SELF-CONSISTENT THEORY OF LARGE AMPLITUDE COLLECTIVE MOTION*

Daniel Almehed and Niels R. Walet

Department of Physics, UMIST, Manchester M60 1QD, United Kingdom

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We investigate the use of an operatorial basis in a self-consistent theory of large amplitude collective motion. For the pairing plus quadrupole model we show that a small set of basis operators is sufficient to approximate the exact solution of the problem accurately.

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In nuclear physics the question "what is the correct choice of collective coordinate in a many-body system" has had quite a few partial answers. In state of the art constrained HFB calculations one chooses a finite number of multipole operators as constraints without any regard to self-consistency [1]. The goal of our approach is to determine a collective path self-consistently, based on knowledge of the Hamiltonian only. We have chosen to use the pairing+quadrupole Hamiltonian as a test-bed for our method (and practical approximations). Here this is illustrated for the γ-soft nucleus ^{58}Fe.

Our formalism, as set out in detail in [2], is based on time-dependent mean-field theory. The determination of the collective coordinate is by means of the solution to the local harmonic approach, which consists of self-consistently solving the force equation and the local RPA equation

$$\mathcal{H}_{qq'} = \Lambda f_{,qq'}\,, \qquad \sum_{rr'ss'} V_{;qq'rr'} B^{rr'ss'} f_{ss'} = (\hbar\Omega)^2 f_{,qq'}\,, \tag{1}$$

where $\mathcal{H}$ is the HFB Hamiltonian and f an RPA vector. The matrices B and V are related to the standard RPA matrices $\mathcal{A}$ and $\mathcal{B}$ [1], and q (r, s) are quasi-particle indices. We look for a path consisting of a series of points where the lowest non-spurious eigenvector of the local RPA equations also

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fulfills the force equation, the first half of Eq. (1). This is done in a double iterative process where we try to fulfill both Eqs. (1) simultaneously. A step in the generalised density, $\Delta\rho$, is made in the direction of the local RPA solution. For each iteration of the local RPA equation we solve the cranking equation to get get the new generalised density. This is done by a constrained steepest decent method where the constraints are that the step length in the collective coordinate is fixed by

$$\Delta Q = [f_{\rm old} + f_{\rm new}] \ \Delta\rho \tag{2}$$

and that $\Delta\rho$ does not change the particle number N_τ.

It has been shown that the RPA equation can be solved to good accuracy by assuming that the RPA eigenvectors can be described by a linear combination of a small number of carefully chosen one-body operators [3], without breaking self-consistency. Assuming that the RPA eigenvectors can be approximated as linear combinations of a small set of one-body operators, $F^{(k)}$, the approximate RPA vector, $\bar{f}_{,qq'}$, is given by

$$f_{,qq'} \approx \bar{f}_{,qq'} = \sum_{k=1}^{n} c_k \mathcal{F}^{(k)}_{,qq'}\,, \tag{3}$$

where $\mathcal{F}^{(k)}$ is the expectation value of $F^{(k)}$. To determine the coefficients c_k the RPA matrices are projected onto the subspace $\{\mathcal{F}^{(k)}_{,qq'}\}$. Then the RPA equation can then be expressed in matrix notation as

$$\mathcal{F}^{(k)\dagger}\ \boldsymbol{B}\ \boldsymbol{V}\ \boldsymbol{B}\ \mathcal{F}^{(l)}\ c_l = \left(\hbar\bar{\Omega}\right)^2\ \mathcal{F}^{(k)\dagger}\ \boldsymbol{B}\ \mathcal{F}^{(l)}\ c_l\,, \tag{4}$$

where $\hbar\bar{\Omega}$ is an eigenfrequency of the projected RPA. The rank of the matrix we need to diagonalise to solve the RPA problem have been reduced from rank of $\boldsymbol{V}$ and $\boldsymbol{B}$, which is equal to the number of 2-quasi-particle degrees of freedom, to the number of one-body operators chosen.

We apply our method to the pairing + quadrupole Hamiltonian as described in [4]. The Hamiltonian can be written as

$$H = \sum_k \varepsilon_k c_k^\dagger c_k - \sum_{\tau=n,p} \frac{G_\tau}{2}\left(P_\tau^\dagger P_\tau + P_\tau P_\tau^\dagger\right) - \frac{\kappa}{2}\sum_{M=-2}^{2} Q_{2M}^\dagger Q_{2M}\,. \tag{5}$$

We rewrite the quadrupole operators as $Q_{2M}^{(\pm)} = \left(Q_{2M} \pm Q_{2-M}\right)/2$ and the pairing operator as $\left(P_\pm\right)_\tau = \left(P_\tau \pm P_\tau^\dagger\right)/2$. After solving the mean-field problem within the Hartree–Bogoliubov approximation, the $\boldsymbol{V}$ and $\boldsymbol{B}$ matrix of Eqs. (1) can be calculated [3]. κ and G_τ are chosen to give realistic

values of deformation and pair-field and ε_k are calculated using the spherical modified oscillator. Our model space consists of two major N-shells and we have followed [4] and multiplied all quadrupole matrix elements with a isospin dependent quenching factor.

The quality of the results achieved by the projection method strongly depends on the choice of the single particle operator basis [3]. In [3] a set of state-dependent Hermitian one-body operators of the structure

$$\tilde{F}^{(k)} \equiv \sum_{qq'} \frac{F^{(k)}(qq')}{E^2_{qq'}} \left(a^\dagger a^\dagger\right)_{qq'} + \text{H.c.} \tag{6}$$

was used where $E_{qq'}$ is the 2-quasi-particle energy. The small set of operators used in [3] gives a good approximation of the β- and γ-vibrations. To do a large amplitude collective motion calculation it is crucial to also have a good approximation of the pairing vibrations. To achieve this we have included a pairing operator active close to the Fermi-surface only. To avoid the problem of having to chose which states have a non-zero matrix element we simply divide the standard pairing operator $P_\pm$ by a large power of $E_{qq'}$. If the suppression factor, $E^k_{qq'}$, is chosen with a large enough k all matrix elements except the once with $E_{qq'}$ closes to zero will become negligible and the result will not depend on k. The basis set will then be

$$\tilde{F}^{(k)} \in \left\{ \left(\tilde{P}_+\right)_\tau, \left(\tilde{P}_-\right)_\tau, \left(\tilde{Q}_{20}+\right)_\tau, \left(\tilde{Q}_{22}+\right)_\tau, \frac{\left(\tilde{P}_+\right)_\tau}{E^k_{qq'}}, \frac{\left(\tilde{P}_-\right)_\tau}{E^k_{qq'}} \right\}, \ \tau = n, p$$

where k will be chosen to be 10. With the improved basis all the low lying vibrational modes are now described with a very high accuracy as can be seen in Fig. 1. The quality of the projection can also be quantified by calculating the overlap of the projected and the full RPA vector. The overlap turns out to be almost 1 which shows that not just the energy but also the wave-functions are well approximated by the projection method.

We have investigated the large amplitude collective axial motion in ^{58}Fe by using both the full RPA and the projected RPA. The results of the two methods are almost identical. From Fig. 1 we can see that the quadrupole moment is approximately proportional to the collective coordinate Q in the region $-2 < Q < 0$. At larger and smaller values of Q, the deformation remains almost constant. Instead, the collective coordinates is now dependent on the pairing fields, for large positive Q proton pairing and for large negative Q neutron pairing. At $Q \approx 1.1$ the proton pair-field collapses to zero, and our collective path ends. The change from quadrupole to pairing mode is dominated by an avoided crossing with the lowest pairing-vibration

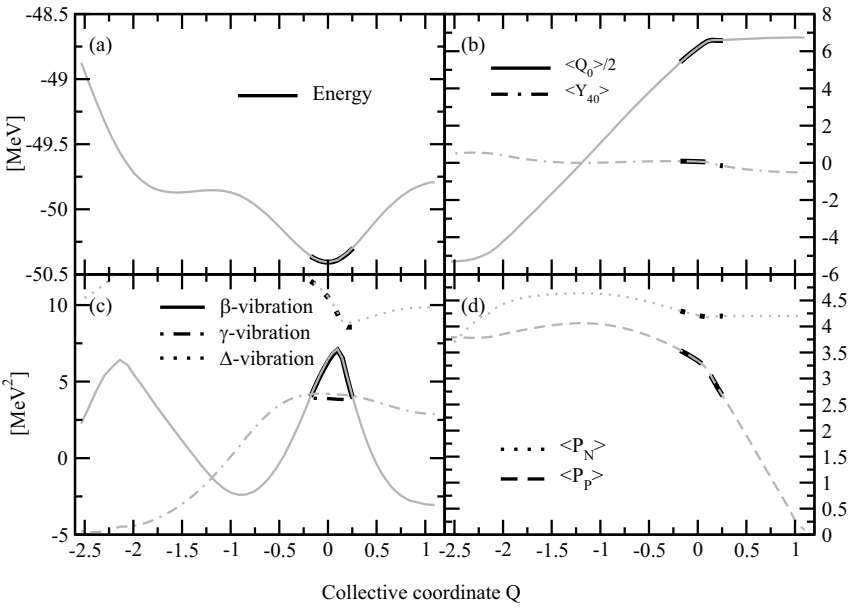

Fig. 1. Axial symmetric large amplitude collective motion in ^{58}Fe. (a) The potential energy along the collective path. (b) The quadrupole and the hexadecapole moments. (c) The lowest RPA frequencies. (d) The expectation-values of the pairing operators. The grey/black curves are the results for the projected/full RPA.

at $Q \approx 0.2$. After this crossing the quadrupole moment, $\langle Q_0 \rangle$ saturates and the $\langle P_p \rangle$ starts changing. The potential energy has a local energy maximum at $Q \approx -1$, which corresponds to a spherical shape, and a shallow oblate minimum at $Q \approx -1.6$. The potential around the minimum show a quadratic behavior which indicates that the harmonic approximation in RPA is well full-filled for small-amplitude vibration, but obviously fails for wave functions that have substantial support away from the minimum.

A more extensive exploration of these methods will be presented in future publications.

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