moving to the right with velocity 0.1. The biggest mass concentrations develop along the axis of symmetry. After initial saturation, the density at the centers of the mass concentrations reach values about 20 times larger that the density of the far field.

5. CONCLUSIONS

Wave collapse, or wave energy/density concentrations in a decreasing volume, appear in many cases where their nonlinear effects dominate the linear effects of dispersion. All known types of the collapse in a wide variety of physical examples arise from the nonlinear Schrödinger equation (NSE):

$$i\Psi_t + \Delta\Psi + f(|\Psi|^2)\Psi = 0; \qquad (62)$$

[see Kosmatov (1991) and references therein]. If $f(u) > Cu^{2/D}$ and $C > 0$, the NSE develops an explosive singularity in a finite time. The perturbation leading to the collapse must exceed some threshold, below which the medium is stable.

If $C < 0$ (62) is "defocusing", meaning that no collapse occurs. The local Gross-Ginsburg-Pitaevskii model (5) is one such example. But this model cannot be considered as realistic for superfluid helium since the roton minimum is missing from the dispersion curve and the properties of superfluid helium depend crucially on the existence of such a minimum. There is a significant interest attached to the question of whether the Gross-Ginsburg-Pitaevskii model with a nonlocal potential that incorporates the correct dispersion curve for ^{4}He will adequately represent the

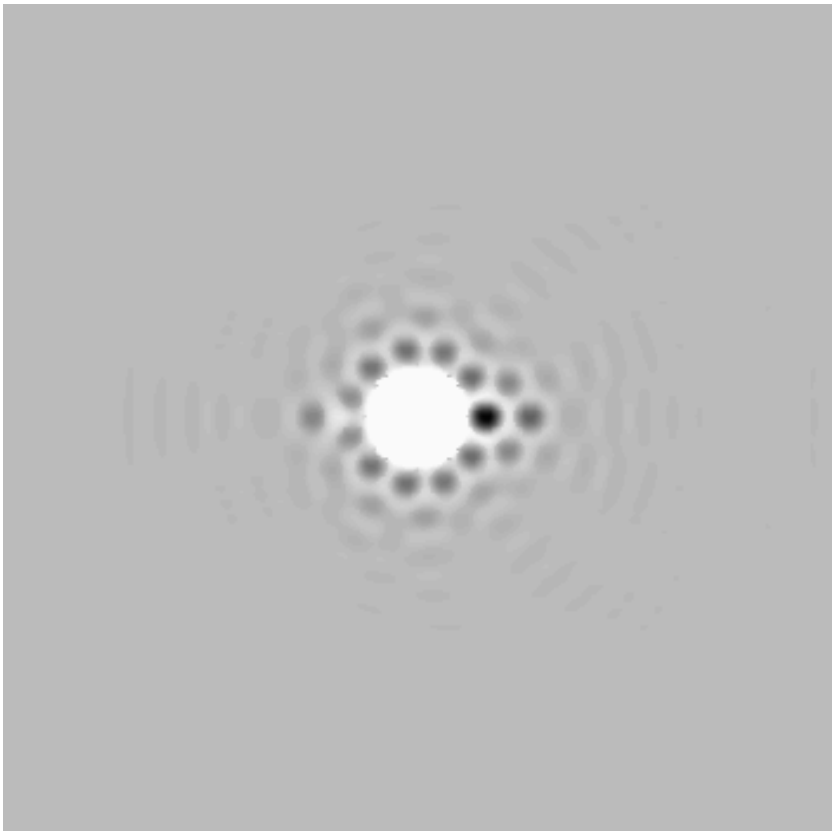

Fig. 4. The solution of (50) for the flow around a sphere of radius 10 moving to the right with velocity 0.1 at (a) $t = 40$, and (b) $t = 120$.

properties of this fluid. The fit to the dispersion curve can be obtained with a variety of nonlocal potentials, but as soon as we require both the position of the roton minimum to be correct and the sound velocity to be correct these nonlocal models lose the advantage of being of "defocusing" type. This changes the properties of the model drastically. The "Eulerian part" of the momentum equation (27) (without the quantum stress tensor) may become no longer hyperbolic in some parts of the integration volume and nondissipative mass concentrations may develop. Such an unphysical behavior indicates that assumptions made in the derivation of the equation must be unjustified. This difficulty could be overcome by introducing into the weakly nonlinear theory dissipation or higher order nonlinear terms. But we would like to preserve the Hamiltonian character of the Ginsburg - Pitaevskii model. Instead, we will take the density - functional approach [Dupont-Roc *et al.* and Dalfovo *et al.*], which tries to introduce an

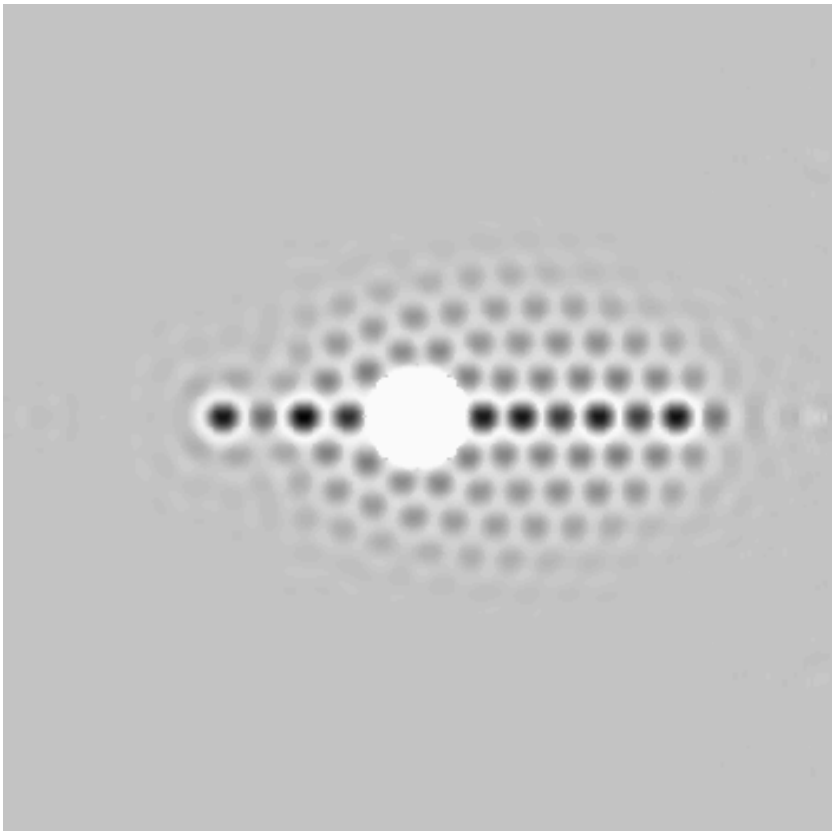

Fig.4. *Continued.*

accurate microscopic picture of liquid helium. We shall elaborate more on this subject in a subsequent paper.

APPENDIX: EQUATION OF MOTION OF THE FLUID MECHANICAL FORMULATION OF THE NONLOCAL MODEL

The derivation of pressure and stress tensor expressions in the fluid mechanical formulation of the local model was obtained by Grant (1973) using a variational principle. We will use this method to find an equation of motion for the nonlocal model. The Lagrangian of the nonlocal model (9) is given by

$$L = \frac{\rho}{2}\left(\frac{\partial\phi}{\partial x_i}\right)^2 + \frac{1}{8\rho}\left(\frac{\partial\rho}{\partial x_i}\right)^2 + \frac{1}{4}\rho(\mathbf{x})\int \rho(\mathbf{x}')U(|\mathbf{x}-\mathbf{x}'|)\,d\mathbf{x}' + \rho\frac{\partial\phi}{\partial t}, \quad (A1)$$

where, as for $|\Psi|^2$ previously, the $t-$dependence of ρ is implied. Using (21) and (22) we can show that

$$\frac{\partial L}{\partial x_i} = \frac{\partial}{\partial t}\Big(\rho\frac{\partial \phi}{\partial x_i}\Big) + \frac{\partial}{\partial x_j}\Big(\rho\frac{\partial \phi}{\partial x_i}\frac{\partial \phi}{\partial x_j} + \frac{1}{4\rho}\frac{\partial \rho}{\partial x_i}\frac{\partial \rho}{\partial x_j}\Big) + \frac{\partial}{\partial x_i}\Big(\frac{1}{2}\rho + \frac{1}{4}\rho\int \rho(\mathbf{x}')U(|\mathbf{x}-\mathbf{x}'|)\,d\mathbf{x}'\Big) - \frac{1}{2}\int \frac{\partial \rho}{\partial x_i}\int \rho(\mathbf{x}')U(|\mathbf{x}-\mathbf{x}'|)\,d\mathbf{x}'. \qquad (A2)$$

After eliminating $\partial\phi/\partial t$ using (22) in (A1) and substituting the resulting expression for L into the left-hand side of (A2) we obtain the equation

$$\frac{\partial}{\partial t}\Big(\rho u_i\Big) + \frac{\partial}{\partial x_j}\Big(\rho u_i u_j - \sigma^q_{ij}\Big) + \frac{\partial}{\partial x_i}\Big(\frac{1}{2}\rho\int \rho(\mathbf{x}')U(|\mathbf{x}-\mathbf{x}'|)\,d\mathbf{x}'\Big) - \frac{1}{2}\frac{\partial \rho}{\partial x_i}\int \rho(\mathbf{x}')U(|\mathbf{x}-\mathbf{x}'|)\,d\mathbf{x}' = 0, \qquad (A3)$$

where the quantum stress tensor is

$$\sigma^q_{ij} = \frac{1}{4}\Big(\frac{\partial^2 \rho}{\partial x_i \partial x_j} - \frac{1}{\rho}\frac{\partial \rho}{\partial x_i}\frac{\partial \rho}{\partial x_j}\Big). \qquad (A4)$$

In order to get hydrodynamical equation of motion we must be able to write

$$\frac{\partial}{\partial x_i}\Big(\frac{1}{2}\rho\int \rho(\mathbf{x}')U(|\mathbf{x}-\mathbf{x}'|)\,d\mathbf{x}'\Big) - \frac{1}{2}\frac{\partial \rho}{\partial x_i}\int \rho(\mathbf{x}')U(|\mathbf{x}-\mathbf{x}'|)\,d\mathbf{x}' = \frac{\partial p}{\partial x_i} - \frac{\partial \sigma^m_{ij}}{\partial x_j}, \qquad (A5)$$

where the pressure, p, and the anisotropic mechanical stress tensor (we use the term 'mechanical' to distinguish this part of the stress tensor from the quantum stress tensor (A4)), σ^m_{ij}, are functions (functionals) of the density, ρ, and derivatives of ρ.

In order to accomplish this task we need to make some simplifying assumptions about the potential $U(|\mathbf{x}-\mathbf{x}'|)$. We will assume that U can be written as a sum of $\delta-$functions and their derivatives:

$$U(|\mathbf{x}-\mathbf{x}'|) = \Big[A_0 + A_2\nabla^2 + A_4\nabla^4 + A_6\nabla^6 + \cdots\Big]\,\delta(\mathbf{x}-\mathbf{x}'), \qquad (A6)$$

where the A_i are constants with $A_0 = 1$, as follows from the normalization condition (10). In fact, a very good fit to the Landau dispersion curve can be obtained by taking only the first three terms in the expression (A6) for the potential U. The integral in (A5) becomes

$$\int \rho(\mathbf{x}')U(|\mathbf{x}-\mathbf{x}'|)\,d\mathbf{x}' = \rho + \sum_{i=1}^{\infty} A_{2i}\nabla^{2i}\rho. \tag{A7}$$

Next we write the left hand side of (A5) as

$$\begin{aligned}&\frac{\partial}{\partial x_i}\Big(\frac{1}{4}\rho\int \rho(\mathbf{x}')U(|\mathbf{x}-\mathbf{x}'|)\,d\mathbf{x}'\Big)\\ &+\left[\frac{\partial}{\partial x_i}\Big(\frac{1}{4}\rho\int \rho(\mathbf{x}')U(|\mathbf{x}-\mathbf{x}'|)\,d\mathbf{x}'\Big) - \frac{1}{2}\frac{\partial\rho}{\partial x_i}\int \rho(\mathbf{x}')U(|\mathbf{x}-\mathbf{x}'|)\,d\mathbf{x}'\right].\end{aligned} \tag{A8}$$

Let

$$p = \frac{1}{4}\rho\int \rho(\mathbf{x}')U(|\mathbf{x}-\mathbf{x}'|)\,d\mathbf{x}, \tag{A9}$$

and expand the term in the square brackets as

$$\begin{aligned}&\frac{\partial}{\partial x_i}\left(\frac{1}{4}\rho\int \rho(\mathbf{x}')U(|\mathbf{x}-\mathbf{x}'|)\,d\mathbf{x}'\right) - \frac{1}{2}\frac{\partial\rho}{\partial x_i}\int \rho(\mathbf{x}')U(|\mathbf{x}-\mathbf{x}'|)\,d\mathbf{x}'\\ &\quad= \frac{1}{4}\left(A_2\Big(\rho\frac{\partial}{\partial x_i}\nabla^2\rho - \frac{\partial\rho}{\partial x_i}\nabla^2\rho\Big) + A_4\Big(\rho\frac{\partial}{\partial x_i}\nabla^2\rho - \frac{\partial\rho}{\partial x_i}\nabla^4\rho\Big)\right.\\ &\qquad\left. + A_6\Big(\rho\frac{\partial}{\partial x_i}\nabla^6\rho - \frac{\partial\rho}{\partial x_i}\nabla^6\rho\Big) + \cdots\right) = \frac{\partial\sigma_{ij}^m}{\partial x_j},\end{aligned} \tag{A10}$$

where

$$\begin{aligned}4\sigma_{ij}^m &= A_2\Big(\rho\frac{\partial^2\rho}{\partial x_i\partial x_j} - \frac{\partial\rho}{\partial x_i}\frac{\partial\rho}{\partial x_j}\Big)\\ &\quad + A_4\Big(\rho\frac{\partial^2}{\partial x_i\partial x_j}\nabla^2\rho - \left[\frac{\partial\rho}{\partial x_i}\frac{\partial}{\partial x_j} + \frac{\partial\rho}{\partial x_j}\frac{\partial}{\partial x_i}\right]\nabla^2\rho + \frac{\partial^2\rho}{\partial x_i\partial x_j}\nabla^2\rho\Big)\\ &\quad + A_6\Big(\rho\frac{\partial^2}{\partial x_i\partial x_j}\nabla^4\rho - \left[\frac{\partial\rho}{\partial x_i}\frac{\partial}{\partial x_j} + \frac{\partial\rho}{\partial x_j}\frac{\partial}{\partial x_i}\right]\nabla^4\rho\\ &\quad + \left[\frac{\partial^2\rho}{\partial x_i\partial x_j}\nabla^4\rho + \nabla^2\rho\frac{\partial^2}{\partial x_i\partial x_j}\nabla^2\rho\right] - \frac{\partial}{\partial x_i}\nabla^2\rho\frac{\partial}{\partial x_j}\nabla^2\rho\Big) + \cdots,\end{aligned} \tag{A11}$$

and, like σ^q_{ij}, is symmetric. Finally the equation of motion (A3) becomes

$$\frac{\partial}{\partial t}\Big(\rho u_i\Big) + \frac{\partial}{\partial x_j}\Big(\rho u_i u_j + p\delta_{ij} - \sigma^q_{ij} - \sigma^m_{ij}\Big) = 0, \qquad (A12)$$

where p, σ^q_{ij}, and σ^m_{ij} are defined by (A9), (A4), and (A11) respectively.

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