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Microscopic description of $\alpha+^{40}$Ca quasimolecular resonances

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A multistep microscopic approach describing the dynamics of quasimolecular resonances is applied to the $\alpha+^{40}$Ca system. The lowest collective two-particle eigenmodes are used as building blocks of the four-particle states. The pair states are built on mean-field single-particle orbitals including also sharp resonances in continuum. The structure of ^{44}Ti is analyzed and strong high-lying α-like resonances are found in good agreement with the experimentally observed quasimolecular spectrum. The resonances turn out to be very collective and contain mostly proton-neutron pairs where the lowest proton single-particle resonance, $\pi p_{3/2}$, couples with the lowest neutron bound state $\nu f_{7/2}$.

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The so-called ''quasimolecular states'' were observed a long time ago as resonances in the α-particle scattering. For a recent review see for instance [1], and references therein. They are connected with the anomalous large angle scattering (ALAS) phenomenon seen in the angular distribution studies. Such states were mainly observed and analyzed in the α scattering on light nuclei such as ^{16}O [2], ^{40}Ca [3], or ^{28}Si [4].

Theoretical interpretation of quasimolecular states is based on the simple picture of a long-living dinuclear rotating system. Therefore all phenomenological treatments suppose a pocketlike potential between the two nuclei. The resonance levels of this potential provide an explanation of the rotational bands seen in the excitation function. Along this line a recent phenomenological description of the $\alpha+^{40}$Ca system was given in Ref. [5].

A lot of work on this problem was also done by using different microscopic approaches. We only mention here the description of the same system within the folding model [6], the resonanting group method (RGM) [7,8], and the orthogonality condition model (OCM) [9–11].

We stress the fact that the shell-model basis involved in all the previous microscopic approaches was restricted to bound single-particle configurations. In a recent paper [12] we obtained within the multistep shell-model (MSM) [13] a very good agreement with experiment for low-lying states in the $\alpha+^{208}$Pb system. We also predicted that some of the high-lying quartet states have a strong overlap with the α-particle wave function, comparable with that of the ground state in ^{212}Po. We called them α-like states and showed that their main components consist of single-particle resonances in continuum. Until now quasimolecular resonances were evidenced only for light nuclear systems as for instance the Ca region. In this Rapid Communication we apply the MSM formalism in order to show that high-lying α-like states exist in ^{44}Ti and they coincide with the resonances seen in the α particles scattering on ^{40}Ca.

It is already known that in describing many-body resonances only the narrow single particle resonances are relevant [14,15]. This was shown to be an adequate approach, for instance, for giant resonances [16], but also for the nucleon decay processes [17]. We will show that single-particle resonances are an important ingredient in the structure of quasimolecular states. Moreover our approach is able to predict the positions of these states in terms of single-particle resonances, without involving additional parameters.

Basically the $\alpha+^{40}$Ca system is very similar to the $\alpha+^{208}$Pb one. As mentioned, we have described the resonance structure of the latter system in terms of quartet excitations built on top of the lowest collective pair states. In the present work we use a similar formalism, but make a more extensive study of the included single-particle resonances. We mention that the inclusion of these resonances in the single particle spectrum to study a system such as $\alpha+^{40}$Ca is a new feature with respect to the previous microscopic calculations. The basic technical details of the present approach can be found in Ref. [12]. Here we will stress only the main points of the four-particle method [12] but discuss the resonance structure of the single-particle states more extensively.

We assume that the wave function $|\Psi_B\rangle$ of ^{44}Ti is a superposition of products of the two-body components acting on the core wave function $|\Psi_A\rangle$ describing ^{40}Ca, i.e.,

$$|\Psi_B\rangle_{\alpha_4}=P^\dagger_{\alpha_4}|\Psi_A\rangle\equiv\sum_{\alpha_2\beta_2}X(\alpha_2\beta_2;\alpha_4)(P^\dagger_{\alpha_2}P^\dagger_{\beta_2})_{\alpha_4}|\Psi_A\rangle, \tag{1}$$

where the indices bear quantum numbers of the angular momentum, parity, eigenvalue number and isospin projections for pairs, $\alpha_2\equiv(J^\pi_{a_2}\tau_1\tau_2)$, and angular momentum, parity, eigenvalue number, $\alpha_4\equiv(J^\pi_{a_4})$, for the quartets. The summation contains $\pi\pi,\nu\nu$ $(\tau_1=\tau_2)$ and $\pi\nu$ $(\tau_1=-\tau_2)$ terms. These three kinds of terms form $\pi\pi\nu\nu$ and $\pi\nu\pi\nu$ quartets corresponding to the couplings $(^{42}\mathrm{Ti}\otimes^{42}\mathrm{Ca})_{\alpha_4}$ and $(^{42}\mathrm{Sc}\otimes^{42}\mathrm{Sc})_{\alpha_4}$, respectively.

The two-particle creation operator for correlated pairs defines the a_2-th eigenstate of the particle-particle Tamm-Dankoff approach (TDA) in terms of the normalized pair operators

TABLE I. Proton/neutron single-particle energies (in MeV). In the second/sixth columns are given the spectroscopic assignments. In the third/seventh columns are given the eigenvalues from the diagonalization and in the fourth/eighth columns the corresponding results from the numerical integration. In the fifth/ninth columns are given the resonance widths.

k	Proton state	E_k (diag.)	E_k (int.)	Γ_k	Neutron state	E_k (diag.)	E_k (int.)	Γ_k
1	$\pi f_{7/2}$	-1.416	-1.417	0.000	$\nu f_{7/2}$	-10.988	-10.988	0.000
2	$\pi p_{3/2}$	1.492	1.408	0.033	$\nu p_{3/2}$	-6.903	-6.908	0.000
3	$\pi p_{1/2}$	3.610	3.401	0.438	$\nu p_{1/2}$	-4.405	-4.418	0.000
4	$\pi f_{5/2}$	6.559	6.601	0.014	$\nu f_{5/2}$	-2.585	-2.587	0.000
5	$\pi g_{9/2}$	7.616	7.622	0.001	$\nu g_{9/2}$	-1.144	-1.147	0.000
6					$\nu d_{5/2}$	0.966	0.657	0.023
7					$\nu h_{11/2}$	8.130	8.351	0.000
8					$\nu d_{5/2}$	7.709	8.467	0.743
9					$\nu g_{7/2}$	7.282	8.724	0.004

$$P^{\dagger}_{\alpha_2}=\sum_{ik} x(ik;\alpha_2)\frac{1}{\sqrt{1+\delta_{ik}}}[c^{\dagger}_i c^{\dagger}_k]_{\alpha_2}, \tag{2}$$

where $c^{\dagger}_i$ stands for the single particle creation operator, with $i\equiv(\tau E l j)$, E is the energy, l the orbital, and j the total angular momentum of the single-particle orbital.

The TDA equations of motion for the two-particle and four-particle systems, respectively,

$$[H,P^{\dagger}_{\alpha_2}]=E_{\alpha_2}P^{\dagger}_{\alpha_2}, \tag{3}$$

$$[H,P^{\dagger}_{\alpha_4}]=E_{\alpha_4}P^{\dagger}_{\alpha_4},$$

lead to the following system of equations describing four-particle excitations:

$$\sum_{\alpha_2'\beta_2'} H(\alpha_2\beta_2;\alpha_2'\beta_2')X(\alpha_2'\beta_2';\alpha_4)$$

$$=E_{\alpha_4}\sum_{\alpha_2'\beta_2'} I(\alpha_2\beta_2;\alpha_2'\beta_2')X(\alpha_2'\beta_2';\alpha_4). \tag{4}$$

Here the Hamiltonian matrix is given only in terms of the metric matrix I and pair energies, as described in Ref. [12].

The single-particle eigenstates form the valence space for the collective pair states. Their radial wave functions $g_{Elj}(r)$ satisfy the Schrödinger equation corresponding to a Woods-Saxon spherical potential, i.e.,

$$\left[-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}+\frac{\hbar^2 l(l+1)}{2\mu r^2}\right]g_k(r)+\langle lj|V(r)|lj\rangle g_k(r)$$

$$=E_k g_k(r), \tag{5}$$

where $k=(\tau E l j)$. They can be found by a diagonalization procedure using the spherical harmonic oscillator basis. This approach gives a very accurate description of the bound states, by including in the basis up to eight major oscillator shells. Concerning the states in continuum the procedure is able to reproduce only the proton resonances in a rather large Coulomb potential. This is because they behave almost like bound states.

Therefore, in our case a numerical integration is necessary. We used a different, but basically equivalent, procedure from Ref. [12] to consider narrow resonances. We found narrow scattering resonances with real energy, instead of Gamow resonances with complex energy. As usual we adopt the regular boundary condition at origin, i.e., $g_k(r)\rightarrow r^{l+1}$, while for large distances we consider the following ansatz:

$$g_k(r)\rightarrow G_l(\kappa r)\cos\delta_k+F_l(\kappa r)\sin\delta_k. \tag{6}$$

Here $G_l(\kappa r)/F_l(\kappa r)$ are the irregular/regular Coulomb functions depending on the momentum κ, and δ_k is the phase shift. The internal and external solutions should be matched at some radius, using the equality of the logarithmic derivatives. In this way one obtains the phase shift as a function of the energy E. The resonance energy corresponds to a sharp change of the phase shift versus the energy E by passing the value $\delta_k=\pi/2$.

The four-body eigenstates resulting from the diagonalization of the system (4) should be compared with the α-particle wave function. As in Ref. [12], let us consider the α-particle formation amplitude defined as the following overlap integral on the internal coordinates:

$$\mathcal{F}_l(R)=\int \mathcal{A}\{[\Psi_\alpha(\xi_\alpha)\Psi_A(\xi_A)Y_l(\hat{R})]^*\Psi_B(\xi_B)\}d\xi_\alpha d\xi_A d\hat{R}, \tag{7}$$

where $\mathcal{A}$ stands for the antisymmetrization operator and $\Psi_\alpha(\xi_\alpha)$ is the Gaussian α-particle wave function [18]. Equation (7) bears the meaning of the α-particle probability inside the ''mother'' wave function $|\Psi_B\rangle$ (^{44}Ti in our case). An eigenstate with a large overlap integral should be seen as a maximum of the excitation function describing the α-particle scattering on ^{40}Ca.

The single-particle eigenstates were found using both diagonalization procedure and numerical integration in a spherical Woods-Saxon potential with universal parametrization [19]. In the diagonalization basis we used 16 major

shells. The result is given in Table I. On the left-hand side of the table the proton states are given, while on the right-hand side are the neutron ones. One can see that the energies for both proton and neutron bound states resulting from the diagonalization procedure (the third/seventh columns) are very close to the values obtained by numerical integration (the fourth/eighth columns). Concerning the states in continuum, due to the Coulomb barrier the proton spectrum obtained by the integration method is much closer to the diagonalization result than in the case of the neutron spectrum. One can also notice the similar relative energies of the first five states for the proton and neutron spectra. In the fifth/ninth columns are given the widths of the resonant states, computed according to the standard relation

$$\Gamma_k = -2\left[\frac{\partial \cot \delta_k}{\partial E}\right]^{-1}_{E=E_r}. \tag{8}$$

By using the states of Table I we obtained the pair eigenstates using the TDA method with the surface-delta residual two-body interaction (SDI) [20]. We adjusted the isoscalar and isovector strengths of the SDI to describe the low-energy spectra [21] of the nuclei ^{42}Ti, ^{42}Ca, and ^{42}Sc, used to generate the needed $\pi\pi$, $\nu\nu$, and $\pi\nu$ pairs for the quartet states in ^{44}Ti. The quartet states, in turn, were obtained by solving the eigenvalue problem (4). To keep the calculations tractable, we considered in the basis the first three collective pair eigenstates. As described in Ref. [12] the metric matrix was first diagonalized and its eigenstates were used to build a new orthonormal basis. Because our initial basis is overcomplete we excluded states having small eigenvalues of the metric matrix. After this the lowest quartet energy in the diagonalization of Eq. (4) is close to the α-particle binding energy. We normalize our four-particle spectrum to this value.

Then we estimated the formation amplitude according to Eq. (7). We varied the center-of-mass (c.m.) radius within the interval $r \in [5,7]$ fm, beyond the nuclear radius $R_c = 4.1$ fm. and divided the result with the ground-state value. The mean value of this ratio we called hindrance factor (HF) and it has almost a constant value within the chosen interval of the radial coordinate. In this region the Pauli principle is less important and the antisymmetrization operation in Eq. (7) can be neglected. This is actually the important region for the α-scattering process. The HF provides a better description of the quartet resonances than the spectroscopic factor, because it takes care only of the external structure of the wave function.

Results for the hindrance factors are shown in Fig. 1 for even spins $J = 0,2,4,6$. One can see that, indeed, for some energies one obtains HF values larger than unity. These states, called α-like states, are the quasimolecular states seen as maxima of the α-scattering excitation function. They are also connected with the ALAS phenomenon as described, for instance, in Refs. [22,23]. We showed in Ref. [12] that the equivalent potential corresponding to the α-particle formation amplitude, considered as a wave function, has indeed a pocketlike shape. This behavior is connected with the peak

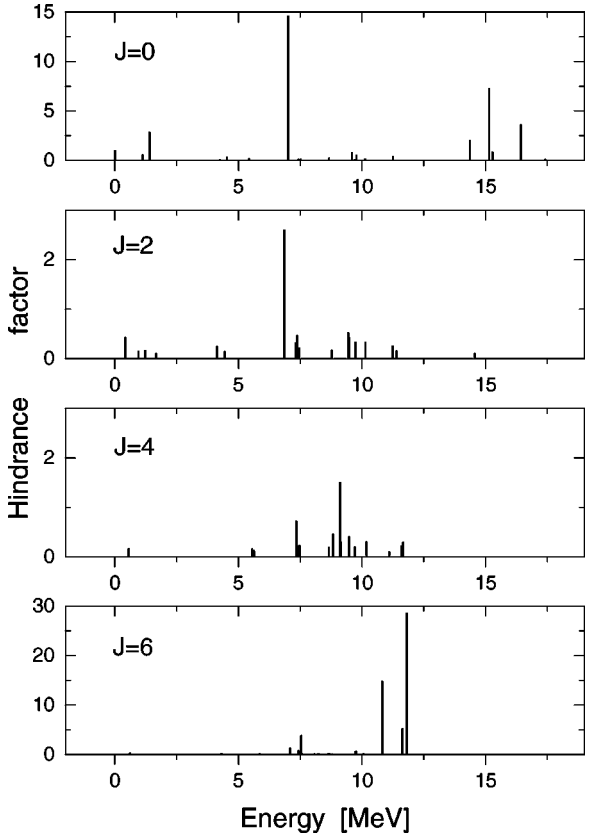

FIG. 1. The hindrance factors as functions of the excitation energy for $J = 0,2,4,6$ four-particle eigenstates.

of the formation amplitude in the nuclear surface region. This means that the nucleons in these quartet states can be found with a larger probability in the touching configuration region, orbiting with some angular momentum.

The microscopic structure of the first high-lying α-like states in terms of collective pairs is given in the second column of Table II for $J = 0,2,4$, respectively. One can observe that these states have a pronounced collective character, with many amplitudes of similar magnitude. In Table III we give the single-particle structure of the pair states involved in the quartet states of Table II. One can see that all of them have practically one dominant component involving only the first proton resonance $\pi p_{3/2}$ and the first neutron bound state $\nu f_{7/2}$. Therefore the structure of the first high-lying α-like states is very simple.

The final results of the resonant states are given in Table IV. Here are given the computed energies of the first high-lying α-like eigenstates (the third column) for each spin (the first column) with comparison to the experimental values (the second column). The experimental energies were obtained using a fitting procedure of the excitation spectrum at large angles [22,23]. For the $J = 2$ case we considered the mean value of the first two states, which are rather close. In Table IV one can notice the good agreement between our calculation and the experiment. This is especially satisfying when taking into account that these numbers were obtained on top of the pair eigenstates, without any additional param-

TABLE II. Quartet structure of the first high-lying α-like 0^+_{11}, 2^+_{33}, and 4^+_{43} eigenstates, respectively, in terms of two-particle pairs (the second column). The amplitudes are given in the third column.

$J^\pi_{a_4}$	$[J^\pi_{a_2}(\tau_1\tau_2)\otimes J^\pi_{a_2}(\tau'_1\tau'_2)]_{J^\pi}$	X
0^+_{11}	$[0^+_2(\pi\pi)\otimes 0^+_1(\nu\nu)]_{0^+}$	0.200
	$[2^+_2(\pi\nu)\otimes 2^+_2(\pi\nu)]_{0^+}$	0.213
	$[3^+_2(\pi\nu)\otimes 3^+_2(\pi\nu)]_{0^+}$	0.155
	$[4^+_2(\pi\nu)\otimes 4^+_2(\pi\nu)]_{0^+}$	0.137
	$[5^+_2(\pi\nu)\otimes 5^+_2(\pi\nu)]_{0^+}$	0.263
2^+_{33}	$[2^+_3(\pi\pi)\otimes 0^+_1(\nu\nu)]_{2^+}$	-0.298
	$[2^+_2(\pi\nu)\otimes 3^+_2(\pi\nu)]_{2^+}$	0.106
	$[3^+_2(\pi\nu)\otimes 3^+_2(\pi\nu)]_{2^+}$	-0.126
	$[2^+_2(\pi\nu)\otimes 4^+_2(\pi\nu)]_{2^+}$	0.218
	$[3^+_2(\pi\nu)\otimes 5^+_2(\pi\nu)]_{2^+}$	0.221
	$[4^+_2(\pi\nu)\otimes 5^+_2(\pi\nu)]_{2^+}$	-0.227
	$[5^+_2(\pi\nu)\otimes 5^+_2(\pi\nu)]_{2^+}$	0.169
4^+_{43}	$[2^+_3(\pi\pi)\otimes 2^+_1(\nu\nu)]_{4^+}$	0.225
	$[2^+_2(\pi\nu)\otimes 3^+_2(\pi\nu)]_{4^+}$	-0.128
	$[2^+_2(\pi\nu)\otimes 2^+_2(\pi\nu)]_{4^+}$	-0.129
	$[3^+_2(\pi\nu)\otimes 4^+_2(\pi\nu)]_{4^+}$	0.112
	$[1^+_2(\pi\nu)\otimes 5^+_2(\pi\nu)]_{4^+}$	0.140
	$[2^+_2(\pi\nu)\otimes 5^+_2(\pi\nu)]_{4^+}$	0.105
	$[5^+_2(\pi\nu)\otimes 5^+_2(\pi\nu)]_{4^+}$	0.325

eters. As a comparison we give in the last column the RGM results of Ref. [7], using the Brink-Boecker interaction B1. Concerning these last values we remark that in Refs. [6,8] better results were obtained by using a similar formalism, but different two-nucleon forces. Actually in Ref. [8] it has been clearly shown that the Brink-Boecker interaction B1 fails in reproducing the angular distribution for $\alpha+$Ca elastic scattering.

We stress the fact that this structure is stable against variations of the number of pair states included in the quartet basis. By increasing the number of pairs the position of the main maxima remains practically unchanged. We also mention that the amount of quartet eigenstates resulting from the diagonalization of the system (4) is much larger, but only a few states, plotted in Fig. 1, have large HF's (actually, a more appropriate name for the HF, which is the generally used term, in the present case of very strong α resonances would be ''enhancement factor'').

From Fig. 1 one can see that our calculations predict a much more complex resonance structure for the $\alpha+{}^{40}$Ca reaction than a simple rotational spectrum, given by the first high-lying α-like states. We predict strong resonances at about 10 MeV for $J=0,2,4,6$ and 15 MeV for $J=0$. We mention here that a similar fragmentation due to the core structure can be seen in the spectroscopic factor of the $\alpha+$Ar system, given by Fig. 2 of Ref. [9].

For states with odd spins we obtained HF's by 2 orders of magnitude smaller than unity implying no α resonances for odd spins contrary to experiment (the strong 1^- resonance obtained in [23]). Our result is consistent with the conclusion

TABLE III. Structure of the low-lying pair states (the second column), entering the quartet structure of Table II, in terms of the single-particle states given in Table I. The corresponding amplitudes are given in the third column.

$J^\pi_{a_2}(\tau_1\tau_2)$	$(\tau_1\otimes\tau_2)_{J^\pi}$	x
$0^+_2(\pi\pi)$	$(\pi p_{3/2}\otimes\pi p_{3/2})_{0^+}$	0.997
$2^+_3(\pi\pi)$	$(\pi p_{3/2}\otimes\pi p_{3/2})_{2^+}$	0.877
$0^+_1(\nu\nu)$	$(\nu f_{7/2}\otimes\nu f_{7/2})_{0^+}$	0.985
$2^+_1(\nu\nu)$	$(\nu f_{7/2}\otimes\nu f_{7/2})_{2^+}$	0.989
$2^+_2(\pi\nu)$	$(\pi p_{3/2}\otimes\nu f_{7/2})_{2^+}$	0.999
$3^+_2(\pi\nu)$	$(\pi p_{3/2}\otimes\nu f_{7/2})_{3^+}$	0.987
$4^+_2(\pi\nu)$	$(\pi p_{3/2}\otimes\nu f_{7/2})_{4^+}$	0.998
$5^+_2(\pi\nu)$	$(\pi p_{3/2}\otimes\nu f_{7/2})_{5^+}$	0.981

of the experimental paper [24]. Here it has been shown that it is difficult to assign this resonance to an α-cluster state. Our belief is that these states are actually connected with the $1\otimes 3$ partitions of the four-particle basis, which we did not consider in our analysis. This is also suggested by Ref. [9].

Regarding the low-lying states, their spectrum is more compressed than the experimental one at variance with the ^{208}Pb case where we obtained a very good agreement. Here the ^{40}Ca core is ''softer'' than ^{208}Pb (less distance between the major shells) and may be the explanation for the compression. This feature, however, seems to affect much less the high-lying part of the spectrum describing quasimolecular states, as can be seen from Table IV. As suggested in Refs. [10,11] it could be that the ^{36}Ar core would give a better description of the low-lying states.

In conclusion, we have described the four-particle eigenstates of the system $\alpha+{}^{40}$Ca within the MSM procedure by using as building blocks two ingredients: (1) the single particle eigenstates generated by the Woods-Saxon mean field including sharp resonances and (2) the pair collective states given by the residual surface-delta interaction.

In this way the result of the diagonalization, giving the four-particle spectrum in terms of the lowest pair eigenstates, is free of any additional parameters. We have predicted the existence of some high-lying states, strongly overlapping with the α-particle wave function. These states we call α-like states. It turned out that the energies of the first high-lying α-like states fit rather well the energies of the observed quasimolecular states. Their microscopic structure is collec-

TABLE IV. The experimental (Refs. [22,23], second column) and theoretical (third column) values of the energies of the quasimolecular resonances versus the spin (first column). In the last column the values of Ref. [7] are given for comparison.

J^π	$E_{\rm exp}$ [MeV]	$E_{\rm th}$ [MeV]	$E_{\rm th}$ [MeV]
0^+	6.67	7.01	5.10
2^+	7.22	7.13	5.69
4^+	7.75	7.34	7.09
6^+		7.53	

tive but has a very simple interpretation: the pair states of the basis contain with a large amplitude the first single-particle proton resonance $\pi p_{3/2}$ coupled with the first neutron bound state $\nu f_{7/2}$.

Our next goal is to generalize this analysis to superfluid nuclei, together with the $1 \otimes 3$ partitions of the four-particle basis, in order to describe the rich experimental data on quasimolecular states in the Ca region.

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