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The effective single particle potential and the tadpole*

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Abstract. The Energy Density Functional (EDF) theory is extremely successful within the effective force approach, noticeably the Skyrme or Gogny forces, in reproducing the nuclear binding energies and other nuclear properties along the whole mass table. The EDF is in this case represented formally as the Hartree-Fock (HF) mean field of an effective force, and the associated single particle states can be considered the eigenstates of the corresponding effective mean field. In general, the phenomenological single particle spectrum is not accurately reproduced. To overcome this difficulty one can improve the functional in order to incorporate in the mean field additional correlations in an effective way. In an alternative viable scheme one can introduce explicitly many-body correlations which affect the single particle motion at both dynamic and static levels. In particular, the particle-vibration coupling scheme modifies the positions of the individual single particle energies. In this case one also introduce the fragmentation of the single particle states, a feature that cannot be described at the mean field level. At the same time the so-introduced correlations modify the static single particle potential, and the single particle states that diagonalize the corresponding density matrix are not the orbitals of a mean field with occupation numbers 1 (occupied orbitals) and 0 (unoccupied orbitals) anymore. In this paper we show that both static and dynamic effects on the single particle motion can be introduced within a previously developed scheme, based on the conserving approximations, and that the static part can be identified with the so-called tadpole term introduced by Khodel in the self-consistent theory of finite Fermi systems. The treatment remains at the formal level, but we hope that several aspects of the particle-vibration coupling scheme will be clarified.

1 Introduction

At normal density the nucleons in nuclear matter and nuclei are delocalized and form a quantum liquid [1,2]. In the independent particle shell model [1], the nucleons move in a one-body potential and the corresponding eigenstates are the building blocks of the many-body wave function, which is then a Slater determinant. In the early time, the model was devised to explain the increasing evidences of the single particle structure of nuclei [3]. As it is well known, this was in serious contrast with the Liquid Drop Model [4] and the optical model [1], which look more consistent with a strong damping of the single particle motion. The solution of the puzzle is based mainly on the observation that in a normal Fermi system the corresponding single particle occupation number has a sharp discontinuity at the Fermi surface, despite the presence of the interaction [5,6]. The latter has only the effect to reduce the size of the discontinuity, which is then smaller than 1. This means that the Pauli principle is still active and the mean free path of nucleons close to the Fermi surface is long. In nuclei, the mean free path is much longer than the nuclear size, and the single particle structure persists despite the interaction, at least to a certain extent. These considerations are at the basis of the Landau theory of Fermi liquid [7] extended to finite nuclei by Migdal [8], with the formulation of the theory of finite Fermi systems (TFFS). In the first version of this theory, only states of low energy excitations or corresponding to the addition of one or few particles were studied. The associated effective Landau-Migdal (LM) interaction amplitudes and the mean field potential were expressed in terms of few independent phenomenological parameters. By means of the self-consistency relations of TFFS [9] the nucleon mean

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field potential can be calculated in terms of the LM amplitudes. The self-consistent version of TFFS was further developed in [10], where it was shown how to calculate the total binding energy and all other ground state properties, in analogous way as in the Skyrme–Hartree–Fock (SHF) method. In ref. [11] the self-consistent TFFS was reformulated in terms of the corresponding energy density functional.

In the SHF method, developed by Vautherin and Brink [12], one expresses all the ground state properties in terms of simple density-dependent interaction. This well known approach can be considered as the EDF method with Skyrme functional.

The connection between the two approaches is discussed in refs. [13–15]. In this case, it is assumed that the effect of correlations beyond the mean field can be embodied in the phenomenological effective interaction between single particle modes, that obey the Pauli principle with a sharp Fermi surface. These single particle modes are indicated as quasi-particles, since they behave as free particle with an effective interaction, the latter being fixed at phenomenological level.

At a more microscopic level, *i.e.* keeping the particle representation, the single particle structure should appear modified with respect to a free Fermi systems, with a reduced discontinuity at Fermi surface and a fragmentation of the single particle strengths. The fragmentation should appear analyzing the one-particle transfer reaction cross sections, where a spread of the single particle levels with given quantum numbers should turn out to be necessary in fitting the data. If the spread is not too large, the single particle structure should be still visible, *e.g.* by introducing the proper centroids of the strength distributions for given single particle quantum numbers. In a fully microscopic approach, *e.g.* the interacting shell model [16, 17], these features should be present, once the single particle strengths have been identified. Unfortunately, the interacting shell model is numerically quite expensive and a systematic application of the method throughout the mass table is still to be developed [17].

As a first step towards a fully microscopic theory, one can take an intermediate approach, by still employing a phenomenological effective interaction or density functional, but introducing explicitly specific correlations which are believed to be particularly relevant and difficult to incorporate in the effective interaction. This line can be followed both within the TFFS and within the EDF approach. In this case, both static and dynamic modifications of the single particle motion are introduced. They are assumed to be the dominant ones in fixing the position and fragmentation of the single particle strengths.

In particular, the correlations produced by the coupling between the particles and the vibrations (phonons) should be of particular relevance since they introduce naturally the fragmentation of the single particle strength. At the same time they are of long range in character and therefore hardly included in the short range effective interactions like Skyrme, Gogny or the LM amplitudes of TFFS. In a previous paper [18], we have presented an approach that develops the particle-vibration scheme to all order at microscopic level, starting from a given EDF. The formalism is conserving, *i.e.* the local current is conserved [19, 20], and the phonons are described microscopically, they are not treated as separated and independent degrees of freedom. In this paper, we further illustrate the method and we show explicitly, how both the static and the dynamic correlations affect the single particle motion. It naturally leads to the introduction of a generalized static single particle potential, which incorporates at static level the effect of correlations introduced by the particle-vibration scheme. This modification of the static single particle potential can be related in a natural way to the so called tadpole term, introduced in the self-consistent TFFS by Khodel [21], see also [10]. Note that in these works only the low-lying strongly collective phonons were considered and they were treated as independent degrees of freedom.

In this paper, we will not face one of the main problem for any many-body theory which is going beyond the mean field within the EDF approach, *i.e.* the possible overcounting of the correlations already incorporated in the functional in an effective way. In principle, one should refit the parameters of the functional or of the effective force with the inclusion of the correlations explicitly introduced. In the case of the particle-vibration approach the ground state energy to be fitted should include correlation terms beyond mean field and consistent with the ones explicitly introduced in the description of the phonons and of the single particle self-energy. In particular if the phonons are described within the Random Phase Approximation (RPA), in order to be consistent, the ground state energy should include the well known RPA correlation energy [22]. The problem of the parameter refitting is beyond the scope of the paper and its practical realization is beyond the present capability of the standard calculation schemes.

The paper is organized as follows. In sect. 2 we recall the formalism and stress that the single particle self-energy contains a static contribution, *i.e.* an energy independent term, beyond the HF term, and a dynamical one, which is determined by the coupling of the particles with the phonons. In sect. 3 it is shown that the static contribution coincides with the so-called tadpole, or non-pole, contribution of the TFFS. In sect. 4 it is discussed the role of the tadpole in the solution of the divergence problem that arises once the coupling to the spurious mode is considered. This result generalize to a generic EDF the procedure developed in the TFFS. We draw our conclusions in sect. 7.

2 The formalism

The approach of choice for a theory that focuses on the single particle structure is the Green's function method. We summarize here the basic equations and their meaning that are at the basis of the formalism developed in ref. [18]. First of all in order to introduce the equations of motion of the Green's function it is necessary to start

from a Hamiltonian formalism. This is done by expanding the functional around the minimum up to second order in the density variations and then introducing the second quantization formalism. The effective Hamiltonian can be written

$$H = H_0 + \frac{1}{4}\sum_{klmn}\langle kl|f|mn\rangle_A N\left(\psi_k^\dagger\psi_l^\dagger\psi_n\psi_m\right), \quad (1)$$

where H_0 is the independent particle Hamiltonian

$$H_0 = \sum_{ij}\epsilon_{ij}\psi_i^\dagger\psi_j \quad (2)$$

where ϵ is the single particle energy matrix in a generic basis. The symbol $N(\ldots)$ indicates the normal ordering with respect to the independent particle ground state. In this way only correlations beyond the mean field are affecting the single particle density matrix and the single particle potential. The indexes $k, l, m\cdots\cdots$ labels the single particle states in a generic basis, and $\psi^\dagger$, ψ the corresponding creation and annihilation operators. In line with the expansion the effective interaction f is the second derivative of the interaction term of the functional with respect to the density matrix ρ

$$\langle us|f|vt\rangle_A = \left(\frac{\delta^2 V}{\delta\rho_{st}\delta\rho_{uv}}\right). \quad (3)$$

The formalism includes a set of coupled equations to be solved by iteration. The first equation is the Dyson equation connecting the single particle Green's function G and the self-energy M

$$\begin{aligned} &i\frac{\partial}{\partial t_1}G_{pq}(t_1,t_2) - \sum_{p'}\epsilon_{pp'}G_{p'q}(t_1,t_2) \\ &-\sum_h M_{ph}(t_1,\overline{t_3})G_{hq}(\overline{t_3},t_2) = \delta(t_1-t_2)\delta_{pq} \end{aligned} \quad (4)$$

The standard definition for G is

$$G_{pq}(t_1,t_2) = -i\langle T\{\psi_p(t_1)\psi_q^\dagger(t_2)\}\rangle, \quad (5)$$

where T indicates the usual fermionic time ordering operator. In eqs. (4), (5) the labels stand for a set of single particle quantum numbers and a bar over a time variable t_i means integration on this variable. The self-energy sums up all the one-particle irreducible diagrams. Finally $\epsilon_{pp'}$ is the unperturbed energy matrix, that for generality is taken possibly non-diagonal, since all the equations are formulated in a generic single particle basis.

The phonons are described by the density-density propagator Π

$$\begin{aligned} \Pi_{sr;km}(t,t') &= -\langle\Psi_0|T\{\rho'_{rs}(t)\rho'_{km}(t')\}|\Psi_0\rangle \\ &= -\langle\Psi_0|T\{\rho'_{sr}(t)^\dagger\rho'_{km}(t')\}|\Psi_0\rangle \\ \rho'_{rs}(t) &= \psi_r^\dagger(t)\psi_s(t) - \langle\psi_r^\dagger\psi_s\rangle, \end{aligned} \quad (6)$$

where Ψ_0 is the (correlated) ground state, $\psi^\dagger$ and ψ are the single particle creation and annihilation operators and the bracket $\langle\ldots\rangle$ indicates mean value in the ground state. This propagator is also the linear response function of the system to an external one-body potential. As mentioned in the introduction the self-energy can be split into a static and a dynamic contribution

$$M_{ph}(t_1,t_3) = U_{ph}(t_1)\delta(t_1-t_3) + \tilde{M}_{ph}(t_1,t_3). \quad (7)$$

The static term is given by the polarization potential U [18,23]

$$\begin{aligned} U_{ph}(t_1) = \phi_{ph}(t_1) &+ \sum_{km}\langle kp|f|mh\rangle_A \\ &\times\left[\langle\psi_k^\dagger(t_1)\psi_m(t_1)\rangle - \langle\psi_k^\dagger(t_1)\psi_m(t_1)\rangle_0\right], \end{aligned} \quad (8)$$

where the brackets $\langle\ldots\rangle_0$ indicate mean value in the independent particle ground state. The expression includes the possible external interaction ϕ, which vanishes for an isolated system. The potential U_{ph} thus receives contributions once there are modifications of the density matrix with respect to the HF one. The diagonalization of the correlated density matrix introduces the so-called "natural orbitals" [24,25], whose occupation numbers in general differ from 0 and 1. In eq. (8) f is the effective two-body interaction.

The second term in eq. (7) describes the dynamical contributions not included in the static single particle potential and can be expressed in term of the particle-vibration coupling

$$\begin{aligned} &\tilde{M}_{ph}(t_1,t_3) \\ &= \frac{1}{2}i\sum_{nrij}W_{pn;ij}(t_1,\overline{t_5})G_{nr}(t_1,\overline{t_4})\Gamma_{rh;ij}(\overline{t_4},t_3;\overline{t_5}) \\ &+\frac{1}{2}\sum_{km}\langle kp|f|hm\rangle_A\langle\psi_k^\dagger(t_1)\psi_m(t_1)\rangle\delta(t_1-t_3), \end{aligned} \quad (9)$$

where the quantity

$$\begin{aligned} W_{pn;ij}(t_1,t_5) = &\langle ip|f|jn\rangle_A\delta(t_1-t_5) \\ &-i\sum_{kmrs}\langle kp|f|mn\rangle_A\Pi_{mk;rs}(t_1,t_5) \\ &\times\langle ri|f|sj\rangle_A \end{aligned} \quad (10)$$

includes indeed the coupling of the single particle to the phonon degrees of freedom. The second term at the r.h.s. of eq. (9) is a direct static interaction, that turns out to be canceled by a term appearing in the expansion of the first term, as it will be shown later, and the expression for $\tilde{M}_{ph}$ is indeed fully dynamical. The function Γ appearing in the self-energy of eq. (9) is the so-called (irreducible) vertex function. The equations for the vertex function and for the phonon propagators close the set of equations that couple the static single particle potential U, the self-energy $\tilde{M}_{ph}$,

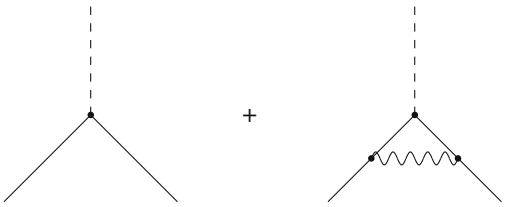

Fig. 1. Starting ansatz for the vertex function Γ of eq. (11).

the phonon propagator and the vertex function. They read

$$\Pi_{mk,rs}(t,t') = \sum_{pqij} G_{mp}(t,\overline{t_1})G_{qk}(\overline{t_2},t)\Gamma_{pq;ij}(\overline{t_1},\overline{t_2};\overline{t_3})$$
$$\times \left[\delta_{ir}\delta_{js}\delta(\overline{t_3}-t') - i\sum_{tu}\langle it|f|ju\rangle_A \Pi_{ut,rs}(\overline{t_3},t')\right],$$
$$\Gamma_{nh;ij}(t_3,t_4;t_5) = \delta_{ni}\delta_{hj}\delta(t_3-t_4)\delta(t_3-t_5)$$
$$-\sum_{rspq}\left(\frac{\delta\tilde{M}_{nh}(t_3,t_4)}{\delta G_{rs}(\overline{t_6},\overline{t_7})}\right) G_{rp}(\overline{t_6},\overline{t_8})G_{qs}(\overline{t_9},\overline{t_7})$$
$$\Gamma_{pq;ij}(\overline{t_8},\overline{t_9};t_5). \qquad (11)$$

These coupled equations have been introduced for an electron gas in refs. [26, 27], where their graphical representation can be found. A more recent presentation can be found in ref. [28]. In the realm of nuclear physics they have been considered in ref. [29]. The novelties of the present formulation is the treatment of a density dependent force, within the EDF scheme, which requires the normal ordering in the Hamiltonian, and the separation of the static contribution to the self-energy, which is the main subject of the paper. The integral equation for the vertex function involves a functional derivative and therefore the set of coupled equations is not solvable in the usual way. In ref. [18] we proposed to expand the equations starting from a guess on the vertex function and solving by iteration for the self-energy, the vertex function and the phonon propagator. A possible starting ansatz for the vertex function is depicted in fig. 1, where the wavy line indicates a phonon propagator. With this initial guess both self-energy and phonon propagator can be derived, which in turn generate the next approximation for the vertex function. The functional derivative of the self-energy with respect to the Green's function can be interpreted as effective interaction in the medium. It plays the key role in generating the various terms of increasing complexity, which can be eventually represented by diagrams. Along the expansion also the static potential U in the self-energy starts to play a role. It has to be stressed that the separation between static and dynamical terms in eq. (7) is an essential consequence of the introduction of the normal ordering in the Hamiltonian. The iterative procedure has been described in details in ref. [18]. Here we limit to report the diagrammatic representation of the terms so generated up to the second iteration, selecting the diagrams with at most two phonons.

At the first iteration one gets the diagrams of fig. 2. The two-phonon diagrams generated at the second iteration are reported in fig. 3

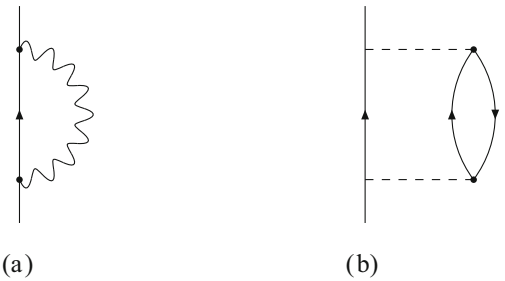

Fig. 2. One phonon contribution to the single particle self-energy (a), and "bubble diagram" (b), see the text. Not all time ordering are displayed.

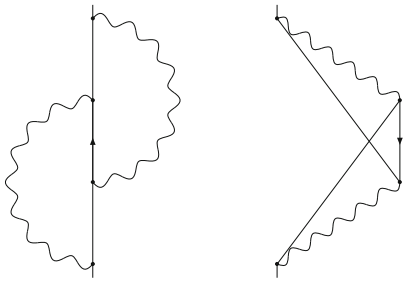

Fig. 3. Two phonon diagrams contributing to the single particle self-energy. Not all time ordering are displayed.

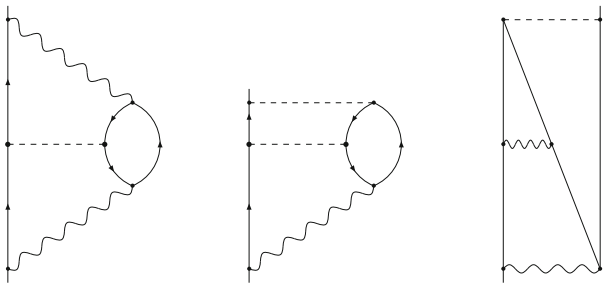

Fig. 4. Additional diagrams of self-energy generated at the second iteration. Not all time ordering are displayed.

It has to be stressed that in the diagrammatic expansion not only the phonon propagator appears, but it is mandatory to include also the bare effective interaction. Indeed at the second iteration also the diagrams of fig. 4 appear, where the dashed line indicates the bare effective interaction. This turns out to be necessary to avoid double counting and respect the correct symmetry factors. Notice that the diagrams are automatically generated by the iterative procedure.

Finally we have to notice that in all practical calculations some selection of particle-hole excitations has to be done. This depends on the considered physical problem. In particular for nuclear structure calculations a good choice can be the inclusion of the most collective modes, the only ones which strictly speaking deserve the name of "phonons". For other scopes, like the calculations of the density of levels, the inclusion also of the non-collective phonons is probably necessary. In any case with zero range forces the introduction of a cut-off or of a model space is mandatory.

3 Single particle potential and the tadpole

In this paper we will focus on the modification of the single particle potential introduced by the one-body term U in the self-energy of eq. (7), as long as the expansion is developed, and on the interplay between static and dynamic contributions to the self-energy.

The expression of eq. (8) for the static correction can be rewritten in terms of the Green's function

$$U_{ph} = \sum_{km} \langle kp|f|mh\rangle_A \times \frac{1}{2\pi i}\int_\Omega \mathrm{d}\omega \left[G_{km}(\omega) - G^{(0)}_{km}(\omega)\right], \quad (12)$$

where G and G^0 are the Fourier transform of the correlated and unperturbed Green's functions, respectively. The integral is taken along the semi-circle Ω surrounding the upper half-plain of the complex ω-plane. In agreement with eq. (4) the difference in the square bracket is directly related to the single particle self-energy

$$U_{ph} = \sum_{km} \langle kp|f|mh\rangle_A \times \frac{1}{2\pi i}\int_\Omega \mathrm{d}\omega \sum_{nl}\left[G^{(0)}_{kn}(\omega)M_{nl}(\omega)G_{lm}(\omega)\right]. \quad (13)$$

This is a complex non-linear integral equation for U. In fact the potential U is again contained in the self-energy M, see eq. (7), which appears in the numerator at the r.h.s., as well as in the denominator of the correlated Green's function G. In any case this equation shows the connection between the static potential U and the self-energy. To a given approximation for the dynamical self-energy $\tilde{M}$ corresponds a well defined approximation for U.

If one approximates the Green's function G, appearing at the r.h.s. of eq. (13), by the unperturbed $G^{(0)}$, and uses the definition of eq. (7), one gets a linear integral equation ($\phi = 0$),

$$\begin{aligned} U_{ph} = &\sum_{km} \langle kp|f|mh\rangle_A \\ &\times \frac{1}{2\pi i}\int \mathrm{d}\omega \sum_{nl} G^{(0)}_{kn}(\omega)\tilde{M}_{nl}(\omega)G^0_{lm}(\omega) \\ &+ \sum_{nl} U_{nl}\left[\sum_{km}\langle kp|f|mh\rangle_A \right. \\ &\left. \times \frac{1}{2\pi i}\int \mathrm{d}\omega G^{(0)}_{kn}(\omega)G^0_{lm}(\omega)\right]. \end{aligned} \quad (14)$$

Taking for $\tilde{M}$ the considered one-phonon diagram of fig. 2(a), this integral equation coincides with eq. (19) for the tadpole as discussed in refs. [21, 30], and introduced in ref. [31], which is also displayed in fig. 3 of ref. [30]. In the present formalism also the diagram of fig. 2(b) should be included (the so-called "bubble diagram"), in order to avoid double counting [18], while in the TFFS approach the diagram is absent because the phonon is treated as a separate unstructured degree of freedom.

However, the integral equation (35) of refs. [30] contains an additional term in the inhomogeneous part. In the TFFS language, it is coming from the variation of the irreducible Landau interaction amplitude. This term will be discussed later, and it corresponds, in the EDF language, to a three-body force (TBF) for the effective interaction. The tadpole has been extensively discussed in ref. [31] within the framework of the Lagrangian formulation of the TFFS and the corresponding self-consistent relations for the single particle Green's function. Apart the TBF term, one can then identify the potential U with the tadpole of the TFFS. Notice that eq. (13) gives the tadpole to all orders. It can be expanded the same way as the dynamical self-energy $\tilde{M}$.

4 Non-linear coupling and the spurious mode

The particle-vibration coupling scheme can be introduced in a macroscopic picture where the phonon degree of freedom is described by a collective variable [32] α. In this case the interaction part of the Hamiltonian (1) is replaced by

$$H_c = \sum_{\lambda\mu}\sum_{km} g^{km}_{\lambda\mu}\left(\psi^\dagger_k\psi_m\alpha_{\lambda\mu} + C.C.\right), \quad (15)$$

where $\lambda\mu$ labels the collective modes of a given multipolarity and $C.C.$ stands for complex conjugate. It turns out [32] that the coupling constants g in the macroscopic picture can be related to the single particle potential V

$$g^{km}_{\lambda\mu} = \left(k\left|\frac{\partial V}{\partial r}RY_{\lambda\mu}(\Omega)\right|m\right). \quad (16)$$

This expression can be obtained from the first order expansion of the single particle potential if one assumes that it is affected by the vibration $\lambda\mu$ according to

$$\begin{aligned} V(\{\alpha_{\lambda\mu}\}) &= V\left((1+\alpha_{\lambda\mu}Y_{\lambda\mu})R\right) \\ &\approx V(R) + \left(\frac{\partial V}{\partial r}\right)R\alpha_{\lambda\mu}Y_{\lambda\mu} + \cdots. \end{aligned} \quad (17)$$

Higher order terms in the expansion correspond to non-linear coupling, *i.e.* processes where a particle is emitting or absorbing two or more phonons simultaneously. These processes are expected to have a weaker strength. However, as discussed in refs. [30,31], they can be essential to handle the coupling with the spurious mode, *i.e.* the 1^- mode of zero energy that must be present due to the breaking of the translational invariance in the ground state of the nucleus. This coupling generates a divergence in *e.g.* the standard one-phonon diagram of fig. 2(a). It turns out [30,31] that when the phonon corresponds to the spurious one the divergence of the diagram is canceled by an analogous divergence occurring in the tadpole generated by the second order term present in the expansion of eq. (17), which corresponds to a two-phonon coupling. It

has to be noticed that the cancellation is valid if the one-phonon diagram is treated at the perturbative level, *i.e.* its contribution to the self-energy is calculated at the unperturbed single particle energy. If cancellation occurs beyond the perturbative scheme has not been demonstrated yet.

This result suggests that the tadpole could play a role in general for the single particle strength distribution, and it should be included in the single particle self-energy. This was checked in refs. [33–35], where the tadpole was included in the calculations of the single particle energies as perturbed by the coupling with the phonons within the TFFS framework. However the tadpole was calculated by including only the non-linear two-phonon coupling discussed above. The relevance of the tadpole terms generated by the linear coupling, as disussed in the previous section, has still to be explored.

Another point that needs to be analyzed is the dependence of the results from the adopted functional and theoretical scheme. In particular one could wonder if the cancellation of the divergence discussed above within the macroscopic approach is still valid for a general microscopic particle-vibration scheme. We show now that this is indeed the case. Let us start from an Energy Density Functional E and call $\mathcal{V}$ its interaction part. The single particle potential $V(r)$ and the effective two-body interaction $f(r,r')$ can be obtained by functional derivatives of $\mathcal{V}$

$$V(r) = \frac{\delta \mathcal{V}}{\delta \rho(r)}\,,$$
$$f(r,r') = \frac{\delta^2 \mathcal{V}}{\delta \rho(r) \delta \rho(r')}\,, \tag{18}$$

where $\rho(r)$ is the density and r stands for coordinate $\mathbf{r}$ and spin-isospin variables σ, τ. The derivative are taken at the density profile that minimizes the functional. The vertex for particle-vibration coupling to a phonon λ can be written [18]

$$\begin{aligned} F^{\lambda}_{qp} &= \sum_{k_1 k_2} \langle \Psi_0 | \rho^{\dagger}_{k_1 k_2} | \lambda \rangle \langle k_1 q | f | k_2 p \rangle_A \\ &= \sum_{k_1 k_2} \langle \Psi_0 | \rho^{\dagger}_{k_1 k_2} | \lambda \rangle \langle k_1 q | \frac{\delta V}{\delta \rho(r)} | k_2 p \rangle_A, \end{aligned} \tag{19}$$

where

$$\rho^{\dagger}_{k_1 k_2} = \psi^{\dagger}_{k_2} \psi_{k_1}. \tag{20}$$

For a local functional the matrix elements of the force are given by

$$\begin{aligned} &\langle k_1 q | \frac{\delta V}{\delta \rho(r)} | k_2 p \rangle \\ &= \int \mathrm{d}^3 r \phi^*_{k_1}(r) \phi^*_q(r) \frac{\delta V}{\delta \rho(r)} \phi_{k_2}(r) \phi_p(r), \end{aligned} \tag{21}$$

where the integration includes the summation over spin and isospin quantum numbers and the ϕ's are the single particle wave functions. This expression can be generalized to include the exchange term and eventually extended to non-local functionals. If the phonon are described within the RPA, the matrix elements of $\rho^{\dagger}_{k_1 k_2}$, appearing in eq. (20), are just the X and Y amplitudes, in the usual terminology [22]. They are in general obtained solving numerically the RPA equations. However for the spurious phonon they have an explicit form, *i.e.* they are the matrix elements [22] of the gradient operator. In fact they must correspond to the matrix elements of the translation operator

$$\begin{aligned} X_{k_1 k_2} &= N \langle k_1 | \frac{\partial}{\partial \mathbf{r}} | k_2 \rangle, \\ Y_{k_1 k_2} &= -N \langle k_2 | \frac{\partial}{\partial \mathbf{r}} | k_1 \rangle, \end{aligned} \tag{22}$$

where k_1 labels particle states and k_2 hole states and N is the normalization of the state. It turns out that it is diverging [22, 32], since $|X| = |Y|$. This divergence can be traced back to the macroscopic phonon model, where the phonon operator is proportional to the zero-point amplitude [4], which is diverging as the inverse of the mode frequency. For an infinitesimal translation δr the density operator $\hat{\rho}(r) = \psi(r)^{\dagger}\psi(r)$ transforms according to

$$\begin{aligned} T(\delta \mathbf{r})^{\dagger} \hat{\rho}(\mathbf{r}) T(\delta \mathbf{r}) &= \rho(\mathbf{r} + \delta \mathbf{r}) \\ &= \rho(\mathbf{r}) - \delta \mathbf{r} \cdot \left[\frac{\partial}{\partial \mathbf{r}}, \hat{\rho}(\mathbf{r}) \right] + O(\delta r^2), \end{aligned} \tag{23}$$

where T is the translation operator

$$T(\delta \mathbf{r}) = 1 + \delta \mathbf{r} \cdot \frac{\partial}{\partial \mathbf{r}} + O(\delta r^2). \tag{24}$$

Equation (23) implies that the derivative of the density $\rho(\mathbf{r}) = \langle \Psi_0 | \hat{\rho}(\mathbf{r}) | \Psi_0 \rangle$ in the unperturbed ground state Ψ_0 can be written

$$\frac{\partial \rho(\mathbf{r})}{\partial \mathbf{r}} = -\langle \Psi_0 | \left[\frac{\partial}{\partial \mathbf{r}}, \hat{\rho}(\mathbf{r}) \right] | \Psi_0 \rangle. \tag{25}$$

In second quantization the derivative operator can be expanded in terms of a set of single particle states ϕ_k

$$\frac{\partial}{\partial \mathbf{r}} = \sum_{k_1 k_2} \langle k_1 | \frac{\partial}{\partial \mathbf{r}} | k_2 \rangle a^{\dagger}_{k_1} a_{k_2}, \tag{26}$$

where $a^{\dagger}$, a are the corresponding creation and annihilation operators.

Working out the commutator in eq. (25) one gets

$$\begin{aligned} \frac{\partial \rho}{\partial \mathbf{r}} &= -\sum_{k_1 k_2} \langle k_1 | \frac{\partial}{\partial \mathbf{r}} | k_2 \rangle \phi^*_{k_1}(\mathbf{r}) \phi_{k_2}(\mathbf{r}) \left[n(k_1) - n(k_2) \right] \\ &= -\sum_{k_1 k_2} \langle k_1 | \frac{\partial}{\partial \mathbf{r}} | k_2 \rangle \\ &\quad \times \phi^*_{k_1}(\mathbf{r}) \phi_{k_2}(\mathbf{r}) \left[n(k_1)(1-n(k_2)) - n(k_2)(1-n(k_1)) \right], \end{aligned} \tag{27}$$

where $n(k)$ is the occupation numbers for Ψ_0, *i.e.* it is 1 for occupied orbits and 0 for non-occupied ones. If one

applies this relationship to eq. (19), with the help of eqs. (21), (22), one realizes that the derivative with respect to density is replaced by the derivative with respect to r. In fact

$$\begin{aligned} F^{\lambda}_{qp} &= \int \mathrm{d}^3 r \phi^*_q(r) \Bigg(\sum_{k_1 k_2} \langle k_1 | \frac{\partial}{\partial r} | k_2 \rangle \phi^*_{k_1}(r) \phi_{k_2}(r) \\ &\quad \times [n(k_1) - n(k_2)] \Bigg) \frac{\delta V}{\delta \rho(r)} \phi_p(\mathbf{r}) \\ &= -\langle q | \frac{\partial \rho(r)}{\partial r} \frac{\delta V}{\delta \rho(\mathbf{r})} | p \rangle \\ &= -\langle q | \frac{\partial V}{\partial \mathbf{r}} | p \rangle, \end{aligned} \tag{28}$$

where the exchange term has been neglected. It has to be stressed that this result in general holds only for the spurious phonon, since it is a consequence of the particular form (22) of the RPA amplitudes. As explained in ref. [31], with the amplitudes of eq. (28) it is possible to demonstrate that the diagram of fig. 2(a), in the case of the spurious phonon, includes a diverging contribution M^{spur}_q given by

$$M^{spur}_q = \langle q | \Delta V | q \rangle N^2. \tag{29}$$

In fact the analytic expression for the one-phonon diagram of fig. 2(a) can be written

$$M_q(\omega) = \sum_{p\lambda} \frac{A^{\lambda}_{qp}}{\omega - \omega_\lambda - \omega_p + i\eta} + \sum_{h\lambda} \frac{A^{\lambda}_{qh}}{\omega + \omega_\lambda + \omega_h - i\eta}, \tag{30}$$

where

$$A^{\lambda}_{qp} = A^{\lambda}_{pq} = |F^{\lambda}_{qp}|^2 \tag{31}$$

and similarly for A^{λ}_{qh}. In eq. (30) p and h label particle and hole states, respectively, and the ω's are the single particle energies. If the phonon λ is the spurious mode, then $\omega_\lambda = 0$ and the vertex F is given by eq. (28). One can then use the identity ($\omega = \omega_q$)

$$\langle q | \frac{\partial V}{\partial \mathbf{r}} | i \rangle (\omega_q - \omega_i)^{-1} = \langle q | \frac{\partial}{\partial \mathbf{r}} | i \rangle, \tag{32}$$

which can be derived from the HF equations, and the resulting relationship

$$\sum_i \langle q | \frac{\partial}{\partial \mathbf{r}} | i \rangle \langle i | \frac{\partial V}{\partial \mathbf{r}} | q \rangle = \langle q | \Delta V | q \rangle, \tag{33}$$

which gives the self-energy of eq. (29). It has the same form as the contribution to the self-energy originating from the two-phonon second order term in the expansion of eq. (17), and indeed the two contributions cancel out provided the same (diverging) normalization is used. After eliminating the divergence one gets from the one-phonon diagram a finite term that is related to the center of mass correction [22,31,34].

This result is actually valid for a general Energy Density functional. In this case, instead of the second order term in expansion (17), one has to consider the third derivative with respect to density of the interaction part $\mathcal{V}$ of the functional, which indeed gives rise to two-phonon processes. Following the same procedure described above for the one-phonon diagram, one can replace the derivatives with respect to the density with the derivative with respect to the coordinate r and get a term of the form (29). As mentioned above, this corresponds to the additional inhomogeneous term contained in the TFFS integral equation for the tadpole [30].

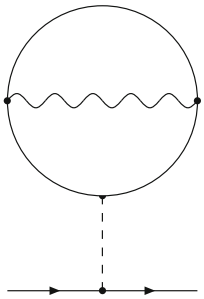

Fig. 5. One phonon contribution to the tadpole of eq. (34).

We stress again that this cancellation is valid only if the one-phonon diagram is evaluated at perturbative level. For a non-perturbative approach, *e.g.* considering the energy dependent Dyson equation, the cancellation can be only approximate. To our knowledge an exact treatment of the spurious mode in this general case has not been formulated and further developments are needed to handle the divergence.

5 Meaning and estimate of the tadpole

At the mean field level the single particle occupation numbers are necessarily 1 or 0. However the effective mean field produced by an effective force should take into account that correlations introduce fractional occupation numbers. Even at static level this modifies the mean field with respect to the HF approximation [36]. We will show now that the tadpole represents the terms of the expansion that take into account this effect. This will also allow for an estimate of the size of the tadpole. We will calculate the tadpole from eq. (14) for a generic single particle state, once the effect of the spurious mode has been properly handled. Let us consider the first term on the r.h.s., corresponding to the diagram of fig. 5 and assume that the Green's function G and the self-energy $\tilde{M}$ are diagonal in the single particle index

$$U_p = \sum_k \langle kp | f | kp \rangle_A \frac{1}{2\pi i} \int \mathrm{d}\omega \left[G^{(0)}_k(\omega) \right]^2 \tilde{M}_k(\omega). \tag{34}$$

Notice that the self-energy M_k includes the summation over the multipolarity of the possible phonons. The factor $[G^{(0)}(\omega)]^2$ has double poles both in the upper half of the energy plain (hole states) and in the lower half plain (particle states). The self energy $\tilde{M}(\omega)$, as it can be seen

from eq. (30), can be split into a component $M^{(1)}$ that has simple poles in the upper half plain, and a component $M^{(2)}$ that has poles in the lower half plain. Applying the residue theorem for double poles, one then gets

$$U_p = \sum_{k<k_F} \langle kp|f|kp\rangle_A \left(\frac{\partial M_p^{(2)}(\omega)}{\partial\omega}\right)_{\omega=-\omega_k} - \sum_{k>k_F} \langle kp|f|kp\rangle_A \left(\frac{\partial M_p^{(1)}(\omega)}{\partial\omega}\right)_{\omega=\omega_k} . \quad (35)$$

In the case of the tadpole diagram of fig. 5 this expression includes all time ordering. It can be verified that if one replaces the phonon propagator by a single particle-hole propagator this contribution to the self-energy reduces to the diagrams M_3 of refs. [36,37].

As it is well known [37,38], the derivative of the self-energy at the unperturbed single particle energy should be negative and it gives the first order depletion of the hole states and the population of the particle states due to the correlations beyond the mean field approximation. In fact the correlated occupation numbers $\overline{n}_p$ can be calculated from the Green's function [39]

$$\overline{n}_p = \int \frac{\mathrm{d}\omega}{2\pi i} G_p(\omega) e^{i\omega\delta}, \quad (36)$$

where $\delta \to 0^+$. The exponential factor assures the convergence of the integral, which can be computed by closing the integration path in the upper complex plain. Expanding the Green's function to first order in the self-energy, one gets

$$\overline{n}_p = \int \frac{\mathrm{d}\omega}{2\pi i}\left[G_p^0(\omega) + \left(G_p^0(\omega)\right)^2 M_p(\omega)\right] e^{i\omega\delta} = n_p + \left(\frac{\partial M_p^{(2)}(\omega)}{\partial\omega}\right)_{\omega=-\omega_p} - \left(\frac{\partial M_p^{(1)}(\omega)}{\partial\omega}\right)_{\omega=\omega_p} . \quad (37)$$

In eq. (37) n_p is the mean field occupation number, *i.e.* it is 1 for occupied orbital and 0 for the non-occupied ones. The explicit expression for the $\overline{n}_p$ can be found within the approximation of eq. (30)

$$\overline{n}_p = n_p + \sum_{q\lambda} \frac{1}{(\omega_p+\omega_q+\omega_\lambda)^2} \times \left[-A^\lambda_{pq}(1-n_q)n_p + A^\lambda_{qp} n_q (1-n_p)\right]. \quad (38)$$

It has to be noted that the total number of particle is not affected by the correlations

$$\sum_p \overline{n}_p = \sum_p n_p \quad (39)$$

i.e. the Luttinger theorem [40] is satisfied, despite the fact that the formalism is not grand canonical as in the original formulation [40]. One consequence of this property is that for an effective force with constant matrix elements the tadpole vanishes. In particular this is true in nuclear matter with a momentum independent Skyrme force.

The tadpole is therefore determined by the variation of the occupation numbers produced by the correlations. This is in line with ref. [36], where it is shown that the static part of the self-energy, *i.e.* the energy independent contribution in the perturbative expansion, is related to the modification of the occupation number due to correlations.

Typical values of the depletion are around 0.1–0.2 [37, 38,41,42], depending on the orbitals, and therefore one can expect that the order of magnitude of the tadpole term is 10–20% of the average particle-hole matrix element. Of course compensations between positive and negative contributions can occur, and indeed in *e.g.* ^{208}Pb the tadpole contribution to the proton single particle energies turns out to be quite small [33]. However, as it has been shown within the TFFS scheme, the contribution can be relevant for the assignment of the single particle levels [42] and the odd-even double mass differences [43,44].

One has also to keep in mind that the fragmentation of the single particle states can play a role. Furthermore, as already discussed, the tadpole can include for a generic orbital the contribution from a possible non-linear particle-vibration coupling, as it can result from an expansion of the functional up to the third order in the density variation.

6 Ground state correlations

According to the Koltun sum rule [22] the correlation energy E_c beyond the mean field can be written

$$E_c = -\frac{1}{2} i \sum_{rs} \int \frac{\mathrm{d}\omega}{2\pi} M_{rs}(\omega) G_{sr}(\omega), \quad (40)$$

where the integral has to be closed in the upper half of the energy plain. Fo simplicity let us take the self energy as diagonal and calculated up to the one phonon contribution, both for the dynamical term of fig. 2(a) and the tadpole term of eq. (35). Accordingly, the Green's function of eq. (40) is calculated at the mean field level. Following the splitting of eq. (7), the static term gives just the sum over the tadpole corrections to the occupied single particle energy. The contribution of the second dynamical term for the self-energy in eq. (7) can be calculated employing the explicit expression of eq. (30). Finally one gets

$$E_c = \sum_{r<k_F} U_r - \sum_{rs} \frac{A^\lambda_{rs}}{\omega_r+\omega_s+\omega_\lambda} \quad (41)$$

where the tadpole term U_r is given by eq. (35) and the second summation runs over the particle-hole pairs. The latter contribution can be depicted with the diagram of fig. 6, which emphasizes how the ground state correlations have a direct effect on the single particle states and the direct link between single particle self-energy and the ground state energy beyond the mean field.

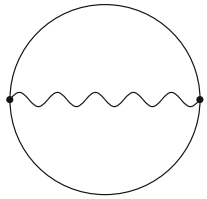

Fig. 6. Diagrammatic picture of the one phonon contribution to the ground state correlation energy beyond mean field.

In the limit of weak collectivity of the phonon, *i.e.* when the particle-hole correlation of the phonon is small with respect to the unperturbed particle-hole excitation energy, the denominator in the second term is of the order of the matrix elements of the effective interaction. It can be expected that the particle-vibration coupling F^λ in the numerator is of the same order and therefore the second term should be of the order of F^λ.

Notice that for the self-energy M one should include also the so called bubble subtraction [18], which gives a final additional contribution to the correlation energy E_c at this order. Its explicit expression can be easily derived along the same lines.

7 Summary and conclusions

In this paper we developed further the many-body theory of ref. [18] of single particle states within the Energy Density Functional method. In this approach one introduces an energy functional which is fitted to reproduce the ground state energy and radii of nuclei throughout the mass table. The method has been very successful and it has been extended to calculate the excited states of nuclei, in particular the giant resonances. In this scheme the ground state energy is calculated within a mean field formalism, which takes the form of Hartree-Fock equations with an effective force.

The calculations generate a set of single particle levels, which is tempting to identify with the physical single particle states that can be extracted from the analysis of *e.g.* one particle transfer reactions. However this is not obvious, since within the EDF method the HF levels are effective ones, introduced merely to minimize the ground state energy. Indeed it turns out that the comparison of the HF levels with the observational data on single particle states is not particularly favorable, even if the ground state energy is well reproduced.

One possible explanation of this drawback is that the HF levels miss some additional correlations, in particular the coupling between the single particle degrees of freedom with the excited states (phonon) of the parent nucleus, the so-called particle-vibration coupling scheme. This particular correlation is systematically developed in ref. [18] and in the present paper within the functional derivative method based on the Green's function formalism. The theory is microscopic since the phonon degrees of freedom are introduced through the particle-hole propagator in a self-consistent scheme, in line with the so-called conserving approximations.

In this work we have shown that the particle-vibration correlation generates, besides the energy dependent single particle self-energy, also an energy independent (*i.e.* static) contribution. It turns out that this contribution, calculated at the lowest order of approximation, coincides with the so called "tadpole" term, first introduced in the Theory Finite Fermi System [10], where the phonon degree of freedom is treated as a separate one, *i.e.* unstructured. In the TFFS scheme calculations of the tadpole has shown that its contribution can be relevant for the energy centroid of the single particle states and for physical quantities like the odd-even double mass differences [42–44].

The introduction of additional correlations for the single particle states in principle demands for consistency that the same correlation is introduced in the calculation of the ground state energy, which would mean a modification of the EDF. Towards the solution of this problem we have calculated and estimated the additional contribution to the ground state energy at the same first order of approximation used for the single particle states.

In conclusion we established a link between the formalism presented in ref. [18] and the TFFS formalism for the particle-vibration coupling scheme. According to both theories the correction to the single particle energies receives a contribution of dynamical character (energy dependent self-energy) as well as a static contribution (tadpole) which is energy independent. Accordingly the EDF should be corrected by the effect of the particle-vibration coupling. The relevance of this correction on the EDF estimate of the ground state energy can be assessed only by numerical calculations.

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Data Availability Statement This manuscript has no associated data or the data will not be deposited. [Authors' comment: The paper is of theoretical chracter and the data are all contained in the text.]

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