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SMALL VIBRATIONS ABOUT EXCITED STATES

W. Besold, C. Toepffer and P.-G. Reinhard

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Résumé — Les équations de l'approximation de phase aléatoire pour de petites vibrations autour des états excités sont établies. La dépendance de la température des excitations collectives sera examinée. Nous appliquons ce formalisme à l'état de base ainsi qu'au premier état excité du noyau 90Zr. Par cela nous allons confirmer l'hypothèse de Brink.

Abstract — We derive Modified RPA-equations for small vibrations around excited states. The temperature dependence of collective excitations is examined. The formalism is applied to the ground state and the first excited state of 90Zr in order to confirm the Brink hypothesis.

1.

Usually, the nuclear giant resonances are described by the Random-Phase-Approximation (RPA) which is a linearized theory of small vibrations about the Hartree-Fock ground-state. Recently, there has come up experimental evidence for giant resonances which are built upon excited states [1]. This has motivated us to investigate a modified RPA (MRPA) which allows for small vibrations about arbitrary states. Thereby we have been concerned mainly with thermally excited "ground-states"; but the formalism of the MRPA is open for any kind of excitation, e.g. particular reoccupations in the shell-model.

There are many ways to derive the RPA-equations. We choose the Green's function formalism and extended it to derive the MRPA, the extension consists in allowing for arbitrary occupation numbers of the single particle states (in the Green's function). Similar derivations have been given by Vautherin and Vinh Mau [2] and by Des Cloizeaux [3] for the special case of thermalized "ground-states".

This contribution is outlined as follows: In section 2 we derive the MRPA equations by means of the Green's function formalism. In order to obtain semi-quantitative predictions for the giant resonances we invoke a sum-rule approximation to the MRPA; it is introduced and discussed in section 3. The results for giant resonances built upon thermally excited ground-states are given in section 4. An example for the case of a particular shell-model excitation is shown in section 5.

2. DERIVATION OF MODIFIED HF- AND RPA-EQUATIONS

We derive the MRPA-equations starting from the equations of motion for the single particle Green's function. The single particle Green's function g(1,1') is defined as follows

\[ g(1,1') = -i \langle T(\hat{\psi}(1) \hat{\psi}^+(1')) \rangle \] (1)

where \( T \) is the time ordering operator, the \( \hat{\psi} \) and \( \hat{\psi}^+ \) are field opera-
tors and \(<\ldots>\) means the expectation value over an ensemble. We use the abbreviation \((1,2)\) for \((r_1, t_1, r_2, t_2)\).

The equation of motion for \(g(1,1')\) is coupled to the two particle Green's function. We employ the Gorkov-factorization of the two-particle Green's function and obtain

\[
\left\{ \frac{\mathcal{H}}{\frac{\partial}{\partial t_1}} + \frac{\hbar^2}{2m} \nabla_1^2 \right\} g^{<}(1,1') = -i \int d^3 r_2 \mathcal{V}(r_1, r_2) (g^{<}(1,1') g(2,2^+)-
\quad - g^{<}(2,2^+) g^{<}(2,1'))
\]

\[
\left\{ -i h \frac{\partial}{\partial t_1} + \frac{\hbar^2}{2m} \nabla_1^2 \right\} g^{<}(1,1') = -i \int d^3 r_2 \mathcal{V}(r_1, r_2) (g^{<}(1,1') g(2,2^-)-
\quad - g^{<}(2,2^-) g^{<}(2,1'))
\]

(2a)

(2b)

Here \(2^+\) means, that \(t_2^+ = \lim(t_2 + \varepsilon)\) and \(2^-\) is defined analogously.

The notation \(g^{<}\) indicates that the eqs. (2) define \(g^{<}\) for \(t_1 < t_1'\); however, the solution can be continued analytically to \(t_1 > t_1'\). One can express the \(g\) in terms of single particle wavefunctions,

\[
g^{<}(1,1') = i \sum_{\lambda, \lambda'} f_{\lambda \lambda'} (t_1, t_1') \phi_{\lambda}(r_1) \phi_{\lambda'}^*(r_1')
\]

(3)

The \(f_{\lambda \lambda'}\), therein is an occupation matrix which allows to describe correlated states or ensembles.

In order to describe the stationary state of the system we choose

\[
f_{\lambda \lambda'}(t_1, t_1') = \delta_{\lambda \lambda'}, f_{\lambda} \exp\left[ -i \omega_{\lambda} (t_1 - t_1') \right]
\]

(4)

In particular, if we set \(f_{\lambda}\) to be the Fermi-Dirac distribution we have the occupation numbers for single particle states with energy \(\epsilon_{\lambda}\) of a fermi-system at finite temperature \(T\) and chemical potential \(\mu\). We insert eqs. (3) and (4) into eqs. (2); then we add eq. (2a) to (2b), take the limit \(t_1 = t_1'\) and project onto single particle states. This yields finally the modified HF-equations

\[
\omega_{\lambda} \delta_{\lambda \lambda'} = \langle s|T|r\rangle + \sum_k f_k <k|v|\tilde{r}\rangle
\]

(5)

where \(\tilde{r}\rangle = |r\rangle - |kr\rangle\). The HF-eqs. are contained in (5) for the special choice \(f_k = 1\) for \(k \leq \text{Fermi surface}\) and \(f_k = 0\) for \(k > \text{Fermi surface}\). These equations are known for long and have been applied by many authors, see e.g. refs. [4,5].

Fig. 1 shows the level scheme for neutrons in \(^{40}\text{Ca}\) calculated with the modified HF-equations and the Fermi-Dirac-distribution.

To get the modified RPA-equations we have to choose the occupation number matrix \(f_{\lambda \lambda'}\) more general as in eq. (4). In analogy with the conventional derivation of RPA we have to add particle-hole-contributions to the HF-state. But in our case we have to take into account, that Pauli-blocking factors \((1-f_{\lambda})\) and \(f_{\lambda}\) will appear, because \(f_{\lambda} \neq 0\) and \(f_{\lambda} = 1\) is possible. Thus the generalized ansatz has to read

\[
f_{\lambda \lambda'}(T+\frac{t}{2}, T-\frac{t}{2}) = \delta_{\lambda \lambda'}, f_{\lambda} \exp(-i \omega_{\lambda} T) +
\quad + f_{\lambda}(1-f_{\lambda})[x_{\lambda \lambda'}^{(v)} \exp(-i \omega_{\lambda} T) + y_{\lambda \lambda'}^{(v)} \exp(i \omega_{\lambda} T)] \exp(-i \omega_{\lambda} T) +
\]
\[ + \sum_{\lambda}(1-R_{\lambda})(x^{(v)}_{\lambda,\lambda} \exp(i\omega^{(v)} \tau) + y^{(v)}_{\lambda,\lambda} \exp(-i\omega^{(v)} \tau)) \exp(-i\omega_{\lambda} \tau) \]

\[ (6) \]

\[ E_{ex}(\text{MeV}) \]

\[ \begin{array}{cc}
\text{kT=0} & \text{kT=5MeV} \\
1h\nu_2 & \\
1g\gamma_2 & \\
2d\gamma_2 & \\
2p\nu_2 & \\
1f\nu_2 & \\
2p\gamma_2 & \\
1f\gamma_2 & \\
2s\nu_2 & \\
1d\gamma_2 & \\
1d\gamma_2 & \\
1p\nu_2 & \\
1p\gamma_2 & \\
1s\nu_2 & \\
\end{array} \]

Fig. 1: neutron single particle levels of \(^{40}\text{Ca}\) at temperature \(kT=0\) and \(kT=5\text{MeV}\), calculated with force Skyrme \(M^*\). The bold part of the lines indicates the occupation probability of the levels. At \(kT=0\) the six lowest levels are occupied with probability 1, at \(kT=5\text{MeV}\) the higher levels also have a finite occupation probability.

The first term therein describes the stationary state as before. The second and third term describe small vibrations about the stationary state. The system is assumed to vibrate in one eigenmode with frequency \(\omega^{(v)}\). We insert the eqs. (6) + (3) into eqs. (2); then we subtract eq. (2b) from (2a), take the limit \(t=0\) and project onto single particle states.

In lowest order we obtain again the MHF-equations. Collecting all terms linear in \(x\) and \(y\) we obtain the MRPA-equations,

\[ \begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} F \\ F_t \end{pmatrix} = \hbar \omega \begin{pmatrix} K & 0 \\ 0 & -K \end{pmatrix} \begin{pmatrix} F \\ F_t \end{pmatrix} \]

\[ (7) \]
where $A_{srkk'} = \frac{\delta k}{\delta k'} \delta_{sk} \delta_{rk'} + (f_r-f_s)(f_{k'}-f_k) \langle sk'|v|rk' \rangle$

$B_{srkk'} = (f_r-f_s)(f_{k'}-f_k) \langle sk|v|rk' \rangle$

$C_{sr} = \frac{f_r(1-f_s) - f_s(1-f_r)}{f_r-f_s}$

$D_{sr} = f_r f_s$

$k > k'$, $s > r$

(8)

The normalization of the eigenvectors $(f_r^s)$ is obtained from identifying $|\hbar\omega|$ with the excitation-energy of the first excited state. It reads

$\sum_{s>r} (f_r - f_s) \{ |F_{sr}|^2 - |F_{rs}|^2 \} = 1$

(9)

3. SUM-RULE APPROXIMATION

A full solution of the MRPA-equations is a formidable task. Therefore we estimate the properties of giant-resonances in the sum-rule approximation to the MRPA-equations (An application of sum-rule techniques in the $T=0$-case can be found in the article of Reinhard and Friedrich in these proceedings; sum-rules with finite temperature have also been investigated by Meyer et al. [6]). Assuming that the giant resonance exhausts the sum-rule for its corresponding multipole operator, we can "solve" the MRPA-equations simply by the ansatz

$f_{sr} = \sqrt{\frac{\lambda}{2}} \frac{Q_{sr} - i \lambda}{f_r - f_s}$

(10)

where $Q$ is the multipole operator,

$\hat{P} = i [\hat{H}, \hat{Q}]$

and $\lambda$ is the oscillator width. Inserting this $f_{sr}$ into the MRPA-equations yields finally simple traces for the width $\lambda$ and the energy $\hbar\omega$ of the giant resonance.

$M^{-1} = \sum f_r ([\hat{Q}, [\hat{H}, \hat{Q}]]_{rr})$ \( f_r \)

$C = \sum f_r ([\hat{P}, [\hat{H}, \hat{P}]]_{rr})$ \( f_r \)

$E = \sqrt{C/M}$, \ $\lambda = \sqrt{C \cdot M}$

(11)

These traces are no more complicated to evaluate than in the $kT = 0$-case.

The exhaustion hypothesis is not perfectly satisfied. Usually the giant resonances are distributed over the states in an energy range $\Delta E$, where we mean with $\Delta E$ the fragmentation width (not the spreading width and not the decay width). Within our sum-rule approach we will
also give an estimate for this fragmentation width $\Delta E$. To that end we exploit the fact, that the sum-rule approximation can also be viewed in terms of a schematic model \cite{7} with $\varepsilon_F$ being the single particle energies and $\varepsilon Q \cdot Q$ being the residual interaction; the actual size of $\varepsilon$ can be evaluated by $Q$-averaging of the true residual interaction. In fact, the sum-rule approximation corresponds to the extreme schematic model where all particle-hole energies are the same. In the following we will derive the expression for $\Delta E$ only for the case $kT=0$.

At $kT=0$ the MRPA-equations reduce to the well-known RPA-equations

$$\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} \chi(v) \\ \psi(v) \end{pmatrix} = \varepsilon \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} \chi(v) \\ \psi(v) \end{pmatrix}.$$  \hspace{1cm} (12)

In the extreme schematic model (equivalent to the sum-rule approximation) we insert

$$A = A_0 = \varepsilon \hat{1} + \kappa \hat{Q} \cdot \hat{Q},$$

$$B = B_0 = -\kappa \hat{Q} \cdot \hat{Q}.$$  \hspace{1cm} (13)

Thus we have the solution for the collective mode

$$\chi_{\nu i}^{(1)} = \frac{Q_{\nu i}}{\varepsilon_1 - \varepsilon}, \quad \psi_{\nu i}^{(1)} = \frac{Q_{\nu i}}{\varepsilon_1 + \varepsilon}, \quad \varepsilon_1 = \sqrt{\varepsilon^2 - 2\varepsilon \kappa \sum_{\nu i} |Q_{\nu i}|^2},$$  \hspace{1cm} (14)

where $\nu$ labels states above the Fermi surface and $i$ below. The other states of the energy spectrum, $\nu \parallel i$, are degenerate at energy $\varepsilon$.

In general the particle-hole energies will not be degenerate. We now consider the fluctuation about the mean value $\varepsilon$ as perturbation; identifying

$$A = A_0 + A_1, \quad (A_1)_{\mu i} n_j = (\varepsilon_m - \varepsilon_i - \varepsilon) \delta_{\mu \nu} \delta_{i j}$$  \hspace{1cm} (15)

and $B = B_0$ remains as before. In first order perturbation theory we obtain, denoting the improved solution by $\chi'$ and $\psi'$,

$$\chi'(\nu) = \chi(\nu) + \sum_{\nu \parallel \mu} x(\mu) \left( \frac{\mu|A_1|\nu}{E_{\nu} - E_{\mu}} \right),$$

$$\psi'(\nu) = \psi(\nu) + \sum_{\mu \perp \nu} y(\mu) \left( \frac{\mu|A_1|\nu}{E_{\nu} - E_{\mu}} \right),$$  \hspace{1cm} (16)

where

$$\mu|A_1|\nu = (x(\mu)^* y(\mu)^*) \begin{pmatrix} A_1 & 0 \\ 0 & A_1 \end{pmatrix} \begin{pmatrix} \chi(\nu) \\ \psi(\nu) \end{pmatrix}.$$  \hspace{1cm} (17)

The first and second order corrections to the energy are

$$\delta E(1) = (\nu|A_1|\nu),$$

$$\delta E(2) = \sum_{\mu \perp \nu} \frac{\varepsilon}{E_{\nu} - E_{\mu}} (\nu|A_1|\mu)(\mu|A_1|\nu).$$  \hspace{1cm} (18)
Note that $\delta E^{(1)} = 0$, because the average $\varepsilon$ has been defined such that

$$\sum_{m,i} |Q_{mi}|^2 (\varepsilon_m - \varepsilon_i - \varepsilon) = 0.$$  

The moments of $\hat{Q}$ are defined as usual by

$$m_N = \sum_{\nu} |\langle \psi_\nu | \hat{Q} | \psi_\nu \rangle|^2 E_\nu^{\text{N}}.$$  

In case of complete exhaustion, only $\nu = 1$ contributes and all moments are given by knowing two of them. In case of incomplete exhaustion various interrelations between the moments carry some information on the fragmentation of the giant resonance. We define the fragmentation width $\Delta E$ from the moments $M_0$, $M_1$ and $M_2$

$$\Delta^2 E = \frac{M_2}{M_0} - \frac{M_1^2}{M_0^2}.$$  

(Note that in case of complete exhaustion $\Delta E = 0$). Inserting the above results for the schematic model in perturbation theory, we obtain the remarkable result

$$\Delta^2 E = \Delta^2 \varepsilon,$$

where $\Delta^2 \varepsilon = \sum_{mi} |Q_{mi}|^2 (\varepsilon_m - \varepsilon_i - \varepsilon)^2 / \sum_{mi} |Q_{mi}|^2$.

This relation is true up to second order in $A_1$. The exhaustion of the $M_1$-sum-rule by the state $|\psi_1\rangle$ can be defined as

$$\eta = \frac{|\langle \psi_0 | \hat{Q} | \psi_1 \rangle|^2 E_1}{\sum_{\mu} |\langle \psi_0 | \hat{Q} | \psi_\mu \rangle|^2 E_\mu}.$$  

Inserting again the schematic model in perturbation theory (up to second order) we obtain

$$\eta = 1 - \frac{\varepsilon}{E_1} \frac{\Delta^2 E}{(E_1 - \varepsilon)^2}.$$  

The perturbation theory is valid if the collective energy is large compared to the fragmentation, i.e. $\Delta E \ll |E_1 - \varepsilon|$. We will use the above formula for $\Delta E$ and $\eta$ also in the case $\Delta E > 0$; in each averaging procedure, of course the thermal occupation probabilities are taken into account.

4. RESULTS FOR TEMPERATURE DEPENDENT GIANT RESONANCES

4.1 Ground-state energies

We first want to look at the relation between thermal excitation-energy and temperature. In the fermi-gas model we have [8]

$$E^* = a \cdot \frac{(kT)^2}{\text{MeV}}, \quad a = 0.25 \cdot A$$

where $a$=nuclear level density parameter, $A$=mass-number, $k$=Boltzmann-constant and $T$=temperature. With our MHF-program we calculated the thermal excitation-energy as a function of temperature for $^{40}$Ca. The results are shown in fig. 2 together with those of the fermi-gas model.
We see that the curve of the MHF-calculation has a smaller slope. Thus the nuclear level-density parameter \(a\), which is the slope of the curves in fig. 2, is smaller for MHF than for the fermi-gas model. That is in good agreement with measurements [9] where the nuclear level density parameter was found to be particularly small for double magic nuclei.

![Fig. 2: Thermal excitation-energy](image)

\[ E^*(T) = E_{\text{MHF}}(T) - E_{\text{MHF}}(0) \]

Fig. 2: Thermal excitation-energy \(E^*(T) = E_{\text{MHF}}(T) - E_{\text{MHF}}(0)\) as a function of \((kT)^2\) (dotted) compared to the fermi-gas formula (24) (full) for \(^{40}\text{Ca}\).

4.2 Collective energies:

With the aid of eqs. (11) we calculated the energies of multipol-giant resonances in \(^{40}\text{Ca}\) for different temperatures and multipolarities.

![Fig. 3: Energy of the different \((L,T)\)-giant resonances in \(^{40}\text{Ca}\) as a function of temperature](image)
In fig. 3 are shown the energies for the isovector-monopole, dipole- and quadrupole-resonance, and the isoscalar monopole- and quadrupole- resonance. The curves for the isovector modes remain nearly constant up to 2 MeV and then start to decrease. This can be understood by the fact, that the phase-space factors in eqs. (8) reduce the residual interaction with increasing temperature (mind that the residual interaction is repulsive for isovector modes). For the isoscalar modes we see the expected increase in energy (the residual interaction is attractive in that case) up to kT = 2 MeV. But then the energies decrease also. This happens because 0Kω-transitions become possible due to heating the ground-state. The whole model works reasonably in 40Ca up to kT ≈ 5 MeV. Above that value substantial fractions (5% for the neutrons and 12% for the protons) of continuum states become occupied in the heated ground-state.

4.3 Fragmentation and exhaustion

In fig. 4 we show ΔE according to eq. (21) for the L=0,1,2-resonance in 40Ca. There is no difference between isoscalar and isovector resonances because ΔZε does not depend on isospin for N/Z-nuclei. The curves are nearly constant up to kT = 0.5 MeV and then increase with temperature, up to nearly double the value at kT = 5 MeV. Nevertheless, the fragmentation remains surprisingly small, in particular for the L=1 mode. Above kT = 5 MeV we observe a decreasing ΔE. There are two possible explanations for that effect:

On the one hand one could say that at temperatures higher than kT=5 MeV the curves are not significant anyway because we do not treat the continuum states properly. On the other hand, we know that we can have a strong collectivity in continuum, for instance zero sound.

It is possible that the decrease of the fragmentation is a physical effect as the result of a new appearance of collectivity by low lying transitions becoming possible. But we cannot be sure to see this effect by our methods.
In fig. 5 we have plotted the loss of exhaustion, $1-\eta$, of the isovector resonances calculated with eq. (23). The loss of exhaustion of the collective state increases for the $(L=1, T=1)$-resonance from about 6% to 18%, for the $(L=0, T=1)$-resonance from about 13% to 27% and for the $(L=2, T=1)$-resonance from 19% to 39% as the temperature increases from 0 to $kT = 5$ MeV. We see therefore from $\Delta E$ as well as from $1-\eta$, that at high temperatures we still have collectivity for the giant resonance modes (except perhaps the isoscalar $L=0$ mode).

5. THE DIPOLE-GIANT-RESONANCE IN $^{90}$Zr

The application of the MRPA is by no means restricted to systems in thermal equilibrium. Indeed, we can use the MRPA-equations with arbitrary occupation-numbers for the calculation of any excited state. As an example we study $^{90}$Zr, where Szeflinski et. al. [10] determined experimentally the energy dependence of the $\gamma$-strength function of the first excited state ($0^+; 1.762$ MeV).

The result confirmed the Brink-Hypothesis which states that identical giant resonances can be built upon each excited state. Within our approach we calculated the energy of the dipole giant resonance built upon the ground-state and the first $0^+$-excited state in $^{90}$Zr as well as the total energies $E_{MHF}(0^+; \text{g.s.})$ and $E_{MHF}(0^+; 1.762$ MeV).

Due to the residual interaction the true ground state of $^{90}$Zr is no longer a pure shell model state with two protons in configuration $(2p_{1/2})^2$ on top of the Sr-core; the proton configuration is a linear combination of $(2p_{1/2})^2$ and $(1g_{9/2})^2$. The orthogonal combination of these two configurations describes the 1.762 MeV-state:

\[
\psi(\text{g.s.}) = a \psi(2p_{1/2})^2 - b \psi(1g_{9/2})^2 \\
\psi(\text{exc.s.}) = b \psi(2p_{1/2})^2 + a \psi(1g_{9/2})^2
\]

The coefficients were estimated to be: $a^2 = 0.72$, $b^2 = 0.28$ [10]. Inserting the corresponding $f_\lambda$ in the MHF and MRPA equations we get the excitation energy of the dipole giant resonance (in sum-rule...
approximation) and the total energies of the ground-state and the excited state. The results are given in the table 1:

<table>
<thead>
<tr>
<th>Table 1: Comparison of the MHF- and MRPA-results with experimental results from [10]</th>
</tr>
</thead>
<tbody>
<tr>
<td>E(L=1,T=1)/MeV</td>
</tr>
<tr>
<td>theory</td>
</tr>
<tr>
<td>(1) 0^+-ground-state</td>
</tr>
<tr>
<td>(2) first excited state</td>
</tr>
<tr>
<td>difference (2) - (1)</td>
</tr>
</tbody>
</table>

For these calculations we used a newly fitted Skyrme force which aims at a good description of the isovector dipole modes.

From table 1 we see that the resonance energy reproduces well the experimental value and that the resonance energy on top of the excited state is shifted upwards just by the excitation energy of this state. For that case, we see the Brink hypothesis being confirmed very well both experimentally and theoretically.

CONCLUSIONS

In order to study the collective excitations of a nucleus which is not necessarily in its ground-state, we derived the modified Hartree-Fock (MHF) and modified RPA (MRPA) equations. The emerging equations are an obvious generalisation of the HF-and RPA-equations, modified by occupation probabilities and phase-space factors. From the temperature-dependence of the MHF energies one can deduce a level density parameter; it comes out to be lower than that of the Fermi-gas model and thus reproduces better the experimental values. Within a sum-rule approximation to MRPA we calculated properties of giant resonances in 40Ca. The resonance energies for the isovector modes decrease as function of the temperature whereas for the isoscalar modes it first increases, up to kT = 2MeV, and then decreases also. These features can be understood by the fact that for the isoscalar modes there are two counteracting effects: the residual interaction decreases with temperature (thus increasing the energy) whereas the average lph-energy decreases because the phase space opens for low-energy excitations. The fragmentation widths increase with temperature up to kT = 5 MeV, but they remain small throughout, in particular for the isovector L=1 mode. The percentage of exhaustion of the sum-rule decreases with temperature, but remains fairly high even at kT = 5 MeV. All the results show the remarkable fact that collectivity does not disappear if a nucleus is excited thermally; at least not up to kT = 5 MeV. Above kT = 5 MeV the results are not reliable, since then a substantial fraction of particles is in continuum states (and these are not handled properly in our treatment). For a more
A complete description one has to study the temperature dependence of the spreading- and the escape- width.

To show the universality of the MRPA, we calculated the $L=1$-resonances on top of the ground-state and of the first excited $0^+$-state in $^{90}$Zr. We found good agreement with experimental results.

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