PAPER

Bistability of Bose–Fermi mixtures

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Abstract

We study formation of a Bose–Fermi droplet in realistic experimental setting. We start with a typical experimental arrangement of two atomic species—bosons and fermions in a harmonic axially symmetric confinement. The variational analysis shows that the system exhibits bistability. For weak repulsion between bosons, one of the equilibrium states, smaller in size, spherically symmetric, and with negative energy, corresponds to quantum droplet; the other with always positive energy represents the elongated droplet-like state immersed in the sea of a fermionic cloud. For stronger repulsion between bosons the bifurcation is seized and only the former state is left. Now it represents an elongated object which, for strong enough boson–fermion attraction, gets negative energy. It becomes an excited Bose–Fermi droplet when the trap is released, what is demonstrated by solving the quantum hydrodynamics equations for the Bose–Fermi system. To depict our ideas we consider the ¹³³Cs–⁶Li mixture under ideal conditions, i.e. we assume no losses.

Quantum mixtures of atomic gases have been studied already for years, both experimentally and theoretically. Of particular interest are degenerate Bose–Fermi mixtures. First experiments in mixtures involving fermionic component were aimed at realization of a degenerate Fermi gas via sympathetic cooling [1–5]. Soon after studies of many-body quantum phenomena followed.

The phase diagram of the harmonically trapped mixture of bosonic rubidium-87 and fermionic potassium-40 atoms was determined in [6, 7]. Tuning the interspecies interactions by Feshbach resonance, the experimentalists observed a collapse of the mixture on the attractive side for interactions exceeding some threshold, and the phase separation on the repulsive side. Binary mixture of potassium-41 condensate immersed in a sea of fermionic lithium-6 atoms was recently realized [8] and collective oscillations of bosonic component were studied. A breathing mode of a condensate was induced by increasing the strength of the boson–fermion forces. On the repulsive side of Feshbach resonance the phase separation is eventually reached and the oscillation frequencies are measured [9]. Here, temperature effects seem to be crucial to explain the experimental results, as shown in [10]. Physics of polarons was probed via radio-frequency spectroscopy of a gas of potassium-41 fermionic impurities immersed in an ultracold atomic gas of rubidium-87 [11] or sodium-23 [12]. The energy, spectral width, and the lifetime of Bose polaron were determined on both sides of a heteronuclear Feshbach resonance, going beyond the standard textbook description in a weakly interacting regime.

A novel quantum mixture, a self-bound system of ultracold atoms has been realized experimentally recently. First quantum droplets were observed in a gas of dysprosium-164 atoms, which possess the largest dipolar magnetic moment among all atoms [13]. Interplay of short range and dipolar forces is crucial for stabilizing such systems. More dipolar droplets were created soon with erbium-166 atoms [14]. Demonstration of existence of different kind of self-bound objects—droplets in a two-component mixture of bosonic potassium-39 atoms has followed [15, 16]. The origin of self-confinement both in dipolar systems as well as in two-component mixtures is due to quantum fluctuations which play essential role at the border of a collapse, as suggested in reference [17]. Quantum droplets in a heteronuclear bosonic mixtures were
also observed [18]. Another new self-bound systems, the Bose–Fermi droplets have been recently elaborated theoretically [19, 20].

Interactions among degenerate identical fermions can be changed by a contact with a Bose–Einstein condensate. For example, a mixture of $^{87}$Rb – $^{40}$ K was used to bring a gas of fermionic potassium to collapse [21, 22]. Indeed, large enough boson–fermion attraction in rubidium–potassium mixture results in an effective attraction between fermions, responsible for the collapse. This attraction, on the other hand, might lead to fermionic superfluidity as in the case of phonon-induced attraction between electrons in superconductors. In fact, a Bose–Fermi mixture in which both the fermionic and the bosonic components are superfluid has been produced [23, 24].

In Bose–Fermi systems, fermions can mediate the interactions between bosons as well. This kind of behavior has been recently observed in an experiment with a mixture of ultracold fermionic $^6$Li and bosonic $^{133}$Cs atoms [25]. If degenerate lithium and cesium atoms attract each other strongly enough, some effective boson–boson attraction might be induced even though the condensed bosons alone were repulsive. This change of the interaction character is caused by a coherent three-body scattering process. It leads to formation of trains of Bose–Fermi solitons as seen in experiment [25] and predicted theoretically a long time ago [26–28].

A crude estimation of the onset of a change of the sign of interactions between bosons, given in reference [26], is as it should take place when

$$\left| g_{BF} \right| > \frac{C}{N_B^{2/5} N_F^{1/2}} \frac{g_B}{g_F}$$

(1)

the bosonic component becomes effectively attractive too. Here, $C = C_1 (a_B^\perp)^3 a_F^\perp \lambda_B^2 / \lambda_F^2$, $a_B^\perp = 3^{1/5} 5^{2/5} \pi / 16$, $a_F^\perp$ is the radial harmonic oscillator length, $\lambda = \omega_z / \omega^\perp$ defines the aspect ratio of the axially symmetric (around $z$ axis) trap, and $a_B$ is the s-wave scattering length for the pure Bose gas related to the interaction strength via $g_B = 4 \pi \hbar^2 a_B / m_B$. The interaction between bosons and fermions is characterized by $g_{BF} = 2 \pi \hbar^2 a_{BF} / \mu$ with $\mu$ being the reduced mass.

To meet the condition (1) scattering lengths of one component must be tuned via Feshbach resonance technique. It can be done in two ways: (i) by tuning $a_B$ to very small values or (ii) by tuning $|a_{BF}|$ to large values.

We consider small $a_B$ case first. For cesium–lithium mixture as in experiment of reference [25], i.e. for $a_{BF} \approx -60 a_0$ ($a_0$ is the Bohr radius), trapping frequencies (130, 130, 6.5) Hz for bosons and (400, 400, 36) Hz for fermions, and particles numbers as $N_B = 30 000$ and $N_F = 20 000$, the equation (1) gives the upper limit $a_B < 0.4 a_0$ (region marked by 1 in figure 1). In fact, the soliton trains were observed in [25] already for $a_B \approx 3 a_0$.

The other way to satisfy the condition (1) is to work close to the Feshbach resonance visible in figure 1, at the magnetic fields around 893 G. Across this resonance one has $a_B \approx 230 a_0$ and the equation (1) is
Figure 2. Upper row: equipotential lines for bosonic component of the Bose–Fermi mixture. Here, the trapping frequencies are $(130, 130, 6.5)$ Hz for bosons and $(400, 400, 36)$ Hz for fermions, $a_{BF} = -60a_0$, $a_B = 3a_0$ (left frame), $a_B = 10a_0$ (right frame), and the number of particles are $N_B = 30,000$ and $N_F = 3000$. Both figures exhibit a minimum (with positive energy) for widths $(\sigma_A, \sigma_r) = (40, 2)$ micrometers. Deeper minima (with negative energy) are at $(\sigma_A, \sigma_r) = (54, 54)$ (left frame) and $(\sigma_A, \sigma_r) = (97, 97)$ (right frame) nanometers. For $N_F = 2 \times 10^4$ there is only the minimum at $(40, 2)$ micrometers. Lower row: here, the confinement is spherically symmetric with trapping frequencies $6.5$ Hz for bosons and $36$ Hz for fermions; other parameters are the same. Deeper minima remain the same in size and depth, whereas the shallower ones now represent spherically symmetric density distributions with $\sigma = 15 \mu m$.

satisfied for large enough $|a_{BF}|$, equal to about $2000a_0$ (region marked by 2 in figure 1). Negative and large values of $a_{BF}$ are explored in reference [29], where the observation of a degenerate Fermi gas trapped by the Bose–Einstein condensate is reported.

In the following we will discuss a scenario of droplet formation. We consider a trapped case with fixed number of fermionic, $N_F$, and bosonic, $N_B$, atoms in a harmonic trap. Although a genuine droplet must be stable without any trapping potential, initially atoms are always kept in a trap. Only then interaction parameters are tuned to required values and a droplet is eventually formed. To this end both kinds of atoms must be mixed in the well prescribed proportions. Typically this condition is not met in a trap with initially prepared atoms. However, droplet can still be formed but then a gaseous cloud of surplus atoms is surrounding a droplet. The cloud is stopped from expansion by the external trap. The liquid droplet is at a stable equilibrium with its vapors then.

This is the situation we are studying here. We show that Bose–Fermi mixture, spanned over parameter regions 1 and 2 in figure 1, shows a bistability phenomenon while trapped by external harmonic potential. For a given set of interaction parameters, there are two minima in the energy landscape, one local and the other global one. Density profiles correspond to two different droplet-like objects immersed in a vapor of surrounding atoms.

To get the idea of possible scenario of droplet formations we start first with simplified variational calculations. Although we consider here one particular set of parameters the scenario we are going to describe is quite general as it follow from the form of the assumed mean field density functional.

The bosonic and fermionic densities are assumed to be axially symmetric distributions of the form of the Gaussian functions with two variational parameters: the axial ($\sigma_A$) and radial ($\sigma_r$) widths. The width of the bosonic cloud is the same as that of the fermionic one. No fermionic background is assumed. These assumptions oversimplifies typical experimental situations, nevertheless quite well illustrate the main idea which will be supported by realistic hydrodynamic simulations in the second part of our paper.

Gaussian ansatz assumes that the densities are proportional to $\exp(-z^2/\sigma_A^2) \exp(-\rho^2/\sigma_r^2)$ and normalized to the number of fermions $N_f$ and bosons $N_B$, respectively. The kinetic fermionic, including the
At the mean-field level, the only interaction energies are $E_{\text{int}} = \frac{1}{\sigma_A^{2/3}} \sigma_B^{4/3}$, $E^{\text{LV}} \propto \left(1/\sigma_A^2 + 2/\sigma_R^2\right)$, and $E^{\text{BF}} \propto \left(1/2\sigma_A^2 + 1/\sigma_R^2\right)$.

At the mean-field level, the only interaction energies are $E_{\text{int}}^B$, $E_{\text{int}}^{BF} \propto 1/\sigma_A^2 \sigma_B^2$ as degenerate fermions do not interact. We consider as well the quantum corrections to the intra- and inter-species interaction energies. The Lee–Huang–Yang correction [31] to the boson–boson interaction is calculated as $E_{\text{LHY}}^B \propto 1/\sigma_A^{3/2} \sigma_B^3$, while the quantum correction to the boson–fermion interaction [32], $E_{\text{q}}^{BF}$, is given in appendix A. Finally, the contributions due to trapping are as follows

$$E_{\text{tr}}^B \propto \left(\omega_B^2 \sigma_A^2 / 2 + \omega_R^2 \sigma_R^2\right)$$

$$E_{\text{tr}}^F \propto \left(\omega_F^2 \sigma_A^2 / 2 + \omega_F^2 \sigma_R^2\right),$$

where $\omega_B^2$ and $\omega_R^2$ are axial and radial trapping frequencies, respectively, for bosons (fermions). Full formulas for all kinds of energy included in the analysis can be found in appendix A.

The variational analysis described above shows the bistability phenomenon, i.e. the existence of two minima in the energy landscape of a trapped Bose–Fermi mixture. The first minimum describes large axially symmetric cloud of mixed species, whereas at the second minimum the mixture forms rather a spherically symmetric droplet. We show the equipotential lines in figure 2 (here, $a_B = 3a_A$ (left upper frame) and $a_B = 10a_A$ (right upper frame)) for the set of parameters close to the region marked by 1 in figure 1, explored in experimental work of reference [25]. For $N_B = 30\,000$ and small number of fermions (here, $N_F = 3000$) we always find two energy minima. One of them, corresponding to a positive energy, represents the elongated axially symmetric object with the axial and radial density widths equal to $(\sigma_A, \sigma_R) = (40, 2)$ micrometers.

The second minimum corresponds to the spherically symmetric atomic clouds. For lower $a_B$ energy at this minimum is negative, i.e. the object, in principle, should remain stable after the trap is removed since the trapping energy is positive. The size of the ‘droplet’ is below 100 nm and increases with $a_B$ (see figure 2). Its energy increases with $a_B$ as well and already for $a_B = 20a_A$ becomes positive and larger than the energy.
corresponding to the first minimum. The atomic densities of spherically symmetric objects are large, too large to resist destruction due to three-body losses. Hence, the regime 1 in figure 1 constitutes rather a good set of parameters for investigating trains of Bose–Fermi solitons. They appear as a result of the modulational instability of bosonic component of elongated cloud assigned to the first minimum (as already observed in [25]). For larger number of fermions, \( N_F = 20,000 \), there exists only one minimum with positive energy. This can be understood based on the Bose–Fermi droplet’s physics —only a particular number of fermions can be associated with a given number of bosons to form a droplet. The surplus particles, fermions in this case, act as a gas being at equilibrium with the droplet.

Our variational calculations are performed for parameters corresponding to a particular experiment [25, 29]. Results were obtained with the help of Gaussian ansatz. The reader should be aware that in principle this approach has severe limitations. For instance results might be correct only in a limited range of parameters or in some particular situations. The density profiles of bosonic and fermionic cloud can be also different from the correct ones. However, as we are going to show in the following where we use more sophisticated approach, the Gaussian based results occurred to be very handy, at least for the experimentally important system studied here. It allowed us to locate the two minima in the energy landscape of the system as well as to determine their character and to estimate the potential barrier separating them. The quality of agreement allows to believe that the main conclusions we have got are of quite general character for the mixtures forming very dilute liquid droplets. In particular the Bose–Fermi mixture confined in a trap exhibits the bistability phenomenon and two distinct regions in parameter space, 1 and 2, naturally appear. Details of emerging minima, of course, depend on the shape of the variational ansatz but overall properties remain unchanged. For example, energies at two minima (region 1) increase with the scattering length \( a_B \).

The energy corresponding to the ‘soliton’ related minimum goes up faster and for some value of \( a_B \) (the bifurcation point) disappears. The bistability persists independently of the trapping geometry, for example the lower row in figure 2 shows the presence of two minima for spherically symmetric confinement.

To verify predictions obtained within the variational analysis we performed numerical simulations based on quantum hydrodynamics equations [19, 20], see also appendix B. We look for the ground state of the system using imaginary time technique. For \( a_B = 3a_0 \) and \( a_{BF} = -6a_0 \) we observe a long plateau in the energy plot while consecutive states generated in imaginary time approach the ground state of the droplet (lower frame in figure 3). We interpret this plateau as a property indicating existence of a local minimum corresponding to an elongated object in figure 2.

When we start the real time evolution choosing as the initial state any of the density distribution belonging to this long plateau then we observe a quick (in duration less than 1 ms) transfer of the mixture toward the state with the droplet, the surplus fermions are being expelled into the fermionic background. Hence, the tunneling from one minimum to the other is possible, with time scale dependent on the height of the barrier separating two minima. For example, analogous simulations for \( a_B = 10a_0 \) reveal a long-living droplet-like object (upper frame in figure 3). This happens because, as shown by variational calculations,
for $a_B = 10a_0$ (figure 2, right frame) there exists a huge barrier separating the two minima. After removing trapping potential this droplet-like object breaks into a train of Bose–Fermi solitons.

To get Bose–Fermi cesium–lithium droplets of larger size, to meet the imaging resolution requirements, one has to move from region 1 to 2 in figure 1, i.e. to increase the value of $a_B$ scattering length. It simultaneously results in decrease of droplet component’s densities making the particle losses less important. An example is shown in figure 4, where the ground state densities, still at the presence of the trap, obtained by imaginary time evolution of quantum hydrodynamics equations for $a_B = 250a_0$ and $a_{BF} = -3.6a_0$ are shown.

It turns out that the variational calculations for such parameters exhibit only one local minimum, corresponding to elongated clouds. See exemplary figure 5 confirming the existence of bifurcation in the system. For strong enough boson–fermion attraction the energy of an elongated mixture becomes negative and the trapping energy is negligibly small. It means that removal of the trapping potential should not destroy the system. One should observe the oscillating Bose–Fermi droplet since its initial shape is far from being spherically symmetric.

It is indeed as shown in the movies [33, 34] resulting from simulations based on hydrodynamics equations, appendix B. For the first case [33], we have $a_B = 250a_0$ and $a_{BF} = -3.6a_0$, i.e. we are deeply in the range of parameters where the droplet exists [19]. The trap is open in 1 ms. When the trap is fully released, the droplet survives and remains very elongated. After a further few milliseconds a rich dynamics

**Figure 5.** Energy, radial and axial widths, and a peak bosonic density of the Bose–Fermi droplet as a function of the scattering length $a_B$, for $a_{BF}/a_B = -3.6$. The numbers of bosons and fermions are $N_B = 10^4$ and $N_F = 1000$, respectively. Black and red curves correspond to the 'droplet' and 'soliton' minima, respectively. The lighter (darker) colors for the size of the system (middle frame) represent the axial (radial) direction.
develops, the droplet becomes soon short in the axial and long in the radial direction. Then opposite happens and the initial shape is restored and the next cycle succeeds. Our simulations firmly prove the existence of the critical ratio \( |\alpha_{BF}| / \alpha_B \) for the formation of Bose–Fermi droplets, see reference [19]. The movie [34] shows what happens with the mixture when \( \alpha_{BF} = -2.8 \alpha_B \). After a few milliseconds the droplet seems to be formed, but eventually it explodes. For even less negative ratio, \( \alpha_{BF} / \alpha_B = -2.0 \), the mixture explodes immediately when the trap is removed, see [35].

The Bose–Fermi droplet can be formed and persist for a longer time if losses due to three-body recombination processes are minimized. For parameters as in the region marked by 1 in figure 1, the atomic densities are certainly too large with respect to the losses (as in figure 5, the lowest frame, for small \( \alpha_B / \alpha_0 \)). The case 2 in figure 1 suggests that the creation of Bose–Fermi droplets is possible. Even more favorable conditions should be accessible for systems with higher boson to fermion mass ratio (see reference [19]) like, for example, bosonic ytterbium–fermionic lithium mixture. Another facilitation in creating Bose–Fermi droplets could be managed by introducing dipolar forces to the scene [13, 14], which can effectively act as an additional, to the contact one, attraction between atoms. In such a case bosonic dysprosium/erbium–fermionic lithium mixtures could be of interest.

In summary, we study the process of formation of a Bose–Fermi mixture and predict the bistability in the presence of the trapping potential. For weak boson–boson repulsion (region 1 in figure 1), there are two minima in the energy landscape of the system. The one has a positive energy and supports axially elongated cloud suitable for soliton formation. The other supports spherically symmetric droplets with negative energy. For stronger intra-bosonic repulsion (region 2 in figure 1) only the first minimum, corresponding to droplets, survive. They form the axially symmetric object. For strong enough boson–fermion attraction its energy becomes negative. Then, when the trapping potential is removed, the system turns into a stable quantum Bose–Fermi droplet. It does oscillate since initially its shape is not spherically symmetric. This behavior is confirmed by simulations based on quantum hydrodynamics. While the case 1 in figure 1 is better suited for studying the physics of Bose–Fermi solitons, we find that the region 2 in figure 1 could be considered as a scene for creating Bose–Fermi droplets.

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Appendix A. Variational analysis: energy contributions

Here we assume that the densities of bosonic and fermionic components are given by

\[
\begin{align*}
n_B(z, \rho) &= \frac{N_B}{\sqrt{\pi} \sigma_B \sigma_f^2} e^{-z^2/\sigma_f^2} e^{-\rho^2/\sigma_f^2} , \\
n_F(z, \rho) &= \frac{N_F}{\sqrt{\pi} \sigma_B \sigma_f^2} e^{-z^2/\sigma_f^2} e^{-\rho^2/\sigma_f^2} ,
\end{align*}
\]

hence are normalized to the number of bosons and fermions, respectively, and are of the same widths. We still admit, however, axially symmetric solutions.

All energy contributions are calculated within the local density approximation. The fermionic kinetic energy due to the Pauli exclusion principle and the gradient corrections (the Weizsäcker one) is

\[
E_{\text{kin}}^F = \kappa_F \int n_F^{5/3} \, d^3 r = \kappa_F \left( \frac{3}{5} \right)^{1/2} \frac{N_F^{5/3}}{\sigma_f^{2/3} \sigma_B^{2/3}}
\]

\[
E_W = \xi \frac{\hbar^2}{8 m_F} \int \left( \nabla n_F \right)^2 \, d^3 r = \xi \frac{\hbar^2}{4 m_F} N_F \left( \frac{1}{\sigma_f^2} + \frac{2}{\sigma_B^2} \right) .
\]

with \( \kappa_F = (3/10) (6\pi^2)^{2/3} \hbar^2 / m_F \) and \( \xi = 1/9 \) [36, 37]. The bosonic kinetic energy is obtained as

\[
E_{\text{kin}}^B = \frac{\hbar^2}{2 m_B} \int (\nabla \sqrt{n_B})^2 \, d^3 r = \frac{\hbar^2}{2 m_B} N_B \left( \frac{1}{2 \sigma_B^2} + \frac{1}{\sigma_f^2} \right) .
\]
We include contact interactions in the analysis. Within mean-field approximation the energies for boson–boson and boson–fermion interactions are

\[
\begin{align*}
E_{\text{tot}}^B &= \frac{1}{2} \sum_\alpha \int n_\alpha^B d^3r = \frac{g_B}{2(2\pi)^{3/2}} \frac{N_B^2}{\sigma_a \sigma_f^2} \\
E_{\text{tot}}^{BF} &= g_{BF} \int n_\alpha n_\beta d^3r = \frac{g_{BF}}{(2\pi)^{3/2}} \frac{N_B N_F}{\sigma_a \sigma_f^2}.
\end{align*}
\]

(A.4)

Degenerate fermions, we assume, do not interact. We consider the quantum corrections as well, including the Lee–Huang–Yang [31] and the Viverit–Giorgini [32] ones for bosons and for bosons and fermions, respectively

\[
E_{\text{LHY}} = C_{\text{LHY}} \int n_B^{5/2} d^3r = \frac{C_{\text{LHY}}}{\pi^{3/4}} \frac{2}{3} \frac{N_B^{5/2}}{\sigma_a^{3/2} \sigma_f^2}
\]

(A.5)

with \( C_{\text{LHY}} = 64/(15\sqrt{\pi}) \ g_B \ d_B^{3/2} \) and

\[
E_{\text{BF}}^\eta = C_{\text{BF}} \int n_B^{4/3} A(w, \alpha),
\]

(A.6)

where \( w = m_B/m_F \) and \( \alpha = 16\pi n_B a_B^3/(6\pi^2 n_F a_F^3)^{2/3} \) are the dimensionless parameters, and the function \( A(w, \alpha) \) has a form:

\[
A(w, \alpha) = \frac{2(1 + w)}{3w} \left( \frac{6}{\pi} \right)^{2/3} \int_0^\infty dk \int_{-1}^{+1} d\Omega \left[ 1 - \frac{3 k^2 (1 + w)}{\sqrt{k^2 + \alpha}} \int_0^{+1} dq \ q^2 \frac{1 - t q (1 - \sqrt{q^2 + k^2 + 2 k q \Omega})}{\sqrt{k^2 + \alpha + w k + 2 q w \Omega}} \right].
\]

(A.7)

The coefficient \( C_{\text{BF}} = (6\pi^2)^{2/3} \hbar^2 a_B^{3/2}/2m_B \).

Finally, the trapping energies are as follows

\[
\begin{align*}
E_{\text{tr}}^B &= \frac{1}{2} m_B \int ((\omega_\alpha^B)^2 z^2 + (\omega_\alpha^B)^2 \rho^2) n_B d^3r \\
&= \frac{1}{2} m_B \left( \frac{1}{2} (\omega_\alpha^B)^2 \sigma_a^2 + (\omega_\alpha^B)^2 \sigma_f^2 \right) \\
E_{\text{tr}}^F &= \frac{1}{2} m_F \int ((\omega_\alpha^F)^2 z^2 + (\omega_\alpha^F)^2 \rho^2) n_F d^3r \\
&= \frac{1}{2} m_F \left( \frac{1}{2} (\omega_\alpha^F)^2 \sigma_a^2 + (\omega_\alpha^F)^2 \sigma_f^2 \right)
\end{align*}
\]

(A.8)

with \( \omega_\alpha^B \) (\( \omega_\alpha^F \)) and \( \omega_\alpha^F \) (\( \omega_\alpha^F \)) being the axial and radial trapping frequencies for bosons (fermions). The total energy functional is \( E_{\text{tot}} = E_{\text{kin}}^B + E_{\text{kin}}^F + E_W + E_{\text{int}}^B + E_{\text{int}}^F + E_{\text{LHY}} + E_{\text{BF}}^\eta + E_{\text{tr}}^B + E_{\text{tr}}^F \).

**Appendix B. Quantum hydrodynamics equations for Bose–Fermi mixture**

The quantum hydrodynamics equations for Bose–Fermi mixture can be brought to life simply by applying the principle of stationary action to the system, in a way already proposed by Dirac [38]. The equations of motion come from the condition

\[
\delta \int d^3r \Psi^* \left( i \hbar \frac{\partial}{\partial t} - H \right) \Psi = 0,
\]

(B.1)

where \( \Psi \) is the system’s many-body wave function, \( H \) is its Hamiltonian, and integration spans over all spatial variables and time. In the simplest approximation the system’s many-body state is just the product of a single-particle bosonic wave function \( \psi_B (r, t) \) and a Slater determinant built of fermionic orbitals \( \psi_{\sigma_j} (r, t) \) (\( j = 1, \ldots, N_F \)). Then the action can be written as

\[
\int d^3r dt \left( i \hbar \psi_B^* \frac{\partial \psi_B}{\partial t} + i \hbar \sum_j \psi_{\sigma_j}^* \frac{\partial \psi_{\sigma_j}}{\partial t} \right) = H^t
\]

(B.2)
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with \( H' = \int d^3 r \delta H(\psi_B, \nabla \psi_B, \psi_F, \nabla \psi_F) \). Equation (B.1) becomes equivalent to a set of equations for single-particle bosonic and fermionic orbitals \( i \hbar \partial \psi_j(\mathbf{r}, t) / \partial t = \delta H' / \delta \psi_j^\dagger(\mathbf{r}, t) \) [39], where \( j = \{ B, F_1, \ldots, F_N \} \). For bosons one has

\[
\tag{B.3}
\frac{i \hbar}{\partial t} \psi_B(\mathbf{r}, t) = \left( -\frac{\hbar^2}{2m_B} \nabla^2 + \frac{\delta E_{\text{tot}}}{\delta \psi_B} \right) \psi_B(\mathbf{r}, t)
\]

with \( E_{\text{tot}} = E_{\text{tot}} - E_{\text{kin}}^B \). For fermions we further assume that all orbitals posses the same phase [40]. In such a case \( i \hbar \sum j \psi_j^\dagger \partial \psi_j / \partial t \) is translated to \( i \hbar \psi_B ^\dagger \partial \psi_F / \partial t \), where a new single-particle wave function \( \psi_F(\mathbf{r}, t) \) is introduced. It has the same phase as orbitals and \( |\psi_F|^2 = n_F = \sum_j |\psi_j|^2 \). Simultaneously, the kinetic energy related term appearing in the last part of equation (B.2) is split into two parts. The first one equal to \( (\hbar^2/2m_F) \sum j (\nabla |\psi_j|^2)^2 \) is approximated by the simplest Thomas–Fermi expression \( E_{\text{kin}}(\psi_F) \) completed by the Weizsäcker correction \( E_W \). The second one, \( m_F n_F \psi_F^2 / 2 \) (with \( \psi_F = (\hbar/m_F) \nabla \phi_F \) and \( \phi_F \) being the orbitals’ phase), describes the macroscopic flow of fermionic component. By assuming the same phase of all fermionic orbitals we allow for collective flows with irrotational velocity only, \( \nabla \times \mathbf{v}_F = 0 \). The resulting equation for fermions takes the form

\[
\tag{B.4}
\frac{i \hbar}{\partial t} \psi_F(\mathbf{r}, t) = \left( -\frac{\hbar^2}{2m_F} \nabla^2 + \frac{\delta E_{\text{tot}}}{\delta \psi_F} \right) \psi_F(\mathbf{r}, t)
\]

with \( E_{\text{tot}} = E_{\text{tot}} - (\hbar^2/2m_F) \int (\nabla |\psi_F|^2)^2 d^3 r \).

In the explicit form equation (B.3) and (B.4) look as

\[
\tag{B.5}
i \frac{\hbar^2}{2m_B} \nabla^2 + \frac{\delta E_{\text{tot}}}{\delta \psi_B} \psi_B + g_{BF} n_F n_B \frac{5}{3} C_{\text{LHY}} n_B^{5/3} + C_{\text{BF}} n_F^{4/3} \mathbf{A}(\omega, \alpha) + C_{\text{BF}} n_B n_F^{4/3} \frac{\partial A}{\partial \alpha} \frac{\partial \alpha}{\partial n_B} \psi_B
\]

and

\[
\tag{B.6}
i \frac{\hbar^2}{2m_F} \nabla^2 + \frac{\delta E_{\text{tot}}}{\delta \psi_F} \psi_F - \frac{\hbar^2}{2m_F} \nabla^2 |\psi_F| + \frac{5}{3} \frac{n_F^{5/3}}{n_B} \nabla \phi_F + g_{BF} n_B \frac{4}{3} C_{\text{BF}} n_F^{4/3} \mathbf{A}(\omega, \alpha) + C_{\text{BF}} n_B n_F^{4/3} \frac{\partial A}{\partial \alpha} \frac{\partial \alpha}{\partial n_B} \psi_F.
\]

Equation (B.5) can be viewed just as the extended Gross–Pitaevskii equation for bosons all occupying the same quantum state \( \psi_B(\mathbf{r}, t) \). The interpretation of the other complex field, \( \psi_F(\mathbf{r}, t) \), is different. Going from hydrodynamic fields \( n_F(\mathbf{r}, t) \) and \( \psi_F(\mathbf{r}, t) \) to the complex quantity \( \psi_F(\mathbf{r}, t) \) in a unique way requires the velocity field to be irrotational. There must exist a scalar velocity potential field. Only then, two scalar functions, the density and the velocity potential, can be uniquely transformed to the real and imaginary parts of the complex field \( \psi_F(\mathbf{r}, t) \). Indeed, in our derivation we make a crucial approximation that all fermionic orbitals have the same phase, i.e. all fermions are forced to move collectively with irrotational velocity \( (\hbar/m_F) \nabla \phi_F \). For less restrictive derivation of quantum hydrodynamics equations for Bose–Fermi mixture see appendix B in reference [20]. We call the quantity \( \psi_F(\mathbf{r}, t) \), fulfilling equation (B.6), the fermionic pseudo-wave function. We solve equations (B.5) and (B.6) by split-operator method, using both imaginary and real time techniques [41].

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