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Electric dipole collectivity in light nuclear systems

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α-^{18}O and α-Ca cluster configurations of ^{22}Ne and the ^{46,48,52}Ti isotopes, respectively, have been studied in a microscopically founded model, treating antisymmetrization between the clusters correctly. Depending on the respective ground state structure, these systems show rotational bands with weak (Ti isotopes) and strong (^{22}Ne) parity splitting. Irrespective of the degree of parity splitting, both cases exhibit $E1$ transitions between these cluster states, which are strong on the appropriate molecular scale. Though the influence of inelastic channels is discussed in qualitative terms only, both ^{22}Ne and the Ti isotopes appear to be promising candidates for the molecular-dipole degree of freedom to be seen in light nuclei.

I. INTRODUCTION

Recent theoretical and experimental studies[1-3] suggest the existence of molecular-dipole modes in heavy and light nuclei in addition to the established single-particle and collective shape degrees of freedom. In the range of light nuclei, strong $E1$ transitions have been observed between excited states in ^{18}O and have been interpreted as evidence for an $\alpha+{}^{14}$C molecular band of strong dipole collectivity.[3] As members of the band, Gai *et al.* suggested the 0_2^+ ($E^*=3.63$ MeV), 1_1^- (4.46 MeV), 2_3^+ (5.26 MeV), 3_3^- (8.29 MeV), and 4_3^+ (10.29 MeV) states in ^{18}O. A band of dipole collectivity should have three characteristics: (1) an alternating parity sequence of 0^+, 1^-, $2^+,\ldots$; (2) large cluster decay widths; and (3) an enhancement of $E1$ transitions. If isospin is a good quantum number, such $E1$ transitions are possible only for cluster configurations with $Z_AN_B-Z_BN_A\neq 0$. As a scale to identify dipole collectivity in light nuclei in terms of the $E1$ transition probability, Alhassid *et al.*[2] derived a sum rule for molecular $E1$ transitions for the case of velocity and/or isospin independent forces. This energy-weighted electric dipole sum rule involving two clusters with atomic and nuclear mass numbers (Z_A,N_A) and (Z_B,N_B), respectively, runs as follows:

$$S_1(E1;A,B)=\frac{9}{4\pi}\frac{(Z_AN_B-Z_BN_A)^2}{(N_A+N_B)N_AN_B}\frac{\hbar^2e^2}{2m}\ . \qquad (1.1)$$

The existence of $\alpha+{}^{14}$C molecular states had been predicted previously on the grounds of microscopic calculations[4,5] which exhibited an $\alpha+{}^{14}$C band of collective states with only little parity splitting. Based on these calculations, Assenbaum *et al.*[6] identified the calculated $\alpha+{}^{14}$C states with the members of the suggested dipole band and obtained $E1$ transition probabilities within the band which are strongly enhanced on the molecular scale of Ref. 2. However, the existence of a mixed parity $\alpha+{}^{14}$C molecular band became questionable by subsequent coupled channel calculations[7,8] studying the $\alpha+{}^{14}$C system on the basis of antisymmetric $\alpha+{}^{14}\mathrm{C}_{\mathrm{g.s.}}$ and $\alpha+{}^{14}\mathrm{C}(2_1^+)$ wave functions. Independently both calculations came to the conclusion that the sequence of ^{18}O states suggested in Ref. 3 as the mixed parity $\alpha+{}^{14}$C dipole band shows a more complex band structure and is apparently a mixture of the molecular $\alpha+{}^{14}$C bands in the elastic (0_2^+, 1_1^-, and 2_3^+ states) and the inelastic (3_3^- and 4_3^+ states) channels. According to the calculation by Suzuki *et al.*,[8] the $\alpha+{}^{14}\mathrm{C}_{\mathrm{g.s.}}$ band is completed by the 3_1^- ($E=5.10$ MeV), 4_2^+ (7.12 MeV), 5_1^- (8.13 MeV), and 6_1^+ (11.69 MeV) states which, however, do not follow the simple energy sequence of a rigid rotor. It should be noted that none of these microscopic calculations was *a priori* able to reproduce the correct energy positions of the $\alpha+{}^{14}$C states compared to the α threshold. In all calculations the energy positions were adjusted to experimental values by the variation of a potential parameter.

The $E1$ transition probabilities calculated in the coupled channel approaches are systematically smaller than in the corresponding single channel studies. This is caused by the fact that the negative parity states have a noticeable shell model component and are strongly affected by the enlargement of the model space through shell model configurations, gained by the introduction of the inelastic $\alpha+{}^{14}$C wave function.[7] On the other hand, the molecular $\alpha+{}^{14}$C states of positive parity are hardly affected by the coupling to the inelastic component. Even the coupled channel calculations predict $E1$ transition probabilities much larger than the experimentally observed values. This discrepancy may be removed by considering more appropriate shell model states in the microscopic models. For example, the $(sd)^2$ component of the ^{18}O ground state band is at most 50% in the calculation of Ref. 7, while the corresponding number is more than 90% in the more elaborate study of Sakuda *et al.*[9]

There is no experimental evidence for molecular dipole collectivity in other light systems yet. It is the aim of the present paper to discuss possible candidates for this novel degree of freedom, based on microscopic one-channel calculations. In view of the above $\alpha+{}^{14}$C results, however, it is necessary to check whether a molecular dipole band, predicted on the basis of a one-channel calculation, will retain its character when other (inelastic) channels are included. A rigorous test would require multichannel calculations which, for systems as heavy as the Ti isotopes discussed below, are out of scope. We shall, therefore, take recourse to qualitative arguments: (1) that molecular states, with the fragments well separated, do not tend to mix with (short-ranged) shell model configurations; and (2) that different molecular states will influence each other only if, incidentally, states of the same spin and parity are (approximately) degenerate in energy. Assumptions (1) and (2) are essential ingredients of the successful band crossing model[10] or the (slightly more general) double resonance model.[11]

II. THEORETICAL BACKGROUND

The many-body wave function of molecular-dipole states is taken as the antisymmetrized product of the internal wave functions of clusters A,B and their relative motion wave function,

$$\Psi=\mathscr{A}[\Phi_A\Phi_B h(\mathbf{r})] \ . \tag{2.1}$$

The internal wave functions Φ_A,Φ_B describe the 0^+ ground states of clusters A,B in the harmonic oscillator shell model; for simplicity the same b value is used for both clusters, which is taken as the weighted mean of the individual b values of A and B. After partial wave decomposition, the relative motion of the two clusters can be determined from a Schrödinger-type equation[12]

$$\Lambda_l \left[-\frac{\hbar^2}{2\mu}\Delta+V_l(r)-E \right] g_l(\mathbf{r})=0 \ . \tag{2.2}$$

The solutions g_l of Eq. (2.2) are related to the relative motion wave functions h_l of Eq. (2.1) by

$$h_l(\mathbf{r})=\sum_n \frac{1}{\sqrt{\mu_{nl}}}\langle U_{nl} \mid g_l \rangle U_{nl}(\mathbf{r}) \ , \tag{2.3}$$

where $U_{nl}(\mathbf{r})$ are the spherical harmonic oscillator wave functions of width $\beta=b/\sqrt{\mu_0}$, μ_0 being the reduced mass number. The m-quantum number of relative motion angular momentum is always suppressed to simplify notation. The normalization constants

$$\mu_{nl}=\langle \Phi_A\Phi_B U_{nl} \mid \mathscr{A} \mid \Phi_A\Phi_B U_{nl} \rangle \tag{2.4}$$

are calculated numerically, using the techniques of Ref. 13. Their appearance in (2.3) is due to the nonorthogonality of the wave functions Ψ of Eq. (2.1) caused by the antisymmetrizer $\mathscr{A}$. The projector Λ_l guarantees that g_l does not contain any Pauli-forbidden components which, when inserted into (2.1), lead to many-body wave functions which are identical zero due to antisymmetrization. The effect of Λ_l is reflected in the nodal structure of $g_l(r)$ in the interaction region.

The potentials $V_l(r)$ in (2.2) are local approximations to the true nonlocal potential of the orthogonalized resonating group method. Following Ref. 5 they can be calculated from the angular momentum projected diagonal matrix elements of the microscopic Hamiltonian $H=T+V-T_{\text{c.m.}}$ in the set of two-center Slater determinants $\Phi(\rho)$ which describe the clusters A and B in their ground states, moving in harmonic oscillator wells of the same width b and mean separation ρ. The functions $\Phi(\rho)$ are closely related to the ansatz (2.1) by virtue of the identity

$$\Phi(\rho)=\mathscr{A}\{\Phi_A\phi_B\exp[-(\rho-\mathbf{r})^2/\beta^2]\} \ . \tag{2.5}$$

In the present calculation $V_l(r)$ is assumed to be a sum of Gaussian functions plus the Coulomb potential of two uniformly charged spheres with radii $r_A=N_A r_c$, $r_B=N_B r_c$, $r_c=1.74$ fm.

The $E1$ transitions between molecular-dipole states of type (2.1) are governed by the matrix elements

$$\langle \Psi_l \mid \mathbf{D} \mid \Psi_{l'} \rangle = \sum_{n,n'} \frac{1}{\sqrt{\mu_{nl}\mu_{n'l'}}} \langle g_l \mid U_{nl} \rangle \langle U_{n'l'} \mid g_{l'} \rangle \times \langle \Phi_A\Phi_B U_{nl} \mid \mathscr{A}\mathbf{D}\mathscr{A} \mid \Phi_A\Phi_B U_{n'l'} \rangle \tag{2.6}$$

of the electric dipole operator $\mathbf{D}$, which can be decomposed into internal and relative motion parts,

$$\mathbf{D}=\mathbf{D}_A+\mathbf{D}_B+\mathbf{D}_r \ . \tag{2.7}$$

The many-body matrix element in (2.6) can be reduced to[6]

$$\langle \Phi_A\Phi_B U_{nl} \mid \mathscr{A}\mathbf{D}\mathscr{A} \mid \Phi_A\Phi_B U_{n'l'} \rangle = \mu_{NL} \langle U_{nl} \mid \mathbf{D}_r \mid U_{n'l'} \rangle \ , \tag{2.8}$$

with $N=n,L=l$ if $2n+l<2n'+l'$, otherwise $N=n'$, $L=l'$; $\mathbf{D}_r$ is proportional to $\mathbf{r}$,

$$\mathbf{D}_r=e\frac{Z_A N_B - Z_B N_A}{N_A+N_B}\mathbf{r} \ . \tag{2.9}$$

The final result,

$$\langle \Psi_l \mid \mathbf{D} \mid \Psi_{l'} \rangle = \langle g_l \mid \mathbf{D}_r \mid g_{l'} \rangle + \sum_{n,n'} \left[\frac{\mu_{NL}}{\sqrt{\mu_{n'l'}\mu_{nl}}} - 1 \right] \langle g_l \mid U_{nl} \rangle \langle U_{n'l'} \mid g_{l'} \rangle \langle U_{nl} \mid \mathbf{D}_r \mid U_{n'l'} \rangle \ , \tag{2.10}$$

contains many-body effects through the second term, which is a direct consequence of antisymmetrization and would be missing in naive, phenomenological models of relative motion. Note, however, that antisymmetrization effects are also contained in the nodal structure of the relative motion wave function $g_l(r)$ obtained from solving Eq. (2.2). The division of the dipole matrix element according to (2.10) is also the appropriate form for numerical computation, since the second term is a short-ranged correction to the first one and converges reasonably fast.

While the expansion of $g_l(\mathbf{r})$ in terms of $U_{nl}(\mathbf{r})$ in (2.6) causes no numerical problems for bound state solutions of (2.2), special care is required for (non-normalizable) resonant states due to the notorious Coulomb oscillations. For the Ti isotopes to be discussed below, no problem occurs since the resonant states of interest have small enough α-decay widths Γ_α to be approximated by bound states. Such an approximation is not reliable for some of the ^{22}Ne states in question (see below) which have large α widths. As long as one of the states is bound (or at least quasi-bound), the $E1$ matrix element (2.6) converges reasonably fast, and we may proceed as follows: In a first step, the $E1$ capture cross section,[14]

$$\sigma(E)=\frac{16\pi}{9}\frac{1}{\hbar v_{\text{rel}}}\left[\frac{E_\gamma}{\hbar c}\right]^3 |\langle \Psi_i(E)|\mathbf{D}|\Psi_f\rangle|^2\,, \tag{2.11}$$

is calculated microscopically as described above, where $\Psi_i(E)$ is a scattering state of type (2.1) and solves Eq. (2.2). A Breit-Wigner fit to $\sigma(E)$ near resonance energy E_R,

$$\sigma(E)=\frac{\pi}{k^2}(2l_i+1)\frac{\Gamma_\gamma\Gamma_\alpha}{(E-E_R)^2+\frac{1}{4}\Gamma_\alpha^2} \tag{2.12}$$

determines the ratio of γ width Γ_γ to α width Γ_α. In the present context, the latter is a safe approximation to the total width Γ_{tot} which originally appears in (2.12). The α width is extracted from elastic scattering phase shifts obtained in the microscopic potential model. With Γ_γ known, the desired $B(E1)$ value is obtained from

$$\Gamma_\gamma=\text{const}\times E_\gamma^3 B(E1)\,. \tag{2.13}$$

If Γ_γ is measured in eV, E_γ in MeV, and $B(E1)$ in $e^2\text{fm}^2$, then the constant in (2.13) takes the value 1.045.

III. APPLICATIONS

A. The α-^{18}O system

The present study uses an oscillator length of $b=1.49$ fm for both the $(1s)^4$ configuration of the α particle and the

$$\{(1s)^4(1p)^{12}(1d_{5/2})^2_{J=0}\}$$

configuration of the ^{18}O ground state. According to Ref. 15 this configuration exhausts about 75% of the ground state wave function and may be considered a reasonable approximation to the ^{18}O ground state. The l-dependent, local potential $V_l(r)$ of Eq. (2.2) is the one obtained by Wintgen *et al.*[5] on a microscopic basis using the V1 force of Volkov. Solving Eq. (2.2) with appropriate boundary conditions one obtains the bound state energies as well as energies and α widths of the low resonances. As for the α-^{16}O case, one finds band structures with substantial parity splitting (of the order of 5 MeV); a negative parity band lies in between two positive parity bands which repel each other. The lower positive parity band corresponds to the ground state band in ^{22}Ne with dominant shell model structure,[4] and is not further discussed in the present context. Both the upper positive and the negative parity bands show pronounced α clustering and are, despite the parity splitting, promising candidates for collective $E1$ transitions. In fact, the $B(E1)$ values (Table I) calculated on the basis of Eqs. (2.6)—(2.9) are large on the scale of the molecular sum rule (1.1). Note that this sum rule represents only a qualitative measure since the assumptions on which (1.1) is based are not fulfilled in the present model where the effective nucleus-nucleus interaction is nonlocal. This is due to the use of antisymmetrized many-body wave functions and, in the present case, essentially introduces a parity dependence.[4] As a first step to coupled channel calculations, one may include the $(2s)^2$ configuration of ^{18}O as a rough approximation of the 0^+ excited state at 5.34 MeV. It turns out[13,16] that the two channels do not influence each other noticeably, apart from the lowest 8^+ states where the requirements of the double resonance mechanism are fulfilled.

B. The α-Ca systems

Molecular structure with little parity splitting ($\approx$0.5 MeV) has been observed[17] in good agreement with microscopic calculations[18] for the α-^{40}Ca system. Analogous calculations for the ^{46,48,52}Ti isotopes[19] predict similar structures for those systems. They cannot be observed in elastic α scattering as they lie well below the Coulomb barrier and absorption is stronger, especially for the α-^{44}Ca system, than for α-^{40}Ca. However, these structures might be detectable in transfer reactions like (^{6}Li,d), and could be identified by strong $E1$ (and $E2$) transitions. We have, therefore, studied the α-^{42,44,48}Ca systems in the elastic channel and calculated $B(E1)$ values, using the microscopically founded potential of Ref. 5, and the corresponding wave functions of Ref. 19. Of special interest is, of course, the α-^{48}Ca system where the $(Z_AN_B-Z_BN_A)^2$ factor is largest and absorptive effects

TABLE I. $E1$ transitions between the α-^{18}O resonances with positive parity and the lowest ^{22}Ne negative parity band. Energies E_i,E_f are taken with respect to the α-^{18}O threshold; the α widths Γ_α refer to the respective final states, and the $B(E1)$ values are given in standard Weisskopf units (W.u.). The last column shows the fraction of the molecular sum rule S_1, Eq. (1.1), corresponding to the various transitions.

J_f	J_i	E_f (MeV)	E_i (MeV)	Γ_α (keV)	$B(E1)$ (W.u.)	Fraction of S_1
0	1	1.93	-5.83	49.6	0.025	0.65
2	1	2.84	-5.83	195.6	0.058	1.70
2	3	2.84	-3.62	195.6	0.032	0.70
4	3	5.07	-3.62	680.3	0.063	1.85
4	5	5.07	0.29	680.3	0.028	0.45

TABLE II. Energy positions (in MeV from Ref. 17) and $E1$ transition probabilities within the suggested α + Ca molecular-dipole band in the ^{46,48,52}Ti isotopes. The $E1$ transition probabilities $B(E1, J-1 \to J)$ are given in standard Weisskopf units (W.u.) and are compared with respect to the molecular sum rule (1.1).

	^{46}Ti			^{48}Ti			^{52}Ti		
J	E^*	$B(E1)$	Fraction of S_1	E^*	$B(E1)$	Fraction of S_1	E^*	$B(E1)$	Fraction of S_1
0	12.63			13.43			10.04		
1	13.23	0.063	1.02	14.10	0.21	1.05	10.97	0.57	1.26
2	13.24	0.042	0.01	14.02	0.08[a]	0.05	10.70	0.22[a]	0.14
3	14.26	0.038	1.05	15.13	0.12	1.02	12.12	0.34	1.13
4	14.65	0.035	0.37	15.40	0.11	0.22	12.31	0.29	0.13
5	16.14	0.031	1.23	16.98	0.11	1.27	13.92	0.30	1.12

[a] In ^{48,52}Ti the 2^+ state is lower in energy than the 1^- state. Hence, the corresponding reduced matrix element is $B(E1, J \to J-1)$.

smallest. Since these structures have comparatively small α widths, one may use the bound state approximation for all states in question.

The energies of Ref. 19 (see Table II) exhibit little parity splitting, as for the α-^{40}Ca system. The corresponding $B(E1)$ values increase from ^{46}Ti to ^{52}Ti. This is due to the $(Z_A N_B - Z_B N_A)^2$ factor, whereas the nuclear matrix elements decrease with increasing mass number, reflecting a decreasing collectivity[19] of the α-Ca dipole states. As an example, the α-^{48}Ca relative motion wave functions have been analyzed in terms of the squares of the expansion coefficients in the oscillator basis (Fig. 1). The distribu-

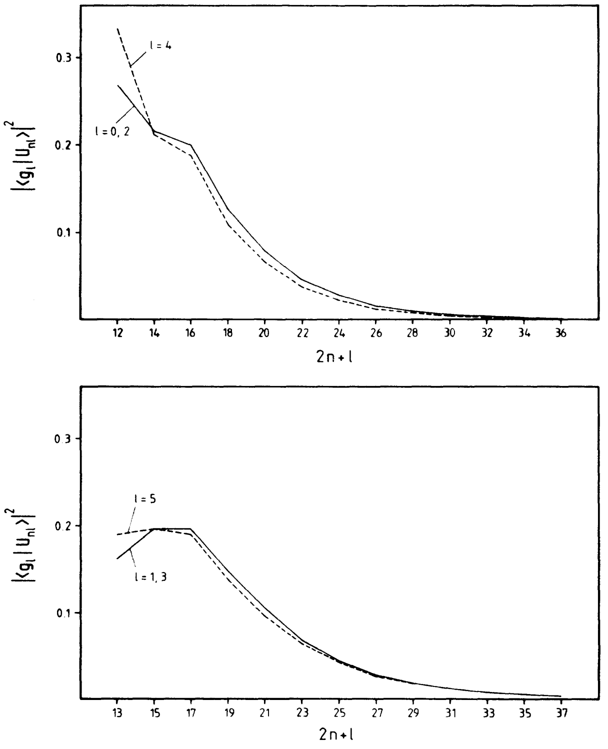

FIG. 1. Absolute squares of the expansion coefficients of the relative motion wave functions g_l of the α-^{48}Ca molecular states in the harmonic oscillator basis $\{U_{nl}\}$ for various partial waves. The values for $l=0,2$ and for $l=1,3$ are identical within drawing accuracy. The oscillator states with $2n+l<12$ and 13, respectively, are Pauli forbidden.

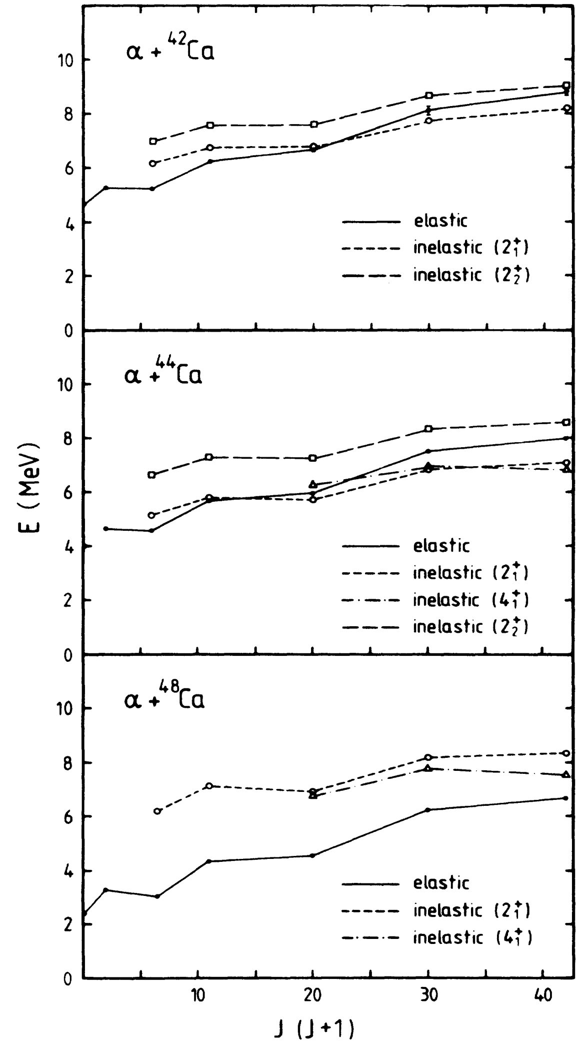

FIG. 2. Schematic band crossing diagrams for the α-^{42}Ca, α-^{44}Ca, α-^{48}Ca systems. The elastic bands have been taken from Ref. 19. Inelastic bands have been derived assuming identical diagonal potentials in the elastic and inelastic channels (Ref. 10) and adopting the experimental values of the respective excitation energies; only aligned bands are shown. The energy scale refers to the relative motion energy in the elastic channel.

tion is similar for positive and negative parity components, and the long tail of the distribution indicates the collectivity of these cluster states. Comparing the various transitions with respect to the sum rule (1.1), one finds enhancement for the $0^+\rightarrow1^-$, $2^+\rightarrow3^-$, and $4^+\rightarrow5^-$ transitions, as expected for collective states of molecular dipole type. Although the absolute $B(E1)$ values are of the same order of magnitude for all transitions, the $1^-\rightarrow2^+$ and $3^-\rightarrow4^+$ transitions seem to be much weaker on the basis of the sum rule. This is obviously a consequence of the (weak) parity splitting which, incidentally, results in the 1^- and 2^+ and the 3^- and 4^+ states, respectively, being almost degenerate. Hence the $1^-\rightarrow2^+$ and $3^-\rightarrow4^+$ transitions are suppressed in (1.1) by the energy weight factor, while for the other group of transitions the parity splitting increases the energy weight factor compared to an ideal rotator. Extrapolating to the ideal rotator case, e.g., for ^{46}Ti with the slope of the band taken from the $0^+\rightarrow2^+$ transition, one finds fractions of S_1 between 35% and 85%. Taken together, one may view these transitions as enhanced on the molecular scale.

In contrast to the α-^{14}C case, both positive and negative parity states are dominantly α-cluster configurations, hence they are unlikely to mix with shell model configurations which are of short range. Coupling to α-cluster configurations of inelastic channels is possible if states with the same spin and parity as in the elastic channel are degenerate in energy. We have, therefore, calculated the corresponding bands in the band crossing model[10] (or the equivalent double resonance model[11]) for the lowest excitations of the Ca isotopes. The result (Fig. 2) shows that there should be no disturbance of the molecular dipole band for α-^{48}Ca where the various bands do not cross. For α-^{42}Ca and α-^{44}Ca there are band crossings, and a disturbance of the elastic molecular dipole bands cannot be excluded by the above qualitative arguments.

IV. SUMMARY

In conclusion, we find that the systems investigated in this paper are potential candidates for the molecular-dipole degree of freedom to be seen in light nuclei. Although the α-^{18}O system shows marked parity splitting, and thus violates criterion (1), one expects strong $E1$ transitions between the positive parity resonances and negative parity states as they all have a well pronounced cluster structure. In fact, the $B(E1)$ values are enhanced on the molecular scale as provided by the sum rule (1.1). A strong enhancement of $E1$ transitions is also found for the α-Ca cluster states of the Ti isotopes for which all three criteria are well fulfilled. With regard to absorption, the α-^{48}Ca system seems to be the best candidate for detecting collective $E1$ transitions in experiment.

The results of the present study rest on the validity of one-channel calculations and may be destroyed if the α-cluster configurations under discussion are disturbed by configurations with internal cluster excitation, as observed for α-^{14}C. As the states (and resonances) of the present study are strongly clustered, the admixture of shell model configurations is unlikely. The influence of collective states with cluster excitation is weak for the α-^{18}O system, according to the coupled channel study of Ref. 13. For the Ti isotopes, a rough estimate on the basis of the band crossing model shows that a disturbance of the single-channel results can be excluded only for the α-^{48}Ca system. Hence ^{52}Ti turns out to be a most promising candidate to find the novel degree of dipole collectivity in light nuclei.

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