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Proton Pygmy Dipole Resonances in ^{17,18}Ne: Collective vs Noncollective

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The proton pygmy dipole resonances (PDRs) in the proton rich nuclei ^{17,18}Ne are investigated in the framework of the interacting shell model. The shell model with the self-consistent Skyrme-Hartree-Fock wave functions well reproduces the experimental data of the ground state properties. The proton PDRs in the neighboring ^{17,18}Ne are predicted. However, the detailed study involving the transition densities and collectivity shows that the PDR in ¹⁷Ne is highly collective and due to the oscillation of the valence protons against the interior core, while in ¹⁸Ne the dipole resonance in the PDR region is noncollective and more likely to be the configuration splitting of the giant dipole resonances.

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The exotic behavior of nuclei approaching the drip lines is one of the top subjects in nuclear physics studies. The loosely bound nucleons can oscillate against the isospin saturated core. Large enhancement of electric dipole (E1) response is expected in the low-energy region, namely the pygmy dipole resonance (PDR). Although PDR exhausts only a few percent of total energy weighted sum rule, nucleon capture rates could be largely enhanced in the r-process nucleosynthesis [1]. The neutron PDRs have been intensely studied in the heavy and medium-heavy nuclei [2–9]. Due to the existence of Coulomb barrier, the proton skin or halo can only appear in the light nuclei and is less profound than the neutron skin or halo. And the proton PDRs are much rarer than the neutron PDRs [10, 11]. However, the nature of PDRs is still controversial since not only the PDRs can be developed by this soft mode, but also the single particle excitation near the threshold can enhance the dipole excitations [3, 12, 13]. The controversy can be further shown by the fact that the mean field theories predicted the increasing integrated strength of neutron PDRs with the increasing of the neutron excess or the neutron skin thickness [2], while the experimental studies show a nontrivial dependence of the total E1 strength as a function of the neutron number, such as in 40,44,48 Ca [14, 15]. In some light and heavy nuclei, the relativistic and nonrelativistic theories also predicted the low-lying strengths to be noncollective nature [16–18].

Most of the studies on the pygmy and giant dipole resonances are based on the mean-field theory with randomphase-approximation (RPA) or quasiparticle RPA. However the mean-field theories can not give the mixing of different configurations, which is critical for loosely bound nuclei. The collectivity of the giant dipole resonances (GDRs) in the light nuclei is less profound than in the medium-heavy and heavy nuclei. Therefore the response function could distribute over several configuration dependent peaks. For electric dipole resonances, most of the contributions come from the cross shell $(\Delta N = 1)$ particle-hole excitations near the Fermi surface. Although conventional configuration mixing shell model is confined in a restricted valence space, it was shown that the GDRs were well reproduced with this model in the light nuclei [19, 20]. Another advantage of the shell model is that the pairing effect is well treated which is very important in the open-shell nuclei especially in the Borromean nuclei, such as 11 Li and 17 Ne. With the pygmy dipole resonances lying in the lower energy region, the fully microscopic shell model calculations could provide more insightful prediction in the light nuclei. In Refs. [21, 22] the shell model studies on the neutron PDRs in light or medium nuclei were reported, with rare examples of the proton PDRs [23]. The PDRs in neutron-rich oxygen isotopes predicted by the shell model [19] were confirmed experimentally [24]. However only transition strength was given in the previous shell model studies. The detailed transition densities and collectivity are very important to reveal the dynamics of the proton PDRs.

¹⁷Ne and ¹⁸Ne exhibit proton halo or skin in spite of Coulomb barrier [25]. The Borromean ¹⁷Ne is a prominent candidate for a two-proton halo, which can be regarded as an ¹⁵O core in its ground state plus two protons in the d^2 or halo like s^2 configurations. The non-resonant soft dipole mode in ¹⁷Ne was predicted by a three-body model [26]. In the present paper, the pygmy dipole resonances in ¹⁷Ne and ¹⁸Ne are predicted in the interacting shell model. The differences of PDRs in these two nuclei are discussed when the transition densities and information on collectivity are available.

The one-body transition density (OBTD) is the standard output of the shell model code such as Oxbash and NuShell@MSU [27]. The OBTDs are unrelated to the radial wave function but related to the angular momentum part between the initial and final states. Thus the transition matrix element can be given by the transition operator and the transition density can be given by the density operator using the same OBTDs. The detailed formulas will be given as follows.

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In the second-quantized representation, the λ -rank one-body operator reads

$$\hat{O}^{\lambda}_{\mu} = \sum_{\alpha\beta} \langle \alpha | O^{\lambda}_{\mu} | \beta \rangle a^{+}_{\alpha} a_{\beta}, \qquad (1)$$

where α stands for the single particle quantum number set $(n_{\alpha}l_{\alpha}j_{\alpha}m_{\alpha})$. In the shell model *M*-scheme, this operator can be written in the tensor coupled form [28],

$$\hat{O}^{\lambda}_{\mu} = \sum_{k_{\alpha}k_{\beta}} \langle k_{\alpha} || O^{\lambda} || k_{\beta} \rangle \frac{\left[a^{+}_{k_{\alpha}} \otimes \tilde{a}_{k_{\beta}}\right]^{\lambda}_{\mu}}{\sqrt{2\lambda + 1}}, \qquad (2)$$

where k_{α} stands for $(n_{\alpha}l_{\alpha}j_{\alpha})$. The reduced transition matrix element between the final state $|J_f\rangle$ and initial state $|J_i\rangle$ can be expressed by the OBTDs and reduced single-particle matrix elements of the valence orbitals,

$$\langle J_f || \hat{O}^{\lambda} || J_i \rangle = \sum_{k_{\alpha} k_{\beta}} \text{OBTD}(fik_{\alpha} k_{\beta} \lambda) \langle k_{\alpha} || \hat{O}^{\lambda} || k_{\beta} \rangle, \quad (3)$$

where J_i and J_f include all the quantum numbers needed to distinguish the states, and OBTD is given by

$$OBTD(fik_{\alpha}k_{\beta}\lambda) = \frac{\langle J_f || \left[a_{k_{\alpha}}^+ \otimes \tilde{a}_{k_{\beta}} \right]^{\lambda} || J_i \rangle}{\sqrt{2\lambda + 1}}.$$
 (4)

The OBTD can also be defined including the isospin freedom [28].

The transition density between the final state $|J_f\rangle$ and initial state $|J_i\rangle$ is defined as

$$\delta\rho(\vec{r}) = \langle J_f | \sum_i \delta(\vec{r} - \vec{r_i}) | J_i \rangle, \tag{5}$$

and the radial transition density $\delta \rho_{\lambda}(r)$ is given by

$$\delta\rho(\vec{r}) \equiv \sum_{\lambda,\mu} \delta\rho_{\lambda}(r) Y_{\lambda\mu}(\hat{r}).$$
(6)

Using the orthonormal relation of spherical harmonics, we have

$$\delta\rho_{\lambda}(r) = \int \langle J_f | \sum_{i} \delta(\vec{r} - \vec{r_i}) | J_i \rangle Y^*_{\lambda\mu}(\hat{r}) d\Omega.$$
(7)

As $\delta(\vec{r} - \vec{r_i}) = \frac{1}{4\pi r^2} \delta(r - r_i) \delta(\hat{r}, \hat{r}_i)$, integrate out the angular part,

$$\delta \rho_{\lambda}(r) \sim \frac{\langle J_f || \sum_i \frac{1}{r^2} \delta(r - r_i) Y_{\lambda} || J_i \rangle}{\sqrt{2J_i + 1}}.$$
 (8)

In order to normalize the radial transition density to the transition strength, we leave out the coefficient in front of Eq.(8) and redefine it as

$$\delta \rho_{\lambda}(r) \equiv \frac{\langle J_f || \sum_{i} \frac{1}{r^2} \delta(r - r_i) Y_{\lambda} || J_i \rangle}{\sqrt{2J_i + 1}} \\ = \frac{1}{\sqrt{2J_i + 1}} \sum_{k_{\alpha}, k_{\beta}} \text{OBTD}(fik_{\alpha}k_{\beta}\lambda) \\ \times \langle k_{\alpha} || \frac{1}{r^2} \delta(r - r') Y_{\lambda} || k_{\beta} \rangle, \tag{9}$$

where

$$\langle k_{\alpha} || \frac{1}{r^2} \delta(r - r') Y_{\lambda} || k_{\beta} \rangle = \psi_{k_{\alpha}}(r) \psi_{k_{\beta}}(r) \langle k_{\alpha} || Y_{\lambda} || k_{\beta} \rangle,$$
(10)

 $\psi_{k_{\alpha}}(r)$ is the radial wave function of the valence orbital k_{α} . For a λ -rank one-body transition operator,

$$\hat{O}^{\lambda}_{\mu}(\vec{r}) = r^{\lambda} Y_{\lambda\mu}(\hat{r}), \qquad (11)$$

using Eq.(3) and Eq.(9), the electric reduced transition probability $B(E\lambda)$ is readily expressed with the proton radial transition densities,

$$B(E\lambda, i \to f) = \frac{\left| \langle J_f || \hat{O}^{\lambda} || J_i \rangle \right|^2}{2J_i + 1}$$
$$= \left[\int e\delta \rho^p_{\lambda}(r) r^{\lambda + 2} dr \right]^2.$$
(12)

However, since the effective charges are frequently used in the calculation of $B(E\lambda)$, Eq.(12) should be modified accordingly using both proton and neutron transition densities,

$$B(E\lambda, i \to f) = \left[\int \left[e_p^{\text{eff}} \delta \rho_\lambda^p + e_n^{\text{eff}} \delta \rho_\lambda^n \right] r^{\lambda+2} dr \right]^2, \quad (13)$$

where e_p^{eff} and e_n^{eff} are the effective charges of protons and neutrons respectively.

In the present shell model calculations. the NUSHELL@MSU code [27] with the WBP10 effective interaction [29] in the spsdpf model space, is used. The Warburton-Brown interaction WBP was originally constructed by fitting the energy levels in the $0 - 1\hbar\omega$ space. In the WBP10 interaction, the coupling between the following multi- $\hbar\omega$ configurations is cut off, i.e. the two-body matrix elements for the $1p - 1h 2\hbar\omega$ excitations are all set equal to 0 due to the Hartree-Fock condition. The cross shell $2\hbar\omega$ two-body matrix elements between $0s^2$ and $0p^2$ are also set equal to 0. The WBP10 interaction is enclosed in the NUSHELL@MSU package. The standard Lawson method is used to remove the center-of-mass spurious components in the wave function by adding a fictitious Hamiltonian which acts only on the center-of-mass excitation [30]. In the present calculation, the $0 - 1\hbar\omega$ configuration space is adopted. Our calculation shows that the whole picture of the calculated E1 response function is similar if the $2-3\hbar\omega$ configurations are included, also see the discussion in Ref. [22].

The s^2 occupation probability of the ground state in ¹⁷Ne is very controversial in theoretical predictions [25, 26]. Three-body cluster theory predicted a large s^2 component and therefore a halo-like structure. However the analysis based on the Coulomb displacement energies [31, 32] or the magnetic moment [33] suggested a

TABLE I: The mass and charge radii in 17,18 Ne. SM(HO) and SM(HF) denote the shell model results using the harmonic oscillator and Hartree-Fock single particle wave functions.

A	J^{π}	proton s^2 probability		δ_{pn} (fm)			mass radii (fm)				charge radii (fm)			
		FMD	SM	FMD	$\rm SM(HO)$	SM(HF)	Exp.	FMD	SM(HO)	SM(HF)	Exp.	FMD	SM(HO)	SM(HF)
17	$1/2^{-}_{g.s.}$	42%	23.6%	0.45	0.17	0.43	2.75(7)	2.75	2.78	2.86	3.042(21)	3.04	2.85	3.02
18	$0_{g.s.}^{+}$	15%	15.0%		0.15	0.25	2.81(14)	2.70	2.78	2.82	2.971(20)	2.93	2.85	2.93
\$ \$		//2	$\langle / m^2 \rangle$											

 ${}^{\$}\delta_{pn} = \sqrt{\langle r^2 \rangle_p} - \sqrt{\langle r^2 \rangle_n}$



FIG. 1: (color online) The nucleon and matter density distributions of the ground states in 17,18 Ne. The experimental errors are indicated by the gray area.

smaller s^2 component. In table I the ground state properties in ^{17,18}Ne calculated by the shell model are compared with the experimental data and Fermion Molecular Dynamic (FMD) model results. Obviously for the nuclei near the drip lines, it is not appropriate to use the harmonic wave functions but Wood-Saxon or mean-field wave functions [19, 34] when calculating physical properties involving single-particle radial wave functions. In our calculations, the self-consistent Skyrme-Hartree-Fock (SHF) wave functions with the SKM^{*} interaction [35] are used in the evaluation of nuclear radii and electric transition matrix elements. The wave functions of positive energy states are obtained by the box approximation. When the harmonic oscillator wave functions is used, the parameter b = 1.8 fm is adopted which is slightly larger than the value $b = \sqrt{41.4/\hbar\omega}$ where $\hbar\omega$ is the global fit $\hbar\omega \approx 45A^{-1/3} - 25A^{-2/3}$ [36]. Clearly from table I, the shell model with the SHF wave functions well reproduces the mass radii and charge radii both in ^{17,18}Ne. In Fig. 1 the calculated nucleon and matter density distributions are compared with the available experimental data. It is worth noting that the halo nucleon can appear in the classically forbidden region for the halo nuclei [37]. In the present calculations, the probabilities of finding one proton at r > 5 fm is 41% and 28% in ^{17,18}Ne respectively. In ¹⁷Ne, this probability is close to the FMD prediction of 40%. Thus by employing the more realistic radial wave functions, the halo-like structure in ¹⁷Ne is reproduced in the shell model without changing the composition of configurations.

To further remove the additional spurious components due to the usage of the Skyrme-Hartree-Fock wave functions, the center-of-mass removed dipole operator is used [38] in the calculation of the dipole transition strength,

$$\tilde{Q}^{\lambda=1}_{\mu} = e \frac{N}{A} \sum_{i}^{Z} r_{i} Y_{1\mu}(\hat{r}_{i}) - e \frac{Z}{A} \sum_{i}^{N} r_{i} Y_{1\mu}(\hat{r}_{i}).$$
(14)

where Z, N and A are proton, neutron and mass number, respectively. The effectiveness of this method was demonstrated in Ref. [19]. In order to smooth out the discrete strengths, the transition strengths are averaged by a Lorentz type factor $\rho(\omega)$

$$\frac{d\bar{B}(E1;\omega)}{d\omega} = \int \sum_{n} B(E1;\omega_n)\rho(\omega-\omega_n)d\omega, \quad (15)$$

where ω is the phonon energy and

$$\rho(\omega - \omega_n) = \frac{1}{\pi} \frac{\Gamma/2}{(\omega - \omega_n)^2 + \Gamma^2/4}.$$
 (16)

The arbitrary total width $\Gamma = 1$ MeV is chosen. In this way, the response function is like the superposition of many isolated Breit-Wigner resonances.

The electric dipole response functions and the B(E1) values of discrete transitions in ^{17,18}Ne are shown in Fig. 2. We have included the contribution from $T = T_z$ and $T = T_z + 1$ states, in order to give the energy-weighed sum rule (EWSR) which is comparable with the Thomas-Reiche-Kuhn (TRK) sum rule. As an odd-A nucleus, the level density in ¹⁷Ne is much higher than in even-A ¹⁸Ne, so the isovector dipole transition strengths in ¹⁷Ne more spread out than in ¹⁸Ne. The shell model predicts two levels in ¹⁷Ne and one level in ¹⁸Ne with strong E1



FIG. 2: (color online) Electric dipole response functions from the excited states to the ground state in 17,18 Ne with the Skyrme-Hartree-Fock single particle wave functions. The thin lines are the B(E1) values of discrete transitions in the shell model calculations, with the cyan lines representing the $J^{\pi}=1/2^+$ ($J^{\pi}=1^-$) states in 17 Ne (18 Ne), the purple lines representing the $J^{\pi}=3/2^+$ states in 17 Ne.

transitions around 10 MeV, which will give appreciable pygmy resonances. In ¹⁷Ne, the shell model also predicts a very low $J^{\pi} = 1/2^+$ state at E = 1.87 MeV which is 0.39 MeV above the proton emission threshold. A B(E1) value 0.00277 fm² could indicate some importance for the astrophysical 2p capture of ${}^{15}O$ in the hot CNO cycle. In 18 Ne, the recent study using the approach of Hartree-Fock-Bogoliubov + quasi-particle random-phase-approximation (HFB+QRPA) with the Gogny force did not predict a PDR around 10 MeV [39]. Although the pairing was included, their calculations gave the lowest resonance at 14.2 MeV whose transition densities behave more close to the giant dipole resonance. For ¹⁸O, the mirror nucleus of ¹⁸Ne, several peaks around 10 MeV were already observed [40, 41]. Only with phonon coupling to the resonance included, the QRPA plus phonon coupling model can give some strength around 10 MeV in 18 O [16].

The sum rule is a useful measure of the collectivity of the giant resonances. For the isovector GDR, the classical energy weighted sum rule is given by

$$S(\text{TRK}) = \sum_{n} \hbar \omega_n |\langle n | \hat{O}_{\mu}^{\lambda=1} | g s \rangle|^2 = \frac{\hbar^2}{2m} \frac{9}{4\pi} \frac{NZ}{A}$$
$$= 14.9 \frac{NZ}{A} e^2 \text{ (MeV} \cdot \text{fm}^2) \tag{17}$$

neglecting the contributions of exchange terms. This is known as the Thomas-Reiche-Kuhn (TRK) sum rule. There is another sum rule, named the energy-weighted cluster sum rule which can be viewed as a measure of

TABLE II: Ground state spins, nonenergy weighted sum rule (NESR) and energy weighted sum rule (EWSR) values of E1 transitions in ^{17,18}Ne. The values are obtained by summing up to $E_x = 40$ MeV. The cluster sum rules are obtained assuming that the valence cluster has Z = 2, A = 2.

Nuclide	$s J_{g.s.}^{\pi}$	Т	$\frac{\rm EWSR}{({\rm MeV}e^2{\rm fm}^2)}$	S(TRK) (MeV e^2 fm ²)	$\frac{\text{EWSR}}{S(\text{TRK})}$ (%)		
17 Ne	$1/2^{-}$	3/2	36.7				
		5/2	30.2	61.4	109		
		Tot	66.9				
$^{18}\mathrm{Ne}$	0^{+}	1	35.8				
		2	47.0				
		Tot	82.8	66.2	125		
Nuclide	$s J_{g.s.}^{\pi}$	T	$\frac{\text{EWSR(pygmy)}}{(\text{MeV}e^2\text{fm}^2)}$		$\frac{\text{EWSR(pygmy)}}{S_{\text{cluster}}}$ (%)		
$^{17}\mathrm{Ne}$	$1/2^{-}$	3/2	3.25	5.73	56.7		
$^{18}\mathrm{Ne}$	0^{+}	1	2.59	6.62	39.1		

the adiabaticity between the giant and pygmy resonances [22, 42]. Assuming that the nucleus (A, Z) can be decomposed into two clusters with (A_1, Z_1) and (A_2, Z_2) , the cluster sum rule is given by

$$S(\text{cluster}) = \frac{\hbar^2}{2m} \frac{9}{4\pi} \frac{(Z_1 A_2 - Z_2 A_1)^2}{A A_1 A_2}.$$
 (18)

Table II gives the sum rules of PDRs and GDRs in ^{17,18}Ne. Since the high-lying $T = T_z + 1$ states do not contribute to the response functions in the pygmy region, only the $T = T_z$ states are included in the lower table. Using E = 12 MeV as a cut energy, the pygmy resonances exhaust 4.9% and 3.1% of the total sum rules in ^{17,18}Ne, respectively. In the FMD calculations, ^{17,18}Ne can be interpreted essentially as the ¹⁵O or ¹⁶O cores plus two protons found mainly in the s^2 or d^2 configurations [25]. If assuming the two protons as the valence nucleons and other nucleons as the core, the pygmy resonances will exhaust 56.7% and 39.1% of the cluster sum rules in ^{17,18}Ne, respectively.

Although the transition strengths in ^{17,18}Ne seem to be similar, however, only the detailed information, i.e. transition densities, can give the possible difference between them. In the previous shell model studies, the transition densities of the pygmy resonances and GDRs have not been included [19, 21–23]. Using the formulas discussed above, the calculated transition densities of the typical resonance states in 17,18 Ne are shown in Fig. 3. Fig. 3(a) and (b) are for the dominant states of 17 Ne in the usually pygmy region. We can see that the proton and neutron move in phase in the nuclear interior, while only protons move in the exterior. This scenario is the typical pygmy resonances of the halo protons oscillating against the inner core. The state in Fig. 3(c) is located in the GDR region. The given transition densities have shown a typical oscillation in the opposite phase between the bulk protons and neutrons. There is no contribution either from protons or neutrons in the exterior region. For comparison, the transition densities of two states in



FIG. 3: (color online) Shell model transition densities of discrete dipole transitions in ^{17,18}Ne.

the PDR region of ¹⁸Ne are displayed in Fig. 3(d)(e). Although the behavior in Fig. 3(d) is somewhat similar to Fig. 3(a)(b), the peaks of proton and neutron transition densities is out of phase about 0.9 MeV. And the B(E1)value of this state is too small comparing with the state at E = 9.413 MeV, not to mention the dominant GDR states. The proton and neutron transition densities in Fig. 3(e) do not show clear-cut in-phase behavior. The interval of the proton and neutron peaks is 1.26 MeV. This state is clearly not the soft mode but more similar to the giant resonances like in Fig. 3(f) where the state is a typical GDR.

Unlike the GDR region, the level density is sparse in the PDR region. Further detailed information on the collectivity of the discrete PDR states can be obtained by viewing the contributions to the total transition matrix element from the valence orbital transitions. These contributions to the isovector operator (14) for the important PDR states discussed in the last paragraph are given in Fig. 4, where the horizontal axis is the single particle excitation energies of valence orbitals. This figure shows that the dominant PDR states in ¹⁷Ne have several components including the transitions $1p \leftrightarrow 2s1d$ and $2s1d \leftrightarrow 1f2p$, which have prominent contributions to the total matrix elements. Together with the discussions on the transition densities, the ¹⁷Ne has shown us an excellent example of collective proton PDR due to the soft mode between the valence protons and the core. However in ¹⁸Ne, the PDR states are much less collective that only a few transitions contribute, most of which comes from the $1p \leftrightarrow 2s1d$ transitions. Together with



FIG. 4: (color online) Contribution to the total matrix elements of valence orbitals for the deexcitations from PDR states in ^{17,18}Ne. The magenta, red and blue bars indicate the transitions between the valence orbitals of $1s \leftrightarrow 1p$, $1p \leftrightarrow 2s1d$, and $2s1d \leftrightarrow 1f2p$, respectively.

the discussions on the transition density, the nature of the E = 9.413 MeV state in ¹⁸Ne is more likely to be the configuration splitting of the GDRs, but in the usually PDR energy region. The different nature of pygmy dipole resonances may also give a possible explanation for the nontrivial dependence of PDRs as a function of the neutron number in the Ca isotopes. Further theoretical investigations on this trend is highly needed.

In summary, we have used the shell model to study the ground state properties and the proton pygmy dipole resonances in ^{17,18}Ne. The shell model with the selfconsistent Skyrme-Hartree-Fock wave functions well reproduces the experimental mass radii and charge radii. The mass density distributions of the ground state in ¹⁷Ne also can be well given. The transition densities of the dipole resonances are calculated from the shell model output. The pygmy resonances around 10 MeV both in ^{17,18}Ne are predicted. However, detailed study involving

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transition densities and collectivity shows that the PDRs in ¹⁷Ne are highly collective and due to the oscillation between the valence protons and the core, while in ¹⁸Ne the dipole resonance in the PDR region is noncollective and more likely to be the configuration splitting of the GDRs.

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