1. INTRODUCTION

The density functional (DF) approach is a well established theory for investigating important ground state properties (energies and density profiles) of quantum many body systems. In the last decades it has been systematically applied (mainly in the so called local density approximation) to a large variety of electronic systems. Applications to strongly interacting quantum systems (helium) has been also become popular in the recent years providing a useful and stimulating alternative (see for example [1]) to microscopic \textit{ab initio} calculations of inhomogeneous systems (free surface, films, clusters ...).

The equations of DF theory for static calculations are derived from a variational principle of the form

\[ \delta \left( E - \epsilon_i \int d\mathbf{r} \, \Psi_i^* \Psi_i \right) = 0 \]  

where

\[ E = \int d\mathbf{r} \, \mathcal{H} \]  

is the energy functional. The energy density \( \mathcal{H} \), characterizing the functional, in general depends on the 1-body density matrix (diagonal as well as non diagonal components). The equations of DF theory have the form of Hartree (or Hartree-Fock) equations for fermions and of an Euler equation for bosons.

It is important to recall the relevant physical quantities that DFT should account for. Concerning bulk properties they are:

- The equation of state
- The static response function.
The equation of state is fixed by the knowledge of $H$ in the homogeneous limit and in particular by its density dependence according to the law

$$P = \rho^2 \frac{\partial}{\partial \rho} \frac{H}{\rho}. \quad (3)$$

The static response function is a key quantity of the theory that should be (in principle) exactly accounted for not only in the macroscopic regime where it coincides with the compressibility, but also at higher wave vectors where the response of the system is sensitive to microscopic details of correlations among particles.

In DFT the static response $\chi(q)$ corresponds to the Fourier transform of the second derivative of the energy functional with respect to the density

$$\chi = \frac{\delta^2 E}{\delta \rho(\mathbf{r}_1) \delta \rho(\mathbf{r}_2)}. \quad (4)$$

The static response is related to the dynamic structure factor through the well known equation [1]

$$\chi(q) = -2 \int_0^\infty d\omega \omega^{-1} S(q, \omega). \quad (5)$$

This equation reveals an important and useful connection between static ($\chi(q, \omega)$) and dynamic ($S(q, \omega)$) features of the system.

In superfluid $^4$He both the equation of state and the static response are well known experimentally in a rather wide range of densities and wave vectors respectively. The most refined phenomenological density functional recently proposed by the Orsay-Trento team accounts with good accuracy for the fine details of these quantities [2] (see figs. 1 and 2).

It is also important to recall that DFT is not suitable to account for all the ground state properties of the system. In particular the pair correlation function and hence its Fourier transform, the static structure factor $S(q)$, lies outside the predictive power of the theory. At zero temperature the quantity $S(q)$ is related to the dynamic structure factor through the most famous relation

$$S(q) = \int_0^\infty d\omega S(q, \omega). \quad (6)$$

Attempts to force the theory to account for the exact value of $S(q)$, through a suitable parametrization of the dynamic structure factor $S(q, \omega)$, should be considered unphysical.

The formalism of DFT can be easily extended to the time dependent case (TDDFT). However, while in the static case the theory is well established and is expected to be, at least in principle, an exact approach for the determination of energy and density profiles of inhomogeneous systems, the applicability of TDDFT to the investigation of dynamic phenomena (for example propagation of collective phenomena) is less obvious especially in the microscopic regime of large wave vectors. The purpose of this paper is to discuss some relevant questions concerning the structure, the ingredients and the applicability of TDDFT. Some emphasis will be also
Figure 1. Equation of state of superfluid $^4$He. The full line corresponds to the density functional of ref.[2]. The dashed line is the prediction of the Monte Carlo calculations of ref.[3]. Points are the experimental values (from ref.[4]).

given to establish important connections between TDDFT and microscopic theories such as the Feynman theory for the elementary excitations of Bose superfluids.

The equations of TDDFT are naturally derived starting from the least action principle

$$\delta \int_{t_1}^{t_2} dt \int d\mathbf{r} \left[ \mathcal{H} - \epsilon_i \Psi_i^* \Psi_i - \Psi_i^* i \frac{\partial}{\partial t} \Psi_i \right] = 0$$

(7)

and take the form of a Schrödinger-like equation

$$(\tilde{H} - \epsilon_i) \Psi_i = i \frac{\partial}{\partial t} \Psi_i$$

(8)

where $\tilde{H}$ is a 1-body density dependent hamiltonian to be determined, together with the solution of the Schrödinger equation, in a selfconsistent way.

In the case of bosons, where a single wave function enters eq.(7), the resulting equations can be more conveniently rewritten by introducing the modulus and the phase of the wave function

$$\Psi = \sqrt{\rho} \ e^{iS}$$

(9)

Here $\rho$ is the (diagonal) density of the system. The resulting equations then take the
Figure 2. Static response function of superfluid $^4\text{He}$. The full line corresponds to the density functional of ref.[2]. Experimental points are from ref. [5].

Form of the equations of hydrodynamics:

$$\frac{\partial}{\partial t} \rho + \nabla (v \rho) = 0 \quad (10)$$

$$\frac{\partial}{\partial t} S + \frac{\delta}{\delta \rho} E = 0 \quad (11)$$

where $v = \frac{1}{m} \nabla S$ is the velocity field and $S$ has the meaning of a velocity potential.

2. TIME DEPENDENT DFT AND RPA

In the bulk the equations of TDDFT can be easily employed to calculate the linear response of the system. Let us consider, for simplicity, the density-density response function and let us assume for the moment (see however the discussion in the second part of the work) that the functional depends, apart from the kinetic energy term, only on the diagonal density $\rho$:

$$\mathcal{H} = -\Psi_i^* \frac{1}{2m} \nabla^2 \Psi_i + V(\rho) \quad (12)$$
The linear response function can then be easily evaluated in this case and takes the familiar form

$$\chi(q, \omega) = \frac{\chi_0(q, \omega)}{1 - v(q)\chi_0(q, \omega)} \quad ,$$

(13)

of the random phase approximation (RPA). In eq.(13) $\chi_0(q, \omega)$ is the independent particle response function given by the Lindhard function for fermions and by the expression

$$\chi_0(q, \omega) = \frac{q^2}{4m} \frac{1}{\omega^2 - (q^2/2m)^2}$$

(14)

for bosons. The quantity $v(q)$ is the Fourier transform of $\delta^2V(\rho)/\delta\rho(r_1)\delta\rho(r_2)$ and is entirely fixed by the static response of the system

$$\chi(q) \equiv \chi(q, \omega=0) = \frac{\chi_0(q)}{1 - v(q)\chi_0(q)} \quad .$$

(15)

For electrons the quantity $v(q)$ is usually written in the form $v(q) = 4\pi e^2q^{-2}(1 - G(q))$, where $G(q)$ is the so called local field correction. Notice that despite the fact that eq.(13) holds for both bosons and fermions, the resulting structure of $\chi(q, \omega)$ and in particular its poles are deeply different in the two cases as a consequence of the different form of $\chi_0$. Equation (13) can be easily generalized to include multi-component systems (for example $^3$He-$^4$He mixtures).

The above discussion reveals that the structure of TDDFT (in its linearized form) is identical to the RPA. These theories are mean field theories and are able to provide an adequate picture of elementary excitations in the low $q$, low $\omega$ regime. Actually in this regime they coincide with the Landau theory of Fermi liquids in the case of fermions and with the equations of classical hydrodynamics in the case of bosons. These are the proper theories to describe macroscopic phenomena in strongly interacting quantum liquids at zero temperature.

In conclusion we can say that TDDFT is well suited to investigate the elementary excitations of quantum many body systems at least in the macroscopic regime. However, due to its mean field nature, this theory cannot account for multi-pair excitations and consequently cannot provide a complete description of $S(q, \omega)$. The situation is schematically drawn in fig.3, where we have distinguished between the low $\omega$ region dominated by elementary excitations (collective modes and, in Fermi systems, single particle transitions) and a higher $\omega$ region dominated by multi-pair effects.

In deriving result (13) for the dynamic response function we have made the assumption that the interaction terms in the energy functional depend only on the diagonal density (see eq.(12). This is clearly an approximation which permits to express the dynamic response in terms of the static response (see eqs.(13-15)). In the language of the Landau theory of Fermi liquids this corresponds to assuming the Landau parameter $F_\ell$ is equal to zero when $\ell \geq 1$. Is this approximation correct enough? The answer is in general negative in strongly interacting liquids and we well know that in liquid $^3$He the dynamic response has a form which differs from eq.(13) due to the presence of the Landau parameter $F_1$. In the language of DFT this means that one cannot ignore the occurrence of current interaction terms in the energy functional. In liquid $^3$He this effect has the important consequence of fixing
the difference between the first sound ($c_1$) and the zero sound ($c_0$) velocity according to the formula (valid within minor approximations):

$$c_1^2 = c_0^2 + \frac{4}{15} \frac{p_F^2}{m^2(1 + F_s^i/3)}$$  \hspace{1cm} (16)

The experimental confirmation of this difference has been shown to be consistent with the measured value of the effective mass

$$\frac{m^*}{m} = 1 + \frac{1}{3} F_s^i$$ \hspace{1cm} (17)

thereby providing a direct check of the correctness of the Landau theory.

3. SUM RULES AND MULTI-PAIR EXCITATIONS

Figure 3 explicitly reveals that if one evaluates suitable moments of the dynamic structure factor

$$m_k = \int_0^\infty d\omega \omega^k S(q,\omega)$$ \hspace{1cm} (18)

the results obtained using TDDFT will differ from the ones derivable from an exact calculation or, in principle, from experiments due to the role played by multi-pair excitations which give a non vanishing contribution to the integrals (18). This question
is relevant because in some cases these moments can be evaluated with the help of sum rule techniques. Many of these sum rules play an important role in the physics of the many-body problem (see for example the f-sum rule) and it is consequently important to understand the relation between sum rules and the TDDFT-RPA scheme.

Due to the occurrence of multi-pair excitations in general mean field theories do not fulfill the sum rules even at small $q$. This statement is important because, for example, one usually expects the Landau theory of Fermi liquids to be exact at small $q$. This is true only if one limits the calculation of the dynamic structure factor to the low $\omega$ regime too. In general the integrals (18) take a significant contribution from the high $\omega$-region, a region where the mean field theory cannot provide a proper description.

The inverse energy weighted moment $m_{-1}$ yielding the static response (see eq.(5)) is an exception in this sense. In fact in the low $q$ limit the multi-pair contribution to this moment is vanishingly small and $m_{-1}$ is consequently exhausted by the collective excitation and (in Fermi systems) by single particle excitations. This property of $m_{-1}$ is especially remarkable in connection with the fact that the static response is exactly reproduced by DFT. It ensures a beautiful self-consistent behavior of the theory.

A different situation occurs with the other moments of the dynamic structure factor. An important question to discuss in this context is whether the f-sum rule

$$\int_0^\infty d\omega \omega S(q, \omega) = \frac{q^2}{2m}$$

(19)

is exhausted by the elementary excitations of the system. Result (19) follows from the use of the completeness relation and holds for velocity independent potentials. Differently from the inverse energy weighted moment the answer to the above question is in general negative even at small $q$. A well known example confirming this statement is given by spin excitations in liquid $^3$He [6] where the Landau theory, which properly accounts for the low $q$, low $\omega$ behavior of the spin dynamic structure factor, gives the result

$$\int_0^\infty d\omega \omega S^L(q, \omega) = \frac{q^2}{2m} \frac{1 + F^q_1/3}{1 + F^s_1/3}$$

(20)

a quantity significantly smaller than the exact result (19) holding for spin independent interatomic potentials. A similar situation occurs in antiferromagnets as well as in bosonic systems in a lattice or in the presence of disorder. The general rule is that the energy weighted sum rule is not exhausted, at small $q$, by the elementary excitations of the system in those systems where the current is not conserved. This happens in general for spin excitations and also for density excitations if the system is not translationally invariant.

4. SUPERFLUID $^4$He

Since the current is conserved in $^4$He the f-sum rule is entirely exhausted by the phonon mode at small $q$ in agreement with the general statements of classical
Figure 4. Dispersion of elementary excitations in superfluid $^4$He. Full line: Feynman approximation. Dashed line TDDFT without current terms (eq.()). Points: experimental data (from [7]).

hydrodynamics. At higher $q$ the relative contribution of the elementary excitations to the integral (19) becomes smaller and smaller and is about one third in the rotonic region as a consequence of the important role played by multi-pair excitations at high wave vectors. Viceversa the inverse energy weighted sum rule even at relatively large $q$ is mainly dominated by the elementary mode due to the occurrence of the $\omega^{-1}$ factor in the integral (5) which quenches the contributions arising from multi-pair excitations located at higher energies.

Let us discuss the implications of the above discussion in the case of $^4$He. In the absence of current interaction terms in the energy functional the dynamic response function takes the form (see eqs.(13-15)):

$$\chi(q, \omega) = \frac{q^2}{2m} \frac{1}{\omega^2 - \omega_0^2(q)}$$ (21)

and exhibits a single pole whose dispersion law is given by

$$\omega_0^2(q) = \frac{q^2}{2m} \left( \frac{q^2}{2m} + 2v(q) \right) .$$ (22)

In fig.4 we report the dispersion law (22). The function $v(q)$ is fixed, through eq.(15), by the static response function which is known experimentally in superfluid
The resulting curve for $\omega(q)$ overestimates the experimental curve. Actually result (22) can be also rewritten in the form

$$\omega_0^2(q) = \frac{m_1(q)}{m_{-1}(q)} = -\frac{q^2}{m\chi(q)}$$

which corresponds to a rigorous upper bound to the dispersion of the collective branch (we ignore here possible decay mechanisms of elementary excitations).

It is interesting to compare result (23) with the prediction of the most famous Feynman approximation

$$\omega(q) = \frac{m_1(q)}{m_0(q)} = \frac{q^2}{2mS(q)}$$

which expresses the energy of the elementary excitation in terms of the static structure factor $S(q)$. The Feynman result (24) also provides a rigorous upper bound to the exact dispersion law. It is important to remark that both the bounds (23) and (24) coincide with the phonon dispersion $\omega = cq$ at small $q$. One has the general inequality

$$\sqrt{\frac{m_1}{m_{-1}}} \leq \frac{m_1}{m_0}.$$  \hspace{1cm} (25)

Inequality (25) reveals that, even in the absence of current terms in the energy functional, time dependent DFT results to be a better approximation with respect to Feynman theory, providing an upper bound closer to the exact dispersion. From a microscopic point of view the quantity $\chi(q)$ is much more difficult to calculate with respect to $S(q)$ though first calculations of $\chi(q)$, based on diffusion Monte Carlo techniques, are now becoming available [8].

We are now ready to discuss the inclusion of current dependent terms in DFT. The explicit form of these new terms is discussed in ref.[2] and will not reported here. The new term is included phenomenologically with the criterium of reproducing the experimental dispersion law of elementary excitations. The following remarks are in order here:

- The new term results in a modification of the equation of continuity (10) which now contains an extra contribution having the form of a backflow effect. Viceversa the Euler equation keeps its form (11).
- The new term does not affect the Galilean invariance and in particular the low $q$ behavior of the response function is not modified. Important changes are instead introduced at higher $q$ especially in the roton region.

The formalism of TDDFT is now ready to be applied to study the dynamics of inhomogeneous helium systems. One can explore, for example, the interesting region where surface excitations can couple with rotons (ripplon-roton hybridization)[9] and where elementary excitations can give rise to particle emission (quantum evaporation)[10]. These investigations are the object of present research and will hopefully provide a test of the quality of the TDDFT formalism and in particular of the new density functional.

Finally one should also be also aware of the limits of the theory. In particular the present formalism cannot account for damping effects associated with the decay of an elementary excitation into two or more excitations. Furthermore the formalism
cannot be pushed upto very high momenta (larger than about $2.5A^{-1}$). In fact at these high values of $q$ the inverse energy weighted moment (5) is no longer exhausted by the elementary excitations: in this regime the static response, major ingredient of DFT, has lost its connection with the physics of elementary excitations.

In conclusion the main message emerging from the present discussion is that the theoretical basis of TDDFT (with the inclusion of current dependent terms) is now reasonably well established and can be applied in a reliable way to investigate important dynamic phenomena of inhomogeneous systems in the microscopic regime.

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