Treatment of the random-phase-approximation including continuum

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The random-phase approximation has been treated in two steps: (a) First, we solve the so-called nuclear structure problem in which the single particle continuum states are excluded. (b) In the second part, we include the continuum utilizing a reformulated version of the random-phase approximation which uses the outcome of the nuclear structure method as an input. Thus the effect of the continuum is directly estimated. Below threshold the excitation energies are shifted; above threshold they obtain additionally a width. Numerical results are presented for ^{16}O and ^{16}N.

[NUCLEAR STRUCTURE RPA calculations for ^{16}O and ^{16}N including continuum.]

In the last years several attempts have been made to include the continuum in the shell-model treatments of nuclear structure and reactions, where in most cases the Tamm-Dancoff-approximation (TDA) has been used.[1] But with respect to numerical expenditure and transparency, the situation is still not very satisfactory.[2] Therefore, we discuss in this investigation a simplified approach, which may also give an adequate estimate of the continuum contributions. We are going to follow the procedure of Ref. 3, in which the random-phase approximation (RPA) problem was reformulated in such a manner that one could use the conventional nuclear structure solution as input for the full problem. The theoretical formulation was worked out in the framework of linear response theory and will not be repeated here in detail. We refer to Ref. 3 in the standard manner, e.g., (W.I.1) means Eq. (I.1) of Ref. 3.

The equations of motion for the quasiparticle matrix between the ground and excited states have the following structure (W.I.12):

$$\tilde{\rho}_{\nu\mu,M}=(n_\nu-n_\mu)[E_M+\epsilon_\mu-\epsilon_\nu-i\eta(n_\nu-n_\mu)]^{-1}\times\left[\delta_{\rho\nu}\delta_{j\mu}(-i\eta)-2\pi\sum_{\lambda\sigma}\tilde{I}_{\nu\sigma\mu\lambda}(\omega)\tilde{\rho}_{\lambda\sigma,M}\right], \quad (1)$$

where the renormalized amplitude is defined by (renormalized quantities are denoted by a tilde)

$$\tilde{\rho}_{\nu\mu,M}\equiv(z_\nu z_\mu)^{-1/2}\langle 0|\psi^\dagger_\mu\psi_\nu|M\rangle. \quad (2)$$

Here, $\tilde{I}$ is the effective p-h interaction (irreducible vertex in the p-h channel). The theory is renormalized according to Migdal's quasiparticle concept, and z_μ denotes Migdal's renormalization constant.[4]

In Eq. (1), $|M\rangle$ denotes a scattering state $|S\rangle$ [defined by the incoming particle with momentum p and (continuous) energy ϵ_p] or a bound state $|B\rangle$ [with the (discrete, complex) energy E_B], respectively.

In the conventional RPA calculation Eq. (1) is diagonalized in a finite space by restricting the single particle states to (quasi) bound state only. Since solutions of such kind are known for many forms of the p-h interaction, we assume for the further procedure that these model states $|n\rangle$ are given. The corresponding phonon creation operator is denoted by $C^\dagger_n$ with $C^\dagger_n|0\rangle=|n\rangle$; $C_n|0\rangle=0$; with amplitudes $\tilde{\rho}_{\mu\nu,n}$.

In order to obtain a full solution for the amplitudes of Eq. (1) with inclusion of the continuum, we split the remaining problem into two parts: (a) the determination of the overlap of the true states with the model, $\langle 0|C_n|M\rangle$, and the additional (bound) correlations in the ground state $\langle 0|C^\dagger_n|M\rangle$ [this is equivalent to determining all amplitudes $\tilde{\rho}_{\mu\nu,M}$ with ν,μ bound, see (W.II.1)]; (b) the determination of the amplitudes $\tilde{\rho}_{\nu\mu,M}$ with one quantum number belonging to the continuum.

So far, one still has to deal with a complicated Fredholm problem. The wanted (complex) energy eigenvalues E_B and the amplitudes are given as the solutions of a homogeneous Lippmann-Schwinger integral equation system. In order to overcome the problem of solving such complicated equations (for a complete treatment of the full RPA problem see Ref. 5), one simplifies the approach by replacing all p-h interaction matrix elements with at least one quantum number belonging to the continuum by a sum of separable forces, e.g.,

$$2\pi\tilde{I}_{\nu\alpha\mu\beta}=D_{(1)}w^{(1)}_{\nu\mu}w^{(1)}_{\alpha\beta}+D_{(2)}w^{(2)}_{\nu\mu}w^{(2)}_{\alpha\beta}. \quad (3)$$

In Ref. 3 the theory was explicitly formulated with one separable term, which turned out not to be sufficient. But the generalization for a force with two separable terms is straightforward. In the notation for single particle states we follow the standard scheme, e.g.,

$\nu, \mu \equiv i, j$ for $\nu, \mu \leq \epsilon_F$, (4a)

$\nu, \mu \equiv m, n$ for $\nu, \mu > \epsilon_F$ (discrete), (4b)

$\nu, \mu \equiv k, p$ for $\nu, \mu > \epsilon_F$ (continuous). (4c)

For the solutions of the problem one obtains the following explicit results:

$$\langle 0|C_n^\dagger|B\rangle = -\frac{1}{E_n + E_B}\sum_{r=1}^{2} D_{(r)} F^0_{(r)n} F_{(r)B}, \tag{5a}$$

$$\langle 0|C_n|B\rangle = -\frac{1}{E_n - E_B}\sum_{r=1}^{2} D_{(r)} F^{0*}_{(r)n} F_{(r)B}, \tag{5b}$$

$$\tilde{\rho}_{ki,B} = [E_B + \epsilon_i - \epsilon_k - i\eta(n_k - n_j)]^{-1} \times \sum_{r=1}^{2} f^{ki}_{(r)}(E_B) F_{(r)B}, \tag{6a}$$

$$-\tilde{\rho}_{ik,B} = (i \rightleftarrows k), \tag{6b}$$

where the following abbreviations have been introduced:

$$F^0_{(r)n} \equiv \sum_{mj} \{\tilde{\rho}_{mj,n} w^{(r)}_{jm} + (m \rightleftarrows j)\}, \tag{7a}$$

$$F_{(r)B} \equiv \sum_{kj} \{\tilde{\rho}_{kj,B} w^{(r)}_{jk} + (k \rightleftarrows j)\}, \tag{7b}$$

$$f^{\alpha\beta}_{(r)}(E) = \left[D_{(r)} w^{(r)}_{\alpha\beta} - D_{(r)} \sum_{s=1}^{2} D_{(s)} w^{(s)}_{\alpha\beta} \sum_{|n>\neq|0>} \left(\frac{F^0_{(r)} F^{0*}_{(s)n}}{(E_n + E)} + \frac{F^{0*}_{(r)n} F^0_{(s)n}}{(E_n - E)}\right)\right]. \tag{8}$$

By inserting the solutions (6) into the definition (7) of $F_{(r)B}$ one obtains the homogeneous eigenproblem:

$$\sum_{s=1}^{2} [\delta_{rs} - D_{rs}(E_B)] F_{(s)B}(E_B) = 0. \tag{9}$$

with

$$D_{rs}(E) \equiv \sum_{kj} \left[(n_j - n_k) \frac{w^{(r)}_{ki} f^{ki}_{(s)}(E)}{E + \epsilon_k - \epsilon_i - i\eta(n_i - n_k)} + (i \rightleftarrows k)\right]. \tag{10}$$

In principle, the determination of the full numerical solution of the problem is very simple. The (complex) eigenenergies E_B are given by the zero points of the determinant $|1 - D(E_B)| = 0$. For the amplitudes one needs, according to Eqs. (5) and (6), the knowledge of the two functions $F_{(r)B}$ defined in relation (7). Because of the homogeneous eigenproblem (9), $F_{(1)B}$ and $F_{(2)B}$ are linearly dependent. Hence, the normalization condition $\langle B|B\rangle = 1$ is sufficient—up to a phase factor—for the determination of these functions. The phase can be chosen in accordance with the outcome of the nuclear structure calculation.

In this initial investigation, we intended to apply the method for the simple case of a nuclear structure RPA calculation (applications for nucleon scattering and phonon processes are also possible) with the main goal of estimating the influence of the continuum. Since many results are available in the oxygen region,[5,6] we have concentrated on ^{16}O and ^{16}N, respectively. The continuum single-particle wave functions were calculated with a Woods-Saxon potential fitted to the experimental single-particle energies. The $1d_{3/2}$ state was included in the nuclear structure calculation. For the separable force we have chosen the surface-delta-interaction[7] (SDI), with the following parameters in the same notation as in Ref. 7:

$$\begin{aligned} &V_0(^{16}\mathrm{O}) = 1650 \ (\mathrm{MeV\,fm^3}),\\ &V_0(^{16}\mathrm{N}) = 1700 \ (\mathrm{MeV\,fm^3}),\\ &\eta = 0.135. \end{aligned} \tag{11}$$

The numerical results for the energies of the negative parity states in ^{16}O are presented in Table I. In order to compare with the structure calculation, we have restricted ourselves to p and d states only. The outcome shows clearly that the low-lying coherent 3^- state is slightly affected by the inclusion of the continuum (being shifted by ≈ 0.2 MeV). The other states are unaffected by the larger basis. The convergence behavior with respect to the included part of the continuum is given in the Table II. The results indicate, that with respect to the real part of the energy eigenvalues, convergence is reached by extending the continuum up to 100 MeV. For the width, the convergence is slightly slower. There is an additional small change of about 0.03 MeV until one reaches convergence at about 400 MeV. In Table III we compare the results with a calculation of Pöpel and Schütte for ^{16}N, who performed a standard TDA-continuum calculation using a SDI force.[9] As anticipated, one gets for these $T = 1$ states almost no change by using the RPA. Since these states are not very coherent, the outcome for the real part does not change by extending the basis to the continuum.

The purpose of this investigation was to test a simplified method for the inclusion of the continuum in TDA or RPA calculations, which avoids the complicated numerical treatment of integral equations. As in the very extended calculations of Ref. 5, we find that the effect of the continuum is rather small and important only for coherent states.

A more sophisticated consideration of the nu-

TABLE I. The calculated energy levels and widths of ^{16}O compared with experiment and some conventional structure calculations.

J^π	T	E_{exp} [a]	Γ_{exp} [a]	E_{ST} [b]	E_C [c]	Γ_C [c]	E_{Mig} [d]	E_{KK} [e]	E_T [f]
0^-	0	10.95		12.29	12.28	0.003	13.67	13.34	12.92
	0			23.35	23.39	0.045	25.40	25.37	24.20
	1	12.80	0.038	12.83	12.80	0.046	12.46	13.93	13.90
	1			25.74	25.81	0.286	22.96	26.94	27.29
1^-	0	7.12		12.80	12.78	0.001	15.04	10.66	10.99
	0	9.63		16.88	16.89	0.286	17.76	16.92	16.73
	0	12.44	0.098	18.44	18.44	0.242	24.08	18.09	17.94
	0			22.81	22.82	0.179	25.87	24.33	23.54
	1	12.80	0.038	12.77	12.81	0.001	12.65	14.07	14.11
	1	13.09	0.100						
	1	17.00							
	1	17.14	0.045	16.94	16.86	0.133	16.81	18.10	18.13
	1	17.29	0.090						
	1	19.48	0.300	19.03	19.04	0.086	18.39	20.31	20.49
	1	20.95	0.150						
	1	22.00		23.17	23.17	0.962	19.12	23.17	24.23
	1	25.00		25.51	25.53	0.438	22.91	26.14	26.89
2^-	0	8.87		11.87	11.87		12.52	12.31	11.95
	0	12.53		16.60	16.61	0.148	17.60	16.77	15.65
	0	(13.98)		18.11	18.02	0.081	19.08	18.59	17.66
	0	15.22	0.075	18.82	18.82	0.016	19.94	19.75	19.18
	0			22.68	22.68	0.061	23.35	23.22	22.92
	1	12.97	0.001	12.52	12.51	0.001	11.59	13.21	13.29
	1	(17.64)		17.44	17.44	0.890	16.67	17.98	18.45
	1	19.24		18.18	18.19	0.260	17.72	19.43	19.41
	1	20.43		20.74	20.76	0.075	18.60	20.86	21.18
	1			23.41	23.41	0.143	22.73	23.95	24.07
3^-	0	6.13		6.54	6.35		6.31	7.09	6.58
	0	(11.62)		15.63	15.63	0.280	15.91	16.18	16.22
	0	18.69	0.280	21.59	21.57	0.420	22.23	21.97	21.15
	1	13.26	0.004	13.23	13.22	0.001	11.76	13.22	13.59
	1			18.86	18.86	0.042	17.78	18.74	19.03
	1			25.04	25.11	0.060	23.07	29.94	25.53
4^-	0			18.34	18.34	0.004	19.28	18.78	17.74
	1			19.79	19.79	0.012	17.77	19.59	19.54

[a] Experimental resonance energies, F. Ajzenberg-Selove, Nucl. Phys. A281, 1 (1977).
[b] Structure calculation without continuum.
[c] Resonance energies with continuum, Migdal's renormalization constant was chosen in accordance with Haug (Ref. 6) as 0.79 for bound states and 1.0 for continuum states.
[d] Structure calculation with Migdal force.
[e] Structure calculation with Kalio-Kolveit potential (Mavromatis *et al.*, Ref. 6).
[f] Structure calculation with (energy-dependent) T matrix (Haug, Ref. 6).

clear structure problem shows that one must add several corrections to the outcome of the conventional RPA. These improvements may alter the result as much as the inclusion of the continuum. For instance, the use of an energy-independent force over a wide energy range in the standard RPA treatments is very questionable.[10] An investigation on the basis of a full many-body theory leads to an identification of the p-h force with the complicated energy-dependent p-h vertex[4,10] which implies at least a different renormalization for the interaction matrix elements with quantum numbers far from the Fermi level. As another point, even if one chooses a less complicated way by utilizing the variational principle for the derivation of the RPA problem, one encounters a nonlinear problem which reduces to the standard RPA only with the assumption that the excited (coherent) states of the nucleus and the neighbor nuclei with plus or minus two particles are pure (noncoherent) shell model states.[11,12,13] That seems like a "contradictio in adjecto," if some of these excited states are a co-

TABLE II. Influence of the size of the configuration space onto the energies and widths for the lowest 3^- states in ^{16}O (in MeV).

Integrated up to (MeV)	E^{3^-}	E^{3^-}	Γ^{3^-}	E^{3^-}	Γ^{3^-}
62	6.364	15.632	0.240	21.574	0.361
104	6.355	15.632	0.258	21.571	0.373
158	6.354	15.632	0.261	21.571	0.380
189	6.353	15.632	0.268	21.571	0.390
223	6.351	15.632	0.274	21.571	0.394
260	6.351	15.632	0.280	21.571	0.420
408	6.350	15.632	0.280	21.571	0.420

herent superposition of p-h amplitudes. Whether such corrections can be incorporated into an effective force in a smaller basis or have a minor influence due to random contributions, respectively, is not known to us. Another way to improve upon the standard RPA is by including higher correlations, for example, of 3p-3h components etc., since one can always use the alternative of treating the problem with more complicated wave functions and simpler forces. In the face of all these complications it seems sufficient—at least for the purpose to obtain a quantitative estimate—to use the simple reduction to a degenerate Fredholm problem for the continuum contributions, with the additional advantage of being able to use the conventional structure calculation as an input.

TABLE III. Calculated energies and widths for N^{16} compared with the TDA result of Pöpel and Schütte (Refs. 8, 9) (MeV).

$T=1$ J^π	E_{ST}	E_C	Γ	E_C^P	Γ^P
0	−3.10	−3.14		−3.00	
	8.01	7.79	0.46	8.01	0.428
1^-	−3.00	−3.02		−2.98	
	1.26	1.25	0.174	1.27	0.172
	3.09	3.06	0.028	3.12	0.028
	4.20	4.10	0.205	4.17	0.202
	7.80	7.79	0.344	7.82	0.346
2^-	−3.71	−3.72		−3.66	
	1.27	1.27	0.181	1.28	0.184
	2.48	2.48	0.011	2.52	0.011
	3.58	3.56	0.018	3.57	0.016
	7.41	7.40	0.155	7.44	0.148
3^-	−3.50	−3.52		−3.49	
	2.53	2.52	0.004	2.54	0.004
	7.91	7.90	0.305	7.91	0.306
4^-	2.90	2.89		2.91	

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[1] C. Bloch, in *Proceedings of the Thirty-Sixth International School of Physics*, Enrico Fermi Course (Academic, New York, 1966); C. Mahaux and H. A. Weidenmüller, *Shell-Model Approach to Nuclear Reactions* (North-Holland, Amsterdam, 1969).

[2] For a recent discussion of different numerical methods, see, M. Micklinghoff, Z. Phys. (unpublished);

[3] M. K. Weigel, Phys. Rev. C 1, 1647 (1970).

[4] A. B. Migdal, *Theory of Finite Fermi Systems and Applications to Atomic Nuclei* (Interscience, New York, 1967).

[5] S. Krewald *et al.*, Nucl. Phys. A281, 166 (1977); thesis, Bonn, 1977 (unpublished). These papers contain an extensive list of references.

[6] For instance, P. Haug, Z. Phys. 238, 289 (1970); H. A. Mavromatis, M. Markiewitz, and A. M. Green, Nucl. Phys. A90, 104 (1967); B. Schwesinger, thesis, Munich, 1976 (unpublished).

[7] J. Letoureux and J. Eisenberg, Nucl. Phys. 85, 119 (1966).

[8] Because of low lying states with positive parity in ^{16}N, the interpretation of the negative parity states as p-h superpositions is even more doubtful than for ^{16}O. Only for the four lowest states can one approximately use this simple picture.

[9] B. Pöpel and G. Schütte, Z. Phys. 231, 48 (1970).

[10] For an approximative inclusion of the energy dependence see, for instance, B. Schwesinger and M. K. Weigel, Phys. Rev. C 16, 493 (1977).

[11] D. J. Rowe, Rev. Mod. Phys. 40, 153 (1968).

[12] M. K. Weigel and J. Winter, J. Phys. G 4, 1427 (1978).

[13] In the many-body theory such contributions are hidden in the irreducible vertex I.