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NUCLEAR FIELD THEORY AS A METHOD
OF ELIMINATING SPURIOUS STATES

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**NUCLEAR FIELD THEORY AS A METHOD
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Теория ядерных полей как метод устранения духовых состояний

Показано, что в рамках ядерно-полевого рассмотрения остаточного взаимодействия можно устранить довольно простым образом большое число духовых состояний, появляющихся при использовании одночастичного, не сохраняющего симметрию, базиса.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

Препринт Объединенного института ядерных исследований. Дубна 1977

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Nuclear Field Theory as a Method of Eliminating Spurious States

It is shown that within the nuclear field treatment of the residual interaction a great deal of the spurious components involved when using a symmetry violating single particle basis can be eliminated in a simple manner.

The investigation has been performed at the Laboratory of Theoretical Physics, JINR.

Preprint of the Joint Institute for Nuclear Research, Dubna 1977

In nuclear theory one frequently uses a single particle basis which violates some symmetry of the real system. For instance the superfluid nuclei are usually described in the Bogolyubov quasiparticle representation which does not conserve the particle number. Further for the description of deformed nuclei one usually starts from deformed single particle states. Even the spherical shell model violates the translational invariance. In all these cases the use of the symmetry violating single particle basis is advantageous. However, such a basis includes a lot of spurious components which are mixed with the true physical excitation states. Thus, one is almost always faced with the problem of eliminating these spurious states. In the present paper we show that within the nuclear field theory (NFT)^{1,2,3/} a great deal of the spurious components can be eliminated in a very simple manner.

In the NFT the nuclear many-body system is described in terms of Feynman diagrams involving both fermion and (collective) phonon degrees of freedom. The rules for the diagrammatic field treatment have been found in ref.^{1/}. The many-body foundation of the NFT has been given in refs.^{2,3/}. As has been stated in ref.^{1/}, the energies of the uncoupled particle fields must con-

tain the Hartree-Fock contribution from the two-body residual interaction. Therefore, if the two-body interaction produces in the Hartree-Fock approximation* a stable shape deformation or a superconducting gap the nuclear field description has to be carried out in the corresponding symmetry violating single particle basis. However, for such cases where the single particle states violate some symmetry property of the real system the equivalence between the conventional Feynmann diagrammatic perturbation treatment and the nuclear field treatment of the residual interaction has not been proved yet. To fill this gap is one of the aims of the present paper. In the following we shall show that the equivalence between both treatments can also be established in the case under consideration where the single particle states do not possess the correct symmetry. Moreover, in showing this we shall see that even a more advantageous description can be obtained within the NFT if one gives up the one-to-one correspondence between both treatments. Then a large part of the involved spurious components can be excluded in the field treatment. This is not only a matter of convenience, but as we shall demonstrate below, there are cases where we have by all means to give up this correspondence in order to obtain physically meaningful results within the NFT. On the contrary, the conventional many-body diagrammatic perturbation theory

* Here the term Hartree-Fock approximation is used in its most general sense. Especially it relates also to the so-called Hartree-Fock-Bogolyubov approximation.

in these cases yields unphysical divergences which are nothing but a consequence of the spurious states involved.

In the NFT the collective modes are utilized as a convenient representation for the partial sums over definite diagram classes. For normal systems, i.e., where the residual interaction does not produce either a stable "shape" deformation or a superconducting gap it has been shown in refs.^{/4,2/} that there exists a holomorphic mapping between the bubble strings of the Feynman-Goldstone diagram formalism and the phonon images of the diagrammatic nuclear field treatment: the bubble diagrams are correctly described by the exchange of the RPA phonons provided all RPA modes are taken into account. Thus the bubble graphs must be disregarded in the NFT (see refs.^{/1,2,3/}). However, if the two-body residual interaction produces a symmetry violating average field, there exists a spurious $\omega=0$ RPA solution and the RPA solutions do not form a complete set (the basis is short by one, see, e.g., ref.^{/5/}). But the completeness of the RPA solutions was a crucial assumption in the proof of the equivalence between the nuclear field and the fermion treatment of the residual interaction given in refs.^{/4,2/}. On the other hand, just in this case where the single particle states do not possess the correct symmetry the use of the RPA modes in a field treatment would be very advantageous. This is because the RPA includes enough of the residual interaction to restore the symmetry. Further, the RPA is probably the only

useful method for defining the collective modes employed in the field treatment; on the one hand, the RPA is simple enough that the corresponding microscopic calculation can be carried out and, on the other hand, it includes enough of the residual interaction that the NFT expansion converges sufficiently fast. Therefore, for practical applications it is of great interest to establish the nuclear field treatment with RPA modes also for such systems where the residual interaction leads to a symmetry violating average field. For this purpose we have to tackle the problems connected with the presence of a spurious RPA solution, e.g., the non-completeness of the RPA eigenvectors. Therefore in sect. 2 we recall some features of the RPA in the presence of a spurious state. In sec. 3 we establish the nuclear field treatment for such systems where the residual interaction produces a symmetry violating average field. A short summary is given in sec. 4.

2. THE RANDOM PHASE APPROXIMATION

For handling the spurious solution it is convenient to cast the RPA equations (see eq. (2.5) of ref. ^{12/}) in the form

$$\begin{pmatrix} \omega_n & -A^- \\ -A^+ & \omega_n \end{pmatrix} \vec{x}_n = 0, \quad \begin{pmatrix} \omega_n & A^- \\ A^+ & \omega_n \end{pmatrix} \vec{y}_n = 0, \quad \omega_n > 0, \quad (1)$$

where

$$\vec{x}_n = \begin{pmatrix} r_n^+ \\ r_n^- \end{pmatrix}, \quad \vec{y}_n = \begin{pmatrix} -r_n^- \\ r_n^+ \end{pmatrix},$$

$$r_n = \frac{1}{\sqrt{2}} (x_n^+ \pm x_n^-),$$

$$A_{ab}^{\pm} = \epsilon_a \delta_{ab} + A_{ab} \pm B_{ab} . \quad (2)$$

The quantities x_n^{\pm} , A_{ab} , B_{ab} and ϵ_a have been defined in ref./2/. The matrices A and B are given by the matrix elements of the residual interaction while x_n^+ and x_n^- are the vectors of the forward and backward RPA amplitudes, respectively. The quantity ϵ_a denotes the Hartree-Fock energies of independent two-quasiparticle configurations which are labelled by the subscript a. The subscript n denotes the different RPA modes with frequency ω_n . As eqs. (1) represent a non-symmetric eigenvalue problem we have also to consider the l.h.s. eigenvectors

$$\vec{X}^n = \begin{pmatrix} r_n^- \\ r_n^+ \end{pmatrix}, \quad \vec{Y}^n = \begin{pmatrix} r_n^+ \\ -r_n^- \end{pmatrix}$$

which are orthogonal to the r.h.s. eigenvectors *

$$\vec{X}_n^t \vec{x}_m = \delta_{nm}, \quad \vec{Y}_n^t y_m = -\delta_{nm}, \quad (3)$$

$$\vec{X}_n^t \vec{Y}_m = \vec{Y}_n^t \vec{x}_m = 0.$$

For existing a spurious solution (which we denote by $n=0$) with $\omega_0=0$ we must have

$$\det(A^+) \det(A^-) = 0. \quad (4)$$

* The letter "t" denotes the transposed quantities.

From the structure of the matrices A^\pm (see eqs. (2)) it is clear that both determinants in eq. (4) cannot vanish simultaneously.

Let us suppose that

$$\det(A^-) = 0, \quad \det(A^+) \neq 0$$

(This is the case for the $J=0$ channel of superfluid nuclei). The spurious solution of eq. (1) is then of the form

$$\tilde{X}_0 = \begin{pmatrix} r_0^- \\ 0 \end{pmatrix}, \quad \tilde{x}_0 = \begin{pmatrix} 0 \\ r_0^- \end{pmatrix}$$

and has zero norm:

$$\tilde{X}_0^t \tilde{x}_0 = 0. \quad (5)$$

The spurious solution is also orthogonal to the remaining RPA eigenvectors with $\omega_n \neq 0$

$$\tilde{X}_{n>0}^t \tilde{x}_0 = \tilde{Y}_{n>0}^t \tilde{x}_0 = \tilde{X}_0^t \tilde{x}_{n>0} = \tilde{X}_0^t y_{n>0} = 0. \quad (6)$$

The vectors $\tilde{x}_0, \tilde{x}_{n>0}, \tilde{y}_{n>0}$ (and analogously the vectors $\tilde{X}_0, \tilde{X}_{n>0}, \tilde{Y}_{n>0}$) do not form a complete set. However, as was shown by Thouless^{6/}, one can construct a complementary vector $\tilde{v}(\tilde{V})$ orthogonal to the RPA eigenvectors with non-zero frequency

$$\tilde{V}^t \tilde{x}_{n>0} = \tilde{V}^t \tilde{y}_{n>0} = \tilde{X}_{n>0}^t \tilde{v} = \tilde{Y}_{n>0}^t \tilde{v} = 0 \quad (7)$$

in order to make the system of RPA eigenvectors complete. In our representation this vector is explicitly given by:

$$\tilde{V} = \begin{pmatrix} 0 \\ v^+ \end{pmatrix}, \quad \tilde{v} = \begin{pmatrix} v^+ \\ 0 \end{pmatrix},$$

where

$$v^+ = (A^+)^{-1} r_0^-.$$

For convenience we choose the normalization

$$r_0^{-1} v^+ = 1. \quad (8)$$

Then it follows

$$\tilde{X}_0^t \tilde{v} = \tilde{V}^t \tilde{x}_0 = 1, \quad \tilde{V}^t \tilde{v} = 2. \quad (9)$$

We are now in a position to establish the relation between the nuclear field treatment of the residual interaction and the Feynman-Goldstone diagram formalism when the perturbation-theoretic approach is performed in a symmetry violating single particle basis.

3. THE NUCLEAR FIELD TREATMENT

Like in ref.^{/2/} we denote the so-called interaction part (see, e.g., ref.^{/7/}) involving, besides the direct two-body interaction, only bubble diagrams by $T^{\text{RPA}}(\omega)$ (see fig. 1(a)). Here ω denotes the energy parameter associated with the two-body interaction \mathbf{V} in the propagator formalism (Green function method)^{/7/}. The partial summation over the bubble diagrams can be carried out explicitly. Using eq. (3.1) of ref.^{/2/} the result can be written as*

$$T^{\text{RPA}}(a\beta\gamma\delta, \omega) = \langle a\beta | \mathbf{V} | \gamma\delta \rangle + T^c(a\beta\gamma\delta, \omega),$$

* Like in ref.^{/2/} the Hartree-Fock single particle states are labelled by Greek letters α, β, \dots

(d)

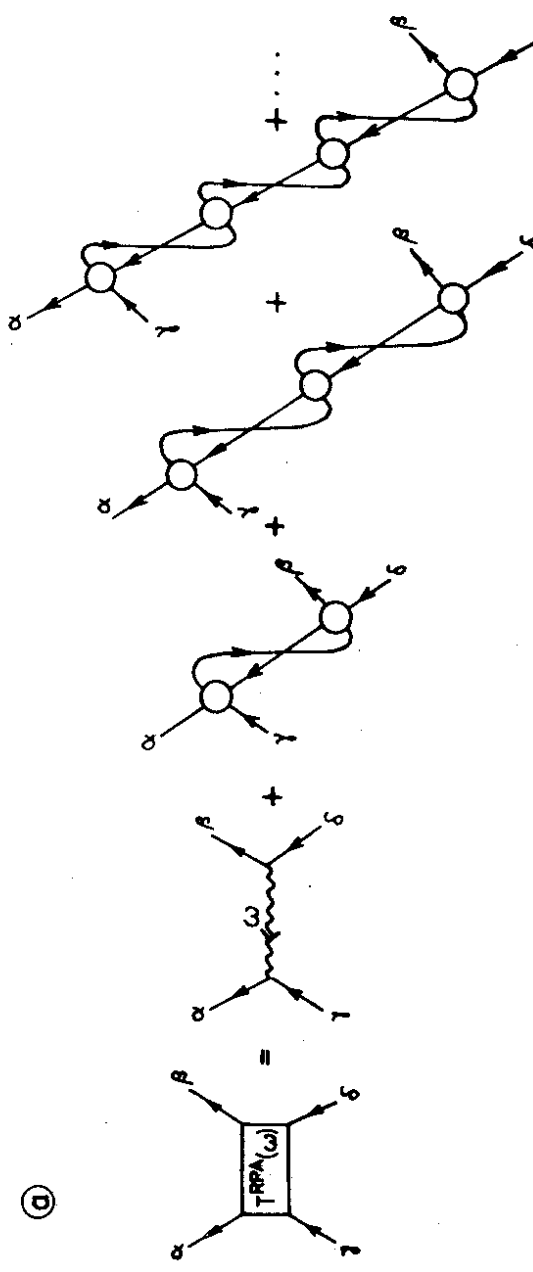


Fig. 1a. Graphical representation of the interaction part in the random phase approximation, $T\text{RPA}(\omega)$, which contains, besides the direct two-body interaction V illustrated by the wavy line, only bubble diagrams. The open circle represents the antisymmetrized matrix element of the two-body interaction. The single particle propagators represented by a full line are chosen in such a way that the backward going bubble strings are already included in the forward going ones.

where the collective interaction part $T^c(\omega)$ which stands for the partial sum over the bubble diagrams reads

$$T^c(a\beta\gamma\delta, \omega) = \mathbf{V}_{a\gamma}^{L^t} \sigma \begin{pmatrix} \omega & -A^- \\ -A^+ & \omega \end{pmatrix}^{-1} \sigma^t \mathbf{V}_{\beta\delta}^R, \quad (10)$$

where

$$\sigma = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}, \quad \tau = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

The vectors $\mathbf{V}_{a\gamma}^L$, $\mathbf{V}_{\beta\delta}^R$ have been defined in ref. /2/. Their components are given by the matrix elements of the residual interaction $\langle a\beta | \mathbf{V} | \gamma\delta \rangle$. Including the complementary vector $\tilde{\mathbf{v}}(\tilde{\mathbf{V}})$ from the RPA eigenvectors we can construct two nonsingular matrices

$$R = \tilde{\mathbf{x}}_0 \tilde{\mathbf{e}}_0^t + \tilde{\mathbf{v}} \tilde{\mathbf{e}}_p^t + \sum_{n>0} (\tilde{\mathbf{x}}_n \tilde{\mathbf{e}}_n^t + \tilde{\mathbf{y}}_n \tilde{\mathbf{e}}_{p+n}^t),$$

$$S = \tilde{\mathbf{X}}_0 \tilde{\mathbf{e}}_0^t + \tilde{\mathbf{V}} \tilde{\mathbf{e}}_p^t + \sum_{n>0} (\tilde{\mathbf{X}}_n \tilde{\mathbf{e}}_n^t + \tilde{\mathbf{Y}}_n \tilde{\mathbf{e}}_{p+n}^t)$$

by means of which we can find the pole decomposition of the interaction part $T^{RPA}(\omega)$ which is needed for its NFT representation*. With the help of the matrices R, S the collective interaction part $T^c(\omega)$ (see eq. (10)) can be written as

$$T^c(a\beta\gamma\delta, \omega) = \mathbf{V}_{a\gamma}^{L^t} \sigma R [S^t \begin{pmatrix} \omega & -A^- \\ -A^+ & \omega \end{pmatrix}^{-1} S^t \sigma^t \mathbf{V}_{\beta\delta}^R.$$

Making use of the RPA equations (1) and the orthogonality relations (3), (5), (6), (7) and using further the normalization (8)

* The quantities $\tilde{\mathbf{e}}_n$ ($n=0,1,\dots,2p-1$) are unit vectors in the $2p$ -dimensional vector space spanned by the RPA eigenvectors $\tilde{\mathbf{x}}_0, \tilde{\mathbf{x}}_{n>0}, \tilde{\mathbf{y}}_{n>0}$ ($\tilde{\mathbf{X}}_0, \tilde{\mathbf{X}}_{n>0}, \tilde{\mathbf{Y}}_{n>0}$) and the complementary vector $\tilde{\mathbf{v}}(\tilde{\mathbf{V}})$.

and (9) after some algebraic manipulations we arrive at the desired NFT representation of the interaction part

$$T^{\text{RPA}}(a\beta\gamma\delta, \omega) = \langle a\beta | \mathbf{V} | \gamma\delta \rangle + T^{\text{S}}(a\beta\gamma\delta, \omega) + T^{\text{C}'}(a\beta\gamma\delta, \omega) \quad (11)$$

which is displayed in fig. 1b. The quantities $T^{\text{S}}(\omega)$ and $T^{\text{C}'}(\omega)$ are defined by

$$T^{\text{S}}(a\beta\gamma\delta, \omega) = \mathbf{V}_{\alpha\gamma}^{L,t} \sigma [(\tilde{\mathbf{x}}_0 \tilde{\mathbf{V}}^t + \tilde{\mathbf{v}} \tilde{\mathbf{X}}_0^t - 2\tilde{\mathbf{x}}_0 \tilde{\mathbf{X}}_0^t) \frac{1}{\omega} + \\ + \tilde{\mathbf{x}}_0 \tilde{\mathbf{X}}_0^t \frac{1}{\omega^2}] \sigma \tau \quad \mathbf{V}_{\beta\delta}^{\text{R}}$$

$$T^{\text{C}'}(a\beta\gamma\delta, \omega) = \sum_{n>0} \mathbf{V}_{\alpha\gamma}^{L,t} \sigma [\tilde{\mathbf{x}}_n^t D_n^+(\omega) \tilde{\mathbf{X}}_n^t + \tilde{\mathbf{y}} D_n^-(\omega) \tilde{\mathbf{Y}}_n^t] \sigma \tau \mathbf{V}_{\beta\delta}^{\text{R}} \\ = \sum_{n>0} [\Lambda_{\alpha\gamma}^n D_n^+(\omega) \Lambda_{\delta\beta}^n + \Lambda_{\gamma\alpha}^n D_n^-(\omega) \Lambda_{\beta\delta}^n] ,$$

where

$$D_n^{\pm}(\omega) = \frac{1}{\pm \omega - \omega_n + i\delta}$$

are the propagators of the RPA phonons with non-zero frequency. The quantity $\Lambda_{\alpha\gamma}^n$ denotes the particle-phonon vertex which has been also defined in ref.^{/2/} Eq. (11) proves the eigenvalence between the usual fermion and the nuclear field treatment of the residual interaction for such systems where the two-body interaction produces a symmetry violating average field and which should, consequently, be described in the corresponding symmetry violating single particle basis (see also the discussion following eq. (3.8) of ref.^{/2/}). Besides the term $T^{\text{C}'}(\omega)$ involving the phonon propa-

(b)

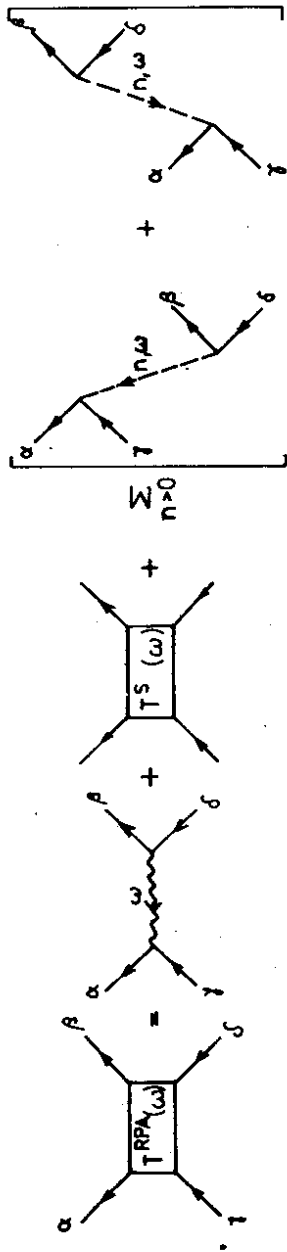


Fig. 1b. Equivalent representation of the interaction part $T^{RPA}(\omega)$ in the NFT. The bubble diagrams of the fermion treatment shown in (a) are described in the NFT by the exchange of the non-zero frequency RPA modes, $D_n^+(\omega)$, (dotted line) plus a four pole term $T^s(\omega)$ illustrated by a rectangle which contains all the spurious correlations involved in the bubble diagrams.

gators $D_n^\pm(\omega)$, which is already known from the NFT for systems having a non-symmetry violating average field, the interaction part contains now a pole term $T^s(\omega)$ arising from the spurious RPA solution ($\omega_0=0$). In calculating the physical properties of the system under consideration this term should be excluded from the interacting part in powers of which the nuclear field expansion is carried out. The explicit separation of the terms resulting from the spurious components, $T^s(\omega)$, and those describing the propagation of true internal excitation modes $T^c(\omega)$ which is obtained here in the NFT representation (11) of the interaction part $T^{RPA}(\omega)$, is by no means a trivial result. It is a consequence of the RPA which "picks out" all the spurious correlations contained in the bubble diagrams and gathers them together to form a spurious $\omega_0=0$ solution which is orthogonal to the remaining non-zero frequency RPA modes ($\omega_n \neq 0$) which, consequently, do not contain any spurious component at all. Hence, all the spurious correlations involved in those Feynman diagrams which are replaced in the field treatment by a combination of collective modes, are automatically eliminated if we exclude the poles corresponding to the spurious $\omega_0=0$ RPA solutions from the NFT representation of the interaction part $T^{RPA}(\omega)$. In this way the NFT eliminates a great deal of the spurious components introduced by the frequently used symmetry violating single particle basis provided the collective modes are appropriately chosen. (We note in this respect that the clear separation of the spurious correlations from

the correlations involved in the true internal excitations were not obtained if the collective modes would be defined in the Tamm- Dankoff approximation). In contrast, in the ordinary many-body perturbation treatment which is carried out exclusively in the fermion basis the spurious components are always mixed with the true physical excitations and there is no "recipe" how to exclude the spurious excitations. Thus, a new advantage of the NFT over the conventional Feynman diagrammatic many-body perturbation theory comes out in the description of finite nuclear systems when some symmetry is violated by the used single particle basis. Note, however, that although in the NFT the spurious correlations are completely eliminated from the interaction part $T^{RPA}(\omega)$ there are still spurious components involved because the field treatment is partly carried out in the fermion basis. Nevertheless, the spurious components involved in a nuclear field description should be by far smaller than the ones contained in the corresponding fermion treatment. This is because the collective modes used in the field treatment are built up just from the most divergent diagrams (bubble diagrams), from which the nuclear field treatment removes all spurious correlations.

We stress, once more, the fact that if the pole term $T^s(\omega)$ corresponding to the spurious mode is excluded from the NFT representation of the interaction part $T^{RPA}(\omega)$ in order to eliminate the spurious correlations, the nuclear field and the fermion treatment of the residual interaction are no longer equivalent. The NFT is superior:

its diagrams contain by far less spurious correlations.

We should further emphasize that in the fermion treatment some divergent diagrams appear whereas the divergences are nothing more than a consequence of the involved spurious excitations and therefore they have no physical meaning. On the contrary, in the NFT the pole terms arising from the spurious excitations, are excluded from the beginning and the corresponding diagrams do not show such an unphysically divergent behaviour. As an illustrative example let us consider the diagrams shown in fig. 2a. For superfluid nuclei they contribute in leading order to the energy of the quasi-particle $(J=0)$ phonon state (see ref. ^{18/}). If we carry out the partial summation over the bubble graphs we get an infinite result. In contrast, the corresponding diagrams (see fig. 2b) of the field treatment which excludes the spurious correlations involved in the bubble diagrams yield quite finite contributions.

4. SUMMARY

The results of the present paper can be summarized in the following way: the NFT provided us with a correct many-body description even when using a symmetry violating single particle basis. Moreover, in this case a new decisive advantage of the NFT over the conventional Feynman diagrammatic many-body perturbation theory emerges which consists in the fact that the NFT removes a great deal of spurious components. As

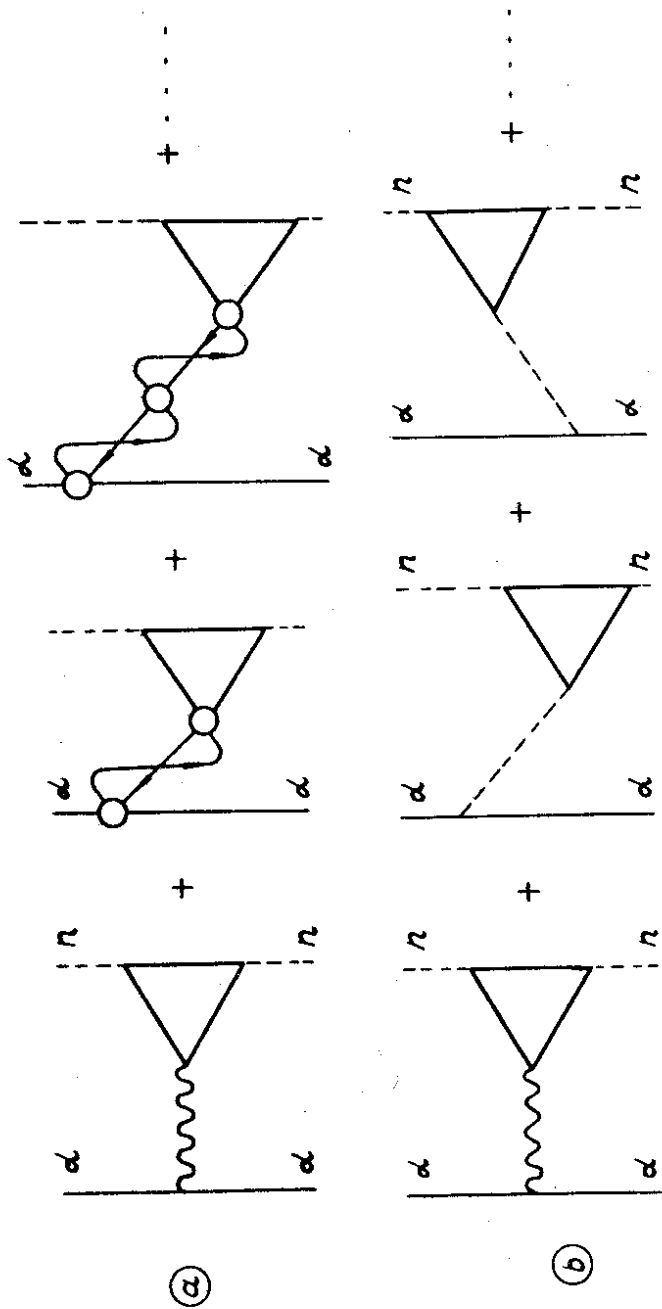


Fig. 2. (a) Feynman diagrams contributing in leading order to the energy of the quasiparticle-phonon state. They give divergent contributions due to the spurious correlation involved in the bubble graphs. (b) in the corresponding nuclear field representation the unphysical poles are removed.

a consequence, in such cases where the conventional many-body perturbation theory yields unphysical poles corresponding to spurious excitations, the nuclear field treatment gives automatically the physically meaningful, finite results.

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