Role of Long-Range Correlations in the Quenching of Spectroscopic Factors

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We consider the proton and neutron quasiparticle orbits around the closed-shell ⁵⁶Ni and ⁴⁸Ca isotopes. It is found that large model spaces (beyond the capability of shell model applications) are necessary for predicting the quenching of spectroscopic factors. The particle-vibration coupling is identified as the principal mechanism. Additional correlations—due to configuration with several particle-hole excitations—are estimated using shell model calculations and generate an extra reduction which is $\leq 4\%$ for most quasiparticle states. The theoretical calculations nicely agree with (e, e'p) and inverse kinematics knockout experiments. These results open a new path for a microscopic understanding of the shell model.

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Introduction.—Single-particle states at the Fermi surface of shell closures (or quasiparticles) play a crucial role in nuclear structure. Their strengths [the spectroscopic factors (SFs)] and energies are essential inputs in largescale shell model (SM) calculations, which provide the most successful description of medium mass 1s0d and 1p0f nuclei [1]. Single-particle wave functions and SFs also enter the nuclear matrix elements that describe nucleon capture and emission in stellar burning processes [2].

The need for understanding quasiparticles has become more compelling in recent years due to the realization that their energies evolve, with changing proton or neutron number, due to the nuclear tensor force [3,4]. The quenchings of absolute spectroscopic factors (SFs) have also been observed to change dramatically at the driplines [5,6]. These effects cause the breakdown of conventional magic numbers far from the valley of stability and can give rise to new exotic modes of excitation. In order to predict the properties of nuclei at the limits of stability, it is imperative to derive robust models for quasiparticle properties. Recently, it has been suggested that relative SFs among small quasiparticle fragments can be described within the SM approach [7]. This Letter discusses the problem of the absolute quenching of SFs and shows that this requires accounting for coupling to collective resonances and large model spaces, beyond the capability of the SM.

The reactions for transfer of a nucleon to or from the initial state $|\Psi_0^A\rangle$ depend on the overlap wave function [8,9]

$$\psi_{\alpha}^{A\pm1}(\mathbf{r}) = \langle \Psi_{\alpha}^{A\pm1} | \psi^{(\dagger)}(\mathbf{r}) | \Psi_{0}^{A} \rangle, \tag{1}$$

where α can label either particle or hole states. SFs are identified with the normalization integral of $\psi_{\alpha}^{A\pm 1}(\mathbf{r})$ and give a "measure" of what fraction of the *final* wave function, $|\Psi_{\alpha}^{A\pm 1}\rangle$, can be factorized into a (correlated) core plus an independent particle or hole. Strong deviations from the independent particle model (IPM)—that is, a Slater determinant with fully occupied orbits—signal substantial correlations and imply the onset of nontrivial many-body dynamics. For stable nuclei, a large body of data has been accumulated from (e, e'p) experiments. These studies showed that proton absolute SFs for isotopes all across the nuclear chart are *uniformly quenched* to 60%–70% of the IPM value [10,11]. Short-range correlations (SRC)—originating from the repulsion of the nuclear force at short distances—have been investigated as a possible cause. However, they explain only a small fraction of the observed reduction [12,13], as confirmed by recent experiments at Jefferson Laboratory [14,15]. Thus, one is left to understand the role of long-range correlations (LRC) effects (see, for example, Refs. [16,17] and references therein).

Successful ab initio calculations have been reported for light nuclei using the variational Monte Carlo method [18]. For larger masses, self-consistent Green's function (SCGF) theory [16,19] gave encouraging results for ⁴⁸Ca and ⁹⁰Zr [20]. However, these early calculations focused only on one particular type of correlations [either coupling to particle-hole (ph) or particle-particle and hole-hole phonons]. Recently, we have improved the SCGF method [21] to include correlations from the remaining collective modes, extended it to large-scale no-core calculations up ⁵⁶Ni, and based our studies on realistic nuclear forces [22,23]. Thus, we are now in the position of making accurate studies of the effects of correlations. In addition, the SCGF equations describe directly the interactions among quasiparticle states, which allows extracting single-particle orbits and effective interactions for the SM. This Letter applies these new capabilities to study in detail quasiparticle states in ⁵⁶Ni and ⁴⁸Ca and to extract an effective Hamiltonian for 1s0d and 1p0f orbits in the SM. The SCGF results will then be compared to the SM ones to investigate the role of *all* different types of correlations on the quenching of SFs.

Formalism.—The calculations were performed in a large model space including up to 10 major harmonic oscillator shells. All details are reported in Ref. [23] and here we give an overview of the points needed for the present discussion. Spectroscopic factors were extracted from the one-body propagator (spin and isospin indices are omitted for simplicity) [19],

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$$g(\mathbf{r}, \mathbf{r}'; \omega) = \sum_{n} \frac{(\psi_{n}^{A+1}(\mathbf{r}))^{*} \psi_{n}^{A+1}(\mathbf{r}')}{\omega - (E_{n}^{A+1} - E_{0}^{A}) + i\eta} + \sum_{k} \frac{\psi_{k}^{A-1}(\mathbf{r})(\psi_{k}^{A-1}(\mathbf{r}'))^{*}}{\omega + (E_{k}^{A-1} - E_{0}^{A}) - i\eta}, \quad (2)$$

where the residues are the overlap amplitudes (1) and the poles give experimental energy transfers. These refer to nucleon pickup (knockout) to the excited states of the systems with A + 1 (A - 1) particles. The propagator (2) is obtained by solving the Dyson equation $[g(\omega) = g^{(0)}(\omega) + g^{(0)}(\omega)\Sigma^*(\omega)g(\omega)]$, where $g^{(0)}(\omega)$ propagates a free nucleon. The information on nuclear structure is included in the irreducible self-energy, which was split into two contributions:

$$\Sigma^{\star}(\mathbf{r},\mathbf{r}';\omega) = \Sigma^{\mathrm{MF}}(\mathbf{r},\mathbf{r}';\omega) + \tilde{\Sigma}(\mathbf{r},\mathbf{r}';\omega).$$
(3)

The term $\Sigma^{MF}(\omega)$ includes *both* the nuclear mean field (MF) and diagrams describing two-particle scattering outside the model space, generated using a G-matrix resummation [24]. As a consequence, it acquires an energy dependence which is induced by SRC among nucleons [23]. The second term, $\tilde{\Sigma}(\omega)$, includes the LRC. In the present work, $\tilde{\Sigma}(\omega)$ is calculated in the so-called Faddeev random phase approximation (FRPA) of Refs. [21,25]. This includes diagrams for particle-vibration coupling at all orders and with all possible vibration modes, see Fig. 1, as well as low-energy 2p1h/2h1p configurations. Particlevibration couplings play an important role in compressing the single-particle spectrum at the Fermi energy to its experimental density. However, a complete configuration mixing of states around the Fermi surface is still missing and would require SM calculations.



FIG. 1 (color online). Left. One of the diagrams included in the correlated self-energy, $\tilde{\Sigma}(\omega)$. Arrows up (down) refer to quasiparticle (quasihole) states, the $\Pi^{(\text{ph})}$ propagators include collective ph and charge-exchange resonances, and the g^{II} include pairing between two particles or two holes. The FRPA method sums analogous diagrams, with any numbers of phonons, to all orders [21,25]. *Right*. Single-particle spectral distribution for neutrons in ⁵⁶Ni, obtained from FRPA. Energies above (below) E_F are for transitions to excited states of ⁵⁷Ni (⁵⁵Ni). The quasiparticle states close to the Fermi surface are clearly visible. Integrating over **r** [Eq. (4)] gives the SFs reported in Table I.

Each spectroscopic amplitude $\psi^{A\pm 1}(\mathbf{r})$ appearing in Eq. (2) has to be normalized to its respective SF as

$$Z_{\alpha} = \int d\mathbf{r} |\psi_{\alpha}^{A\pm 1}(\mathbf{r})|^2 = \frac{1}{1 - \frac{\partial \Sigma_{\hat{\alpha}\hat{\alpha}}^{\star}(\omega)}{\partial \omega}} \Big|_{\omega = \pm (E_{\alpha}^{A\pm 1} - E_{0}^{A})}, \quad (4)$$

where $\sum_{\hat{\alpha}\hat{\alpha}}^{\star}(\omega) \equiv \langle \hat{\psi}_{\alpha} | \Sigma^{\star}(\omega) | \hat{\psi}_{\alpha} \rangle$ is the matrix element of the self-energy calculated for the overlap function itself but normalized to unity $(\int d\mathbf{r} | \hat{\psi}_{\alpha}(\mathbf{r}) |^2 = 1)$. By inserting Eq. (3) into (4), one distinguishes two contributions to the quenching of SFs. For model spaces sufficiently large, all low-energy physics is described by $\tilde{\Sigma}(\omega)$. Then, the derivative of $\Sigma^{\text{MF}}(\omega)$ accounts for the coupling to states outside the model space and estimates the effects of SRC alone [26].

In general, the self-consistent (SC) self-energy (3) is a functional of the one-body propagator itself, $\Sigma^* = \Sigma^*[g]$. Hence, the FRPA equations for the self-energy and the Dyson equation have to be solved iteratively. The mean-field part, $\Sigma^{MF}[g]$, was calculated exactly in terms of the fully fragmented propagator (2). For the FRPA, this procedure was simplified by employing the $\tilde{\Sigma}[g^{IPM}]$ obtained in terms of a MF-like propagator

$$g^{\text{IPM}}(\mathbf{r}, \mathbf{r}'; \omega) = \sum_{n \notin F} \frac{(\phi_n(\mathbf{r}))^* \phi_n(\mathbf{r}')}{\omega - \varepsilon_n^{\text{IMP}} + i\eta} + \sum_{k \in F} \frac{\phi_k(\mathbf{r})(\phi_k(\mathbf{r}'))^*}{\omega - \varepsilon_k^{\text{IMP}} - i\eta}, \quad (5)$$

TABLE I. Spectroscopic factors (given as a fraction of the IPM) for valence orbits around ⁵⁶Ni. For the SC FRPA calculation in the large harmonic oscillator space, the values shown are obtained by including only SRC, SRC and LRC from particle-vibration couplings (full FRPA), and by SRC, particle-vibration couplings and extra correlations due to configuration mixing (FRPA + ΔZ_{α}). The last three columns give the results of SC FRPA and SM in the restricted 1p0f model space. The ΔZ_{α} s are the differences between the last two results and are taken as corrections for the SM correlations that are not already included in the FRPA formalism.

	10 osc. shells			Exp. [29]	1p0f space		
	FRPA	Full	FRPA				
	(SRC)	FRPA	$+\Delta Z_{\alpha}$		FRPA	SM	ΔZ_{α}
⁵⁷ Ni:							
$\nu 1 p_{1/2}$	0.96	0.63	0.61		0.79	0.77	-0.02
$\nu 0 f_{5/2}$	0.95	0.59	0.55		0.79	0.75	-0.04
$\nu 1 p_{3/2}$	0.95	0.65	0.62	0.58(11)	0.82	0.79	-0.03
⁵⁵ Ni:							
$\nu 0 f_{7/2}$	0.95	0.72	0.69		0.89	0.86	-0.03
⁵⁷ Cu:							
$\pi 1 p_{1/2}$	0.96	0.66	0.62		0.80	0.76	-0.04
$\pi 0 f_{5/2}$	0.96	0.60	0.58		0.80	0.78	-0.02
$\pi 1 p_{3/2}$	0.96	0.67	0.65		0.81	0.79	-0.02
⁵⁵ Co:							
$\pi 0 f_{7/2}$	0.95	0.73	0.71		0.89	0.87	-0.02

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which was updated *at each iteration* to approximate Eq. (2) with a limited number of poles. Equation (5) defines a set of undressed single-particle states that can be taken as a basis for SM applications. This feature will be used below to estimate the importance of configuration mixing effects on the quenching of spectroscopic factors. The present calculations employed the N3LO interaction from chiral perturbation theory [27] with a modification of the tensor monopoles to correct for missing three-nucleon interactions [28].

Results.-The calculated single-particle spectral function $[S_{56}_{Ni}(\mathbf{r}, \omega) = \frac{1}{\pi} |g(\mathbf{r} = \mathbf{r}'; \omega)|^2]$ is shown in Fig. 1 for the case of neutron transfer on ⁵⁶Ni. This picture puts in evidence the quasiparticle and quasihole states associated with valence orbits in the 1p0f shell. The corresponding SFs are reported in Table I, including both protons and neutrons. The first column is obtained by including only the derivative of $\Sigma^{MF}(\omega)$ when calculating Eq. (4). Since N3LO is rather soft compared to other realistic interactions the effect of SRC is relatively small. From other models one could expect a quenching up to about 10% [16], as confirmed by recent electron scattering experiments [14,15,30]. This difference would not affect sensibly the conclusions below. The complete FRPA results for SFs are given in the second column. For the transition between the ⁵⁶Ni and ⁵⁷Ni ground states, our result agrees with knockout reactions with fast beams within the given error bar [29]. Note that ⁵⁶Ni is close to the stability line, where the analysis of these reactions has been tested against electron scattering results. The remaining orbits have similar quenchings and are in line with results expected for stable nuclei [10]. This shows that the dominant mechanism in reducing the spectroscopic strength is to be looked for in LRC involving configurations among several shells around the Fermi surface.

We now turn to the question of what are the relevant lowenergy degrees of freedom and the importance of configurations with multiple ph excitations. Excitations beyond 2p1h and 2h1p are partially included by the SC FRPA, from which one can expect an accurate description of quasiparticles around shell closures. This was checked by comparing SC FRPA and large-scale SM calculations in the 1p0f shell. The basis and the interaction were constructed using the "undressed" single-particle orbits $\phi_{\alpha}(\mathbf{r})$, defined by Eq. (5), and the same G-matrix interaction used in the full-space FRPA calculations. Shell model calculations used the code ANTOINE [1,31] and included up to 6p6h excitations for the A = 57 systems and up to 8p8hfor A = 55. The resulting SFs are shown in the last three columns of Table I. As an example, the quenching for the $p_{3/2}$ ground state of ⁵⁷Ni, is predicted to be 0.82 by FRPA and 0.79 by the SM. Comparing with the full-space result of 0.65, one infers that about half of the quenching is driven by degrees of freedom from outside the 1p0f space. In particular, giant resonances originating from $1\hbar\omega$ and $2\hbar\omega$ excitations carry enough collectivity to influence the quenching of orbits close to the Fermi surface. The difference between SM and FRPA in the 1p0f space is $\Delta Z_{\alpha} = 0.79 - 0.82 = -0.03$, which is smaller than the typical model dependence of SFs extracted from experiments. One can treat the ΔZ_{α} s as small perturbations and add them to the full-space FRPA results, leading to our final predictions for absolute SFs (third column of Table I). Relative SFs with respect to the other states in ⁵⁷Ni have been studied by reanalyzing all the available (*d*, *p*) data [7]. These results agree with the SM and, hence, with FRPA ones (see Table I). However, the model dependence of this analysis appears too large to constrain absolute values of SFs.

Table II reports the results of the same analysis for ⁴⁸Ca. Also in this case, degrees of freedom from outside the first 10 oscillator shells have a small effect, of 3%-6%, on the absolute SFs. The SC FRPA coupling to collective modes reduces these to about 80% of the IPM, and even lower for proton holes to ⁴⁷K. The SM calculations employed the undressed single-particle orbits (5) generated by the large space SC FRPA for this nucleus. We adopted a model space (which will be named sd_3pf) consisting of the $(1s_{1/2},$ $0d_{3/2}$, $1p_{3/2}$, $0f_{7/2}$) orbits for protons and of $(1p_{1/2})$, $1p_{3/2}, 0f_{5/2}, 0f_{7/2}$) for neutrons. This can be handled by present day computers with up to 10p10h configurations and includes the most important excitations across the Fermi surface. The SM results in the sd_3pf model space do not give additional quenchings for the valence orbits in the 1p0f shell. Hence, multiple ph configurations are suppressed even more than for the ⁵⁶Ni case. Note that the $\nu 0 f_{5/2}$ quasiparticle in ⁴⁹Ca splits in two main fragments but their total strength remains unchanged. Experimental

TABLE II. Same as Table I but for ⁴⁸Ca. The $\nu 0f_{5/2}$ particle ($\pi 1s_{1/2}$ hole) fragments in ⁴⁹Ca (⁴⁷K) with lowest excitation energy are indicated by an asterisk. The experimental SFs for ⁴⁹Ca are from Ref. [32], those for ⁴⁷K are form Ref. [11].

	10 osc. shells			Exp.	sd ₃ pf space		
	FRPA	Full	FRPA				
	(SRC)	FRPA	$+\Delta Z_{\alpha}$		FRPA	SM	ΔZ_{lpha}
⁴⁹ Ca:							
$\nu 0 f_{5/2}$	0.97	0.10	0.16		0.19	0.25	+0.06
$\nu 0 f_{5/2}^{*}$	0.97	0.69	0.62		0.77	0.70	-0.07
$\nu 1 p_{1/2}^{3/2}$	0.97	0.82	0.82	$0.71(^{+20}_{-12})$	0.96	0.96	< 0.01
$\nu 1 p_{3/2}$	0.97	0.78	0.78	0.53(11)	0.94	0.94	< 0.01
⁴⁷ Ca:							
$\nu 0 f_{7/2}$	0.96	0.80	0.80		0.97	0.97	< 0.01
⁴⁹ Sc:							
$\pi 1 p_{3/2}$	0.95	0.52	0.48		0.74	0.70	-0.04
$\pi 0 f_{7/2}$	0.95	0.74	0.73		0.94	0.93	-0.01
⁴⁷ K:							
$\pi 0d_{3/2}$	0.94	0.67	0.59	0.56(4)	0.87	0.79	-0.08
$\pi 1 s_{1/2}^{*}$	0.95	0.52	0.36	0.53(4)	0.64	0.48	-0.16
$\pi 1 s_{1/2}$	0.95	0.24	0.14	0.08(1)	0.34	0.23	-0.10

SFs for the ground $(\nu 1 p_{3/2})$ and first excited $(\nu 1 p_{1/2})$ states, have been extracted from a combined analysis of (d, p) and (n, γ) reactions [32].

Proton-hole states in 47 K are a case in which SM correlations start becoming important. The FRPA in the sd_3pf space describes about a half of the quenching of the $0d_{3/2}$ orbits in the full space. The SM calculations induce a further reduction of $\approx 8\%$. Adding this estimate brings the $0d_{3/2}$ SF to 0.59, in agreement with the experimental (e,e'p) value of 0.56(4) [11]. Shell model correlations are even more substantial for the $1s_{1/2}$ fragments: here the sd_3pf space is sufficient to reproduce almost all of the quenching obtained in the largest space. Configurations not included in the FRPA are also more important and induce a further reduction of up to 16% for the ground state of 47 K. The total predicted strength of the two $1s_{1/2}$ peaks is 0.50, somewhat lower than the (e, e'p) value of 0.61(5).

Utsuno and collaborators have also calculated the spectral strength for proton removal from ⁴⁸Ca [33]. They found that the spin-orbit splitting between the 0*d* states and the ordering of single-particle energies are sensitive to the tensor force. These calculations also show that the fragmentation pattern in ⁴⁷K is well reproduced by the SM, as suggested in [7]. The experimental strength is however lower by an overall factor of ≈ 0.73 . This is nicely explained by the combined SC FRPA and SM results, where the final corrected strengths of Table II are smaller than the pure SM ones by 0.75 for the 0*d*_{3/2} peak and by 0.70 for the summed 1*s*_{1/2} strength.

Summary.-In conclusion, we have studied the effects of correlations on the quenching of absolute spectroscopic factors. The present work does not support the assumption that the uniform quenching observed in stable nuclei originates from a unique mechanism such as short-range correlations. SRC have been predicted [12,16] and experimentally confirmed [14,15] to influence just a small fraction of the total strength. We find that spectroscopic factors for valence orbits result from a combination of configuration mixing at the Fermi surface and coupling to collective resonances. The former can usually describe the relative spectroscopic factors (hence, the fragmentation pattern at low energy) and it will be crucial in open shell nuclei. On the other hand, the overall quenching of absolute spectroscopic factors requires both the coupling to collective modes at higher energies and large model spaces that cannot be approached by usual shell model calculations. This work reported on the first consistent calculation of all these effects in the medium-mass region and was based on a realistic interaction.

It was also found that quasiparticles around shell closures can be described accurately by self-consistent Green's function theory in the FRPA approximation. Moreover, the theory links the interactions among quasiparticle states with the underlying nuclear forces. This opens a new possibility for deriving single-particle orbits, effective charges and interactions for the shell model form realistic nuclear interactions.

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