Success and Limitations of Two- and Four-Quasiparticle Tamm-Dancoff Theories of Vibrational States: Applications to Even Tin Isotopes with a Realistic Nucleon-Nucleon Potential*

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(Received 10 May 1968)

Extensive calculations of the spectra of the even Sn isotopes with the two- and four-quasiparticle (qp) Tamm-Dancoff theories are performed. The effective nuclear forces are the Tabakin and the Yale-Shakin potentials renormalized for core polarization involving up to all the subshells between the magic numbers 8 and 126. Several different sets of single-particle energies are considered, one of which corresponds to a Woods-Saxon potential. Over-all semiquantitative agreement with the data is obtained. We show how relative large values of the quadrupole moment of the 2_1^+ state [such as $Q(2_1^+)=+0.125$ b] may arise from large two-qp–four-qp cross terms even in cases where four-qp components are small. Many aspects of the theory are critically examined; in particular, several different approximations in projecting out spurious kets of the nucleon-number nonconservation. Projected improvements and developments of the theory are outlined.

I. INTRODUCTION

THE one-three-quasiparticle and the two-four-quasiparticle (qp) Tamm-Dancoff (TD) theories have been extensively applied to studying both parity states of even and odd tin and nickel isotopes.[1–11] In particular, the even tin isotopes are generally believed to be representative of the so-called vibrational region and at the same time a good testing ground for such theories. The reason for the latter point is that, while the Bardeen-Cooper-Schrieffer (BCS) pairing effect of the many valence neutrons in subshells of rather large degeneracies is important, strong mixing of shell-model configurations and, in particular, formation of collective states, is also characteristic of these nuclei due, in part, to a relatively high single-particle (or qp) level density. The quasiparticle Tamm-Dancoff (QTD) method involves excitations belonging to the class of seniorities zero and two, while the quasiparticle second Tamm-Dancoff (QSTD) also embraces certain particular excitations of seniority four of the shell model. The great power of the methods of mixing qp configurations lies in the fact that while it probably comprises, in general, all the most important dynamical effects of the residual interactions, it allows at the same time a relatively large number of active subshells to be taken explicitly into account for a large number of interacting nucleons. For example, in describing tin isotopes which involve numbers of active neutrons of the order of 20, one can in QSTD get away with including all the five valence subshells and reaching dimensions of only up to about 200×200; the corresponding dimensions of exact shell-model calculations or even of complete seniority-four calculations would lead to quite ridiculous dimensions. The quasiparticle methods, justified physically by the importance of the BCS pairing component of the nuclear force, seem thus to be the only feasible ones in such cases. They are based on a statistical mechanical description of the nucleus as a grand canonical ensemble. The conservation of the true particle number only on the average allows, in this picture, secular matrix dimensions independent of the exact nucleon number of a given nuclide determined only by the angular-momentum geometry and selection rules and the qp anticommutation relations.

The price for the above simplifications is heavy: One must face the problem of spurious states due to the above nonconservation, i.e., of fluctuations of the $\hat{N}$ operator and of its powers $\hat{N}^{n+1}$, $n=1, 2, \cdots$, in all the excited modes and of $\hat{N}^{n+1}$ even in the qp vacuum. In a given orthonormal basis such spurions are explicitly constructed and projected out of the secular matrices before their diagonalizations. This must be done but can be done in a QTD Hilbert space only for spurious

* Supported in part by Istituto Nazionale di Fisica Nucleare.

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kets which are entirely contained within that given Hilbert space (we call them "basic spurions"). One is then always left with a parasitic contamination of the final "physical" eigenvectors by higher-order spurions which are partly inside and partly outside our Hilbert space. It is believed that such kets are not too dangerous, since generally they have only small (after normalization) components inside our Hilbert space. The projection out of basic spurions can be performed either by the secular matrix projection described in Refs. 2 and 8 or, completely equivalently, by projection of spurions and the Schmidt procedure, i.e., by an explicit construction of the physical (nonspurious) orthonormal basis vectors in which to set up the secular matrix (this procedure is used in Refs. 9 and 11). There arises an ambiguity about the treatment of the 0^+ states in QSTD and in higher TD theories, an ambiguity connected with the approximations involved and with the peculiar character of the 0^+ states as the only ones involving the qp vacuum $|0\rangle$ as one basic vector of the Hilbert space and with the fact that the ground state 0_1^+ itself belongs to the set. This ambiguity and related interpretational problems are described in Sec. II.

The exact number projection after[11] or before[12] a QTD or QSTD diagonalization is very interesting for evaluating our residual (higher-order) spuriousness; however, while it sacrifices, in general, the relative simplicity of the qp formalism, introducing a heavy mathematical apparatus, it is also entangled in interpretational difficulties.

In a series of papers,[4–6] the QTD and QSTD theories have been applied to the even tin isotopes with the realistic nucleon-nucleon potentials of Tabakin[13] and of Yale.[14] For such potentials (reaction matrix of Shakin *et al.*[15] for Yale) a renormalization is necessary for the core polarization, i.e., by including virtual excitations and de-excitations of the core protons and neutrons in the sense of the double scattering terms of the Brueckner theory. Such a renormalized effective realistic nuclear force in Sn differs from the corresponding one as derived by Kuo and Brown[16] for light and almost mirror nuclei by an unsymmetrical treatment of the core neutron and proton parts due to a large separation of the respective two Fermi levels and a different treatment of the Pauli principle for the two nucleonic charge states of the particle-hole pairs. In Refs. 4–6, only the apparently most important four highest-lying core subshells of both the protons and neutrons between the magic numbers 28 and 50 have been included in the core-polarization corrections. In the present paper, we extend our analysis also to cases in which we include all the core (hole) subshells between the magic numbers 8 and 50 and the extra higher (particle) subshells of the upper major shell between the magic numbers 82 and 126.

One of the greatest limitations of the previous and current QTD calculations is the lack of a self-consistent determination of the single-qp parameters in the sense of the Hartree-Fock-Bogolubov (HFB) procedure. In fact, the independent qp model (IQM), and thus the single-qp basis, should ideally be determined just from such self-consistent calculations. Such calculation, particularly with a reaction matrix for a realistic potential and with the condition of the double self-consistency,[17] is a formidable task in itself and has not yet been reported in the literature. Instead, we have used several more or less purely phenomenological approaches in determining our single-qp (QTD, QSTD input) parameters. The question is delicate, as some results (particularly the noncollective states and properties) are moderately sensitive to these input parameters. Clearly, provided one stays within a reasonable range of parameters, the results are much less sensitive to their details for even isotopes than they are for odd isotopes.

One of the recipes applied in the present paper is that of a best-fit-type parameter search for the "unperturbed" single-particle energies within quite restricted reasonable ranges of variation (the restrictions imposed are those of compatibility with the Mayer-Jensen shell-model spectrum and qualitatively with the odd isotopes). A subsequent solution of the BCS equation gives a desired set of QTD, QSTD input parameters.

Another series of our present results is based on the set of energy eigenvalues of the best Woods-Saxon potential reported by the Bonn group.[18] In this case the corresponding qp input parameters are fixed from an independent calculation and involve no free parameters. Details of these procedures are given below.

In the present paper, we do not investigate the question of a possible (even partial, mixed) "stable" deformation of the Hartree-Fock average nuclear field of the tin isotopes. We keep the assumption of a basic spherical shape. We pay particular attention to the reported large observed values[19] of the quadrupole moments of the first excited 2_1^+ states, $Q(2_1^+)$. We show how such large values of $Q(2_1^+)$ can be understood without invoking the assumption of a stable quadrupole deformation for the single-particle basis.

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II. DISCUSSION OF APPROXIMATIONS AND RESULTS

Let us first examine the question of the 0^+ QSTD spurions. The lowest-order spurion of the number nonconservation is, as in Eq. (21) of Ref. 2,

$$|\psi_{\rm sp2}\rangle = N_{\rm sp2}(\hat{N}-N_0)|0\rangle = \sum_a \zeta_a A_{a00}^\dagger(aa)|0\rangle, \quad (1)$$

where N_0 is the exact particle (neutron) number; $A_{JM}^\dagger(aa')$ is a two-qp basic operator of Ref. 2 and $\zeta_a = -N_{\rm sp2}\sqrt{2}\hat{\jmath}_a u_a v_a$. $|\psi_{\rm sp2}\rangle$ of (1) is the only basic spurion of QTD. In QSTD one clearly has basic spurions containing four-qp components. Such spurions are of "higher order" for QTD and their scalar products with the final "physical" QTD vectors measure their higher-order spuriousness, i.e., the nonprojected unphysical ingredients. Similarly, the particle nonconservation spurions with six-qp components are of "higher order" for QSTD, and their scalar products with the final "physical" QSTD eigenvectors would measure the degree of parasitic contamination of those vectors due to the failure to project out the exact nucleon number before diagonalization.

The natural definition of a spurion seems to be

$$|\psi_{{\rm sp},x_n}(JM)\rangle = \tilde{N}_{{\rm sp},x_n}(\hat{N}-N_0)X_{n,JM}|0\rangle, \quad (2)$$

where $X_{n,JM}|0\rangle$ is a vector of our Hilbert space. If we choose $X_{n,JM} \equiv A_{JM}^\dagger(cc')$, we obtain

$$|\psi_{\rm sp4}(cc',JM)\rangle = N_{\rm sp4}(cc',J)[\delta_{J0}\delta_{M0}\delta_{cc'}2\hat{\jmath}_c u_c v_a + (N_0-N_{cc'})(1+\delta_{cc'})^{1/2}A_{JM}^\dagger(cc') + \textstyle\sum_b \hat{\jmath}_b u_b v_b \mathbf{B}_{(0J)JM}^\dagger(bbcc')]|0\rangle, \quad (3)$$

where $N_{\rm sp4}$ is the normalization factor, $N_{cc'} = N_0 - v_c^2 + u_c^2 - v_{c'}^2 + u_{c'}^2$ is the average nucleon number in the state $A_{JM}^\dagger(cc')|0\rangle$,

$$N_{cc'} = \langle 0|A_{JM}(cc')\hat{N}A_{JM}^\dagger(cc')|0\rangle,$$

and $\mathbf{B}^\dagger$ is an unnormalized four-qp basis operator defined in Eq. (10) of Ref. 2. The term containing $(N_{cc'}-N_0)$ is generally small; we call it the "blocking term." In our results presented below, we refer to $|\psi_{\rm sp4}\rangle$ of Eq. (3) as to spurions with no "blocking." Almost numerically equivalent solutions are obtained if one replaces N_0 in the right-hand side of Eq. (2) by $N_{cc'}$, i.e., when the term containing $(N_{cc'}-N_0)$ drops out. Below we refer to this case as with "blocking" (this approximation is, in practice, a useful simplification; most of our results reported here as well as those of Refs. 2–10 correspond to this case). In both the variants a Schmidt orthonormalization of the set of $|\psi_{\rm sp4}\rangle$ is necessary, in general.

The specificity of the 0^+ spurions is their nonvanishing $|0\rangle$ vacuum component. This obviously implies a depletion of this component in the ground state, 0_1^+, the lowest eigenstate of the secular matrix for $J^\pi = 0^+$. In fact, this implies a criticism of and a correction to the particular given BCS solution (or to $|0\rangle$) assumed in the TD formalism to be a zero-order approximation to the ground state. As we shall see, this depletion effect is a measure of the spuriousness in $|0\rangle$ rather than of a dynamical effect of the H_{40} part of the Hamiltonian (coupling of the four-qp excitations to $|0\rangle$). In particular, by projecting out the spurions $|\psi_{\rm sp4}\rangle$ of Eq. (3) we automatically project out the well-known most important spurion $\mathfrak{N}(\hat{N}^2-N_0^2)|0\rangle$ of the BCS solutions [the large fluctuations of the $\hat{N}^2$ operators; in fact, this spurion is a linear combination of the spurions of Eq. (3)]. Fluctuations of $\hat{N}^3$, $\hat{N}^4$, etc., which are part of the remaining higher-order spuriousness, remain unprojected.

Another approach implicit in Refs. 9–11 consists in insisting on the physical purity (correctness) of the unprojected BCS ground state $|0\rangle$, as a good nonspurious basis vector. This means assuming that it is practically an eigenstate of $\hat{N}$ and that the spurions $|\psi_{\rm sp4}\rangle$ have no qp–vacuum components [the constant term with δ_{J0} in Eq. (3) is dropped and the new $|\psi_{\rm sp4}\rangle$ is renormalized]. Formally it can be done by the redefinition

$$|\psi_{\rm sp4}'(cc',JM)\rangle = \mathfrak{N}_{\rm sp4}'(cc'J)A_{JM}^+(cc')(\hat{N}-N_0)|0\rangle. \quad (4)$$

Actually, the technical prescription of Refs. 9 and 11 is different, but the results are equivalent to those based on Eq. (4). The projection out of $|\psi_{\rm sp4}(cc,00)\rangle$ by the Schmidt procedure is then particularly simple. The definition of Eq. (4) is clearly a limitation and in contrast to the basic notion of a spurious ket as $(\hat{N}-N_0)$ applied to a ket belonging to our Hilbert space, and it is a sacrifice of the theory in this sense. Clearly, the depletion of the $|0\rangle$ component of $|0_1^+\rangle$ of QSTD will now be small, as it is due practically to the small dynamical effect of H_{40} only. The advantage of this approach over that of Eq. (3) is the unity of description one obtains in this way between the $|0_1^+\rangle$ and all the QSTD excited states. In fact, the exclusion of all the six-qp excitations in the QSTD states means, in particular, the exclusion of the six-qp spurions which have (small) nonvanishing two-qp components. These spurious two-qp components are small but analogous to the $|0\rangle$ component of $|\psi_{\rm sp4}\rangle$ of Eq. (3) for $J=0$. Somewhat consistently, both are not projected out in the present approach, which should tend to preserve correct interrelations (level spacings, etc.) of 0_1^+ and all the other states. The states $J^\pi \neq 0^+$ are defined in QSTD as two- and four-qp excitations out of $|0\rangle$. In the approach of Eq. (4), this means that such excitations are generated almost out of the ground state itself. This seems to have a particular advantage; for example, in the corresponding description of two-nucleon transfer reactions. On the other hand, in QSTD with the projection of $|\psi_{\rm sp4}\rangle$ of Eq. (3), $|0_1^+\rangle$ is markedly different from $|0\rangle$, and the excited $J^\pi \neq 0^+$ QSTD states can no longer have the interpretation in terms of simple

TABLE I. QTD and QSTD eigenvalues of 0^+ states of Sn^{116} calculated with the Tabakin potential with core polarization (*S2*) of Gmitro *et al.*[a] the four-qp percentage weights of QSTD vectors are given in parentheses; three cases of spurions projected out, as discussed in the text, are compared.

QTD	QSTD $\langle\langle 0\|\psi_{sp4}\rangle\neq 0\rangle$ no "blocking"	QSTD $\langle\langle 0\|\psi_{sp4}\rangle\neq 0\rangle$ with "blocking"	QSTD $\langle\langle 0\|\psi_{sp4}'\rangle=0\rangle$ with "blocking"
0.0	−0.102(35.3)	−0.098(36.0)	−0.121(2.1)
2.054	1.979(6.3)	1.942(4.2)	1.942(6.9)
2.904	2.921(14.6)	2.756(6.1)	2.756(6.1)

[a] References 4 and 5.

TABLE II. QTD and QSTD $J^\pi\neq 0^+$ states of Sn^{116} with the renormalized Tabakin potential of Table I; the spurions $|\psi_{sp4}\rangle$ are with "blocking."

2^+		4^+		3^-	
QDT	QSTD	QTD	QSTD	QTD	QSTD
1.439	1.391(1.4)	2.268	2.200(2.6)	2.673	2.828(2.7)
2.621	2.515(4.6)	2.814	2.714(4.7)	3.380	3.054(3.7)
	5^-		6^-		7^-
QTD	QSTD	QTD	QSTD	QTD	QSTD
2.371	2.335(1.1)	2.607	2.565(1.4)	2.429	2.322(4.1)
2.754	2.712(1.2)	2.751	2.687(2.3)	2.880	2.790(3.0)

basic excitations out of the ground state of the same QSTD theory.

Neither of the approaches to the problem of QSTD spurions is entirely satisfactory and calculations based on exact number projection before diagonalizing secular matrices of a QSTD-type theory would be very interesting.

In Table I, we illustrate some of the points discussed above on the example of the Tabakin potential with the second-order core-polarization corrections of Ref. 4 and the single-particle energies of Bando[20] as used in Refs. 4 and 5. The nucleus is Sn^{116}. The harmonic-oscillator parameter is $\sqrt{\nu}=0.454$ F^{-1}.

The number of orthonormal spurions $|\psi_{sp4}\rangle$ is always equal to the number of $A_{00}^\dagger(cc)$, i.e., to the number of subshells. In our case, it means six spurions altogether: five $|\psi_{sp4}\rangle$ of the five valence neutron subshells plus $|\psi_{sp2}\rangle$ of Eq. (1). In the case "with blocking" one can also include the (otherwise redundant) seventh spurion, $\mathfrak{N}(\hat{N}^2-N_0^2)|0\rangle$. A diagonalization shows that, for example, in the case of the results of Table I this gives no significant modification of the corresponding results with $\langle 0|\psi_{sp4}\rangle\neq 0$, with blocking. The exact QSTD 0^+ matrices are 56×56 with 50 nonspurious eigenstates.

From Table I, we see that while the 0^+ eigenvalues for all the cases in question are quite close to each other, the only striking difference lies in the four-qp percentage weight (in parentheses) of the ground state (0_1^+ eigenvector). The lowering of the 0_1^+ energy with respect to the qp vacuum is small in all cases. Since the total weight of $A^\dagger|0\rangle$ is almost negligible in $|0_1^+\rangle$, we find only about 64% of the $|0\rangle$ weight in $|0_1^+\rangle$ (a 36% depletion) in the cases of $\langle 0|\psi_{sp4}\rangle\neq 0$ [$|\psi_{sp4}\rangle$ of Eq. (3)] and a 98% $|0\rangle$ weight for $\langle 0|\psi_{sp4}'\rangle=0$ [$|\psi_{sp4}'\rangle$ of Eq. (4)]. The case of no "blocking" and no $|0\rangle$ components of $|\psi_{sp4}'\rangle$ gives almost the same result. In order to see that the $|0\rangle$ depletion effect is practically independent of the H_{40} coupling, we have diagonalized the 0^+ QSTD matrix with $|\psi_{sp4}\rangle$ of Eq. (3), inconsistently setting H_{40} equal to zero. Again we find the depletion by about 36% of the $|0\rangle$ component. Only the 0_1^+ eigenvalue is shifted a little; the other results remain unchanged. We can conclude that the 36% depletion effect is due almost exclusively to $\langle 0|\psi_{sp4}\rangle\neq 0$.

One striking feature of our results is the smallness of the 0_1^+ energy shift in relation to the BCS ground. This means that the four-qp correlation components are randomly distributed and, in the 0^+ matrix diagonalization, shift the 0^+ energy only a little, at least for our particular nuclear force. In particular, a perturbation estimate where all the individual four-qp modes contribute a positive shift is not justified here. In principle, one should add the negative of this shift to obtain each J^π excitation energy. However, this shift is actually connected with H_{40}, which is left out in QSTD for $J^\pi\neq 0^+$. It is probable that similar shifts will occur for $J^\pi\neq 0^+$ states in a six-qp Tamm-Dancoff calculation.[21] These could, at least in part, compensate for the corresponding ground-state shift. It is then safer not to count the QSTD 0_1^+ shift in interpreting other QSTD J_n^π eigenvalues. Moreover, our calculations containing no HFB self-consistency are particularly unreliable for the ground state.

Dimensions of the other J^π QSTD Hilbert spaces are much larger, but do not exceed $204\times 204(4^+)$. We have used a special FORTRAN code due to Ottaviani for computing all the diagonal and all the four-qp–two-qp coupling elements in each given case. This serves as a guide in deciding truncations of the complete secular matrices by numerical saturation of successive diagonalizations of matrices with increased dimensions (computer experiments). This allows the complete dimensions to be reduced by 50% or more.

In Table II, we give our results for $J^\pi\neq 0^+$ for the same renormalized Tabakin force and for Sn^{116}. There is no difference here between $|\psi_{sp4}\rangle$ of Eq. (3) and $|\psi_{sp4}'\rangle$ of Eq. (4); we use the variant with "blocking." The four-qp percentages are indicated in parentheses for QSTD. The observed levels of Sn^{116} are: $0_{2,3}^+$:1.76, 2.02; $2_{1,2}^+$:1.29, 2.11; $4_{1,2,3,4}^+$:2.39, 2.53, 2.80, 3.05; 3_1^-:2.27; 5_1^-:2.364; 6_1^-:2.774, and 7^-:2.909 (all in MeV). The identification of the quoted 7^- state as 7_1^- would appear very hard to understand.

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[21] J. Hendekovič has performed, as examples, some "caricature" calculations in this direction.

TABLE III. QTD and QSTD states of Sn^{116} for the renormalized Yale-Shakin force SHA I described in the text; $|\psi_{sp4}\rangle$ are with "blocking."

0^+		2^+		4^+	
QTD	QSTD	QTD	QSTD	QTD	QSTD
0.0	(−0.192)(37.0)	1.376	1.307 (2.2)	2.120	2.009 (4.0)
2.040	1.889 (6.7)	2.530	2.444 (6.2)	2.901	2.722 (7.6)
2.892	2.613 (20.2)	3.134	2.972(64.7)	3.240	3.062(54.4)

3^-		5^-		6^-		7^-	
QSTD	QTD	QSTD	QTD	QSTD	QTD	QSTD
2.269(3.0)	2.311	2.261(1.3)	2.537	2.479(1.6)	2.709	2.628(2.4)
3.064(8.8)	2.746	2.677(1.8)	2.859	2.781(2.4)	2.968	2.853(3.7)

TABLE IV. QTD and QSTD states of Sn^{120} for the renormalized Yale-Shakin force SHA II described in the text; $|\psi_{sp4}\rangle$ are with "blocking."

0^+		2^+		4^+	
QTD	QSTD	QTD	QSTD	QTD	QSTD
0.0	(−0.210)(37.0)	1.187	1.158(0.8)	2.006	1.975(1.1)
2.074	1.971 (4.1)	2.593	2.530(3.5)	2.946	2.662(77.3)
3.002	2.794 (40.9)	3.171	3.000(52.5)	3.371	2.899(30.7)

3^-		5^-		7^-	
QTD	QSTD	QTD	QSTD	QTD	QSTD
2.503	2.414 (3.9)	2.281	2.253(1.0)	2.530	2.490(1.4)
3.209	3.079 (11.1)	2.783	2.740(1.5)	2.952	2.892(2.5)

The over-all agreement with experiment is not very satisfactory. Moreover, the renormalized Tabakin force is so weakly attractive that it gives only very small four-qp percentages of the lowest $|J^\pi\rangle$ vectors. With 1.4% of the four-qp components of $|2_1^+\rangle$ we find, with the neutron effective charge $e_{\rm eff}^{(2)}=1$, only a small quadrupole moment $Q(2_1^+)=0.042$ b. The observed value[19] is $Q(2_1^+)=(0.4\pm0.3)$ b. The transition rate $B(E2,2_1^+\rightarrow 0_1^+)=270.6e^2F^4$ is found in QSTD and $=354.9e^2F^4$ in QTD with the same $e_{\rm eff}^{(2)}=1$. The latter difference is particularly striking because of the small four-qp percentage in $|2_1^+\rangle$; however, since it is the QSTD 0_1^+ state with $\langle 0|\psi_{sp4}\rangle\neq 0$ (with "blocking") which is used here, the difference is due mainly to the destructive effect of the four-qp components of $|0_1^+\rangle$.

In the following series, we present some QTD and QSTD results for the Yale-Shakin force[14,15] and with slightly modified (adjusted) single-particle energies. For example, reasonable results are obtained for the reasonable set of energies "SHA I": $2d_{5/2}$:0.0; $1g_{7/2}$: −0.5; $3s_{1/2}$:1.0; $2d_{3/2}$:2.5; $1h_{11/2}$:2.0; $1g_{9/2}$:−4.0; $1f_{5/2}$, $2p_{1/2}$, $2p_{3/2}$:−12.0 (all in MeV). Again the core renormalization of the force is limited to the four most important neutron and proton subshells. The results or Sn^{116} are summarized in Table III. The QSTD 0^+ results refer to $\langle 0|\psi_{sp4}\rangle\neq 0$, with blocking. The 0_1^+ energy shift is larger here than in Table I. Again the core-renormalized force is only weakly attractive and QSTD is generally well approximated by QTD except for $Q(2_1^+)$ for which even the small (2.2%) four-qp admixture in $|2_1^+\rangle$ is most important (with the 94-component $|2_1^+\rangle$ vector); we find here $Q(2_1^+)=+0.10$ b.

In the isotope Sn^{120}, the 7_1^- state has been identified at a much lower energy, at 2.483 MeV, and no observed 6^- state has been reported. In Table IV, we summarize our QTD and QSTD results for the renormalized Yale-Shakin force and for the somewhat modified set of the single-particle energies: $2d_{5/2}$:0.0; $1g_{7/2}$:0.5; $3s_{1/2}$:1.75; $2d_{3/2}$:2.3; $1h_{11/2}$:1.4; $1g_{9/2}$:−4.0; $1f_{5/2}$, $2p_{1/2}$, $2p_{3/2}$: −12.0 (all in MeV). This force we call SHA II. The results of Table IV are generally very similar to those of Table III. No observed value of $Q(2_1^+)$ has been reported. The observed energy levels of Sn^{120} are: 0_2^+:1.89; 2_1^+:1.17; 4_1^+:2.18; 3_1^-:2.39; 5_1^-:2.28, and 7_1^-:2.48 (all in MeV). Except for 0_2^+, the agreement with the data is better here than that for Sn^{116} in Table III.

In the following series, we give results based on the single-particle unperturbed energies obtained by the Bonn group[18] with their best Woods-Saxon potential. The energies (in MeV) for the five valence (nl_j) subshells are: −10.52($2d_{5/2}$), −9.36($1g_{7/2}$), −8.45($3s_{1/2}$), −7.78($2d_{3/2}$), −7.16($1h_{11/2}$), for all the other proton and neutron subshells between the magic numbers 8 and 126 we have: −30.09($1d_{5/2}$), −27.93($1d_{3/2}$),−27.07 ($2s_{1/2}$), −22.91($1f_{7/2}$), −19.07($1f_{5/2}$), −18.82($2p_{3/2}$), −17.28($2p_{1/2}$), −15.24($1g_{9/2}$), −2.56($2f_{7/2}$), −1.14 ($3p_{3/2}$), −0.23($3p_{1/2}$), +1.01($2f_{5/2}$), +1.04($1i_{13/2}$), +1.07($1h_{9/2}$). In all our previous results of Tables I–IV we were, in our core-polarization corrections, applying the variant "*S2*" of Ref. 4, i.e., simplified energy denominators and the ansatz of a $\frac{1}{2}$ occupation of the neutron valence subshells. In the following we use in the same corrections, the exact (full) energy denominators, the variant "*C2*" of Ref. 4. In Table V, we give results where only the four core subshells of $1g_{9/2}$ and $1f2p$ (as in Tables I–IV, without $1f_{7/2}$) are included in the core corrections to the effective force. Comparison is given between the Tabakin and the Yale-Shakin potentials. In the latter case, we use a slightly different value of $\sqrt{\nu}=0.46\text{F}^{-1}$. The isotope is Sn^{116}. The results of Table V are generally similar for both potentials. Only small four-qp weights are found in all the first excited J^π states. The definition of $|\psi_{sp4}\rangle$ for $J^\pi=0^+$ is the same as for the results of Tables III and IV. While the 2_1^+ energy is rather high for the Tabakin force, the general over-all agreement with all the other observed energies is somewhat better for the Tabakin force than for the Yale-Shakin force. This agreement is not bad (except for the dubious 7_1^- case) if one realizes that we have in this variant no *ad hoc* adjustable parameter at all. With the neutron $E2$ effective charge $e_{\rm eff}^{(2)}=1$ we find for Tabakin: $B(E2, 2_1^+\rightarrow 0_1^+)=304.3$ (QTD) and $=210.8$ e^2F^4(QSTD); $Q(2_1^+)=+0.034$ b (QTD) and $=+0.098$ b (QSTD). Similarly, for Yale-Shakin we find: $B(E2, 2_1^+\rightarrow 0_1^+)=303.1$ (QTD) and $=216.8$ e^2F^4 (QSTD); $Q(2_1^+)=+0.043$ b (QTD) and $=+0.122$ b (QSTD). These results are quite reasonable. We see

TABLE V. QTD and QSTD states of Sn^{116} for the renormalized Tabakin and Yale-Shakin forces with the core polarization determined with the single-particle energies of Bleuler *et al.*,[a] including only the four highest-lying core subshells; $|\psi_{sp4}\rangle$ with "blocking."

	0^+		
	Tabakin		Yale
QTD	QSTD	QTD	QSTD
0.0	(−0.114)(35.7)	0.0	(−0.286)(37.5)
2.050	1.926 (4.4)	2.336	2.134 (10.0)
2.481	2.224 (9.7)	2.862	2.579 (12.4)
	2^+		
	Tabakin		Yale
QTD	QSTD	QTD	QSTD
1.427	1.313 (3.6)	1.369	1.251 (3.8)
2.429	2.249 (5.9)	2.708	2.488 (9.4)
2.474	2.307 (6.3)	2.798	2.614 (7.0)
	4^+		
	Tabakin		Yale
QTD	QSTD	QTD	QSTD
2.263	2.171 (2.9)	2.382	2.286 (3.5)
2.679	2.552 (6.0)	2.894	2.709 (12.9)
2.712	2.617 (3.2)	3.021	2.921 (4.2)
2.947	2.717 (11.2)	3.156	2.947 (8.2)
	3^-		
	Tabakin		Yale
QTD	QSTD	QTD	QSTD
2.904	2.784 (4.2)	3.080	2.949 (4.7)
3.810	3.673 (22.8)	3.905	3.750 (19.0)
	5^-		
	Tabakin		Yale
QTD	QSTD	QTD	QSTD
2.404	2.355 (1.3)	2.593	2.544 (1.2)
2.670	2.616 (1.7)	2.887	2.824 (1.8)
	6^-		
	Tabakin		Yale
QTD	QSTD	QTD	QSTD
2.558	2.486 (2.3)	2.782	2.697 (2.8)
2.767	2.666 (4.4)	2.984	2.852 (4.2)
	7^-		
	Tabakin		Yale
QTD	QSTD	QTD	QSTD
2.269	2.197 (2.3)	2.496	2.416 (2.6)
2.728	2.628 (3.0)	2.925	2.820 (3.0)

[a] Reference 18.

TABLE VI. QTD and QSTD states of Sn^{116} for the Yale-Shakin force; the core-polarization calculation includes all the subshells between the magic numbers 8 and 126, and the single-particle energies are all from Bleuler *et al.*[a]

0^+		2^+		4^+	
QTD	QSTD	QTD	QSTD	QTD	QSTD
0.0	(−0.363)(39.0)	1.259	1.153(3.3)	2.755	2.565(13.8)
2.427	2.029 (15.2)	3.074	2.804(13.7)	3.380	3.041(52.5)

5^-	6^-	7^-
QTD	QTD	QTD
2.943	3.236	2.896
3.241	3.324	3.454

[a] Reference 18.

that the two-qp–four-qp interference terms in QSTD are able to increase $Q(2_1^+)$ by a factor of the order of 3 in the direction of a better agreement with experiment.[19]

Clearly, the weakness of the effective attractive part of the core-renormalized two-nucleon force depends rather critically on the smallness of the separation of the highest core subshells (of $1g_{9/2}$, in particular) from the valence subshells. According to general experience and to the related evidence from $(e,e'p)$ reaction on other nuclei on the deepness of lower core subshells, the Woods-Saxon eigenvalues of Ref. 18 for $1f_{7/2}$ and lower subshells should probably be separated further from the four high-lying core subshells. This would mean that the effect of the so-modified lower subshells on the core polarization would be actually much smaller than the one we find and present below for the Woods-Saxon single-particle energies of Ref. 18. The deep-lying subshells in Table VI still give appreciable contributions towards reducing the general over-all attraction of the effective force, and the resulting calculated levels of Sn^{116} are shifted upwards in relation to those of Table V. In Table VI, we give several of our lowest states of Sn^{116} for the Yale-Shakin force with the second-order core-polarization renormalization involving all the subshells between the magic numbers 8 and 126. All the specific assumptions for the calculations are here exactly as in those of Table V. Except for 2_1^+ the energy levels lie typically too high; the QSTD ground-state energy shift is large (Yale potential) and $|0_1^+\rangle$ has a large depletion of the $|0\rangle$ component due to the removal of the QSTD spurions. In the case with $e_{\text{eff}}^{(2)}=1$, we find $B(E2, 2_1^+ \rightarrow 0_1^+)=317.0e^2F^4$ in QTD and $=273.7e^2F^4$ in QSTD; the corresponding values of $Q(2_1^+)$ are $+0.036$ b (QTD) and $+0.125$ b (QSTD). These values are slightly higher than those corresponding to the eigenvectors of the states of Table V. The most important contributions to the differences between Tables V and VI are due to the $1f_{7/2}$ subshell, although the effect of the upper major shell is important. All the level spectra for cases intermediate between those of Tables V and VI lie in between the spectra of Tables V and VI and vary with the number of core subshells included in a smooth, uniform manner. We do not give here our results for such intermediate cases. Somewhat better results are systematically obtained if one uses in the core-polarization terms the simplified (S) energy denominators of Ref. 4 which were systematically used by Kuo *et al.*[15] This difference means that, in the case of a vibrational nucleus such as Sn, with many relatively wide-spread valence subshells, single-particle excitations within the valence subshells are important corrections to the core particle-hole excitations.

An interesting observable quantity is the magnetic moment of the 5_1- state. The observed g factor for Sn^{116} given by Bodenstaedt *et al.*[22] is $g_{5_1}\text{-}(116) = -0.065 \pm 0.005$. If we limit ourselves to the contribution of the valence neutron spin part of the $\hat{\mu}$ operator,[23] we find the following values of this quantity: (1) with the Tabakin force of Table V: $g_{5_1}\text{-}(116) = -0.238$ (QTD) and $= -0.253$ (QSTD) [it is interesting to mention that if we do not use the "blocking" approximation for $|\psi_{sp4}\rangle$ we find $g_{5}\text{-}(116) = -0.150$ (QSTD) for the same force]; (2) with the Yale-Shakin force of Table V: $g_{5_1}\text{-}(116) = -0.198$ (QTD) and $= -0.221$ (QSTD). In order to fit the observed value of Ref. 22, we have undertaken a calculation involving the contributions of the neutrons and protons of the core explicitly, in addition to the valence neutrons.[24] Our preliminary results show that the absolute values of g_{5_1}- given above get reduced by the contributions of the core nucleons.

III. CONCLUSIONS

We have examined several aspects of the power and of the limitations of the microscopic spectroscopy of superconductor vibrational nuclei based on the QTD methods. We have seen how, with realistic nuclear forces renormalized for core polarization, reasonable semiquantitative agreement with experiment can be obtained by solving secular problems of dimensions reduced by many orders of magnitude with respect to those of the exact shell-model-configuration problem.

The pure two-qp QTD theory with the projection out of the $(\hat{N}-N_0)|0\rangle$ spurion is a very good approximation (except for the 0^+ states) of the QSTD eigenstates; this means only very small four-qp (or seniority $v=4$) admixtures in such states. In particular, if one wants to interpret QTD modes as "phonons," the excited 0^+, 2^+, and 4^+ "triplet" and other excited states certainly are *not* of the two-phonon type. Similar conclusions apply to the simply related quasiparticle random-phase approximations (QRPA and QSRPA). On the other hand, the four-qp components of QSTD eigenvectors are, even though small, very important for single-particle observables. In particular, they considerably enhance the diagonal elements of the $E2$ operator [in $Q(2_1^+)$].

The theory presupposes here the predominance of the BCS (or qp vacuum, $|0\rangle$) component in the ground state ($|0_1^+\rangle$). In principle, the QTD and QSTD theories should be based on self-consistent solutions of the HFB problem. Presumably, such bases, being a better (variational) approximation to the ground state, should tend to decrease the ultimate configuration mixing and, in particular, to reduce the spuriousness of the particle-number nonconservation and thus the depletion of the $|0\rangle$ component in $|0_1^+\rangle$. In such a situation, the QTD, QSTD modes have a clear interpretation of simple operators generating excitations directly from the ground state.

One very interesting question is that of possible deformed HFB solutions; it would be natural to expect a further reduction of the four-qp modes in QSTD with an HFB deformed basis. This question remains completely open. A QSTD description in terms of a purely spherical basis may turn out to be equivalent to a QTD description with a deformed HFB basis.

Unfortunately, in practice HFB bases are not available, especially in the Sn region, and one is forced to use bases defined in a purely phenomenological way. This is, of course, a very bad limitation. With the definitions applied in the present paper we find generally unpleasant ambiguities and also rather large depletions of the $|0\rangle$ component of $|0_1^+\rangle$. This renders the interpretation of all other QTD and QSTD eigenstates somewhat obscure. In collaboration with Alzetta and Gambhir,[25] the present authors are now performing calculations for both even and odd Sn isotopes where the BCS solutions would be based on a modified inverse-gap-equation (IGE) method. The qp basis is in this method defined by the lowest experimental energies of the odd mass isotopes and the one- and three-qp Tamm-Dancoff (QTD 13) solutions. It is hoped the method will give a considerable general improvement of our theory of the even isotopes in addition to assuring good agreement with the observed energy spectra for the odd isotopes.

The basic spurions due to the nucleon-number nonconservation must always be projected out before diagonalization. Their importance depends on the set of the single-particle parameters used as input in a given secular problem. The "blocking" or any other approximation of the basic spurions may not be very good for inappropriately chosen single-particle parameters. There always remains a higher-order spuriousness of spurions with components outside our Hilbert space. Their parasitic role is probably not very dangerous for the lowest-lying states but may become so for higher-lying Tamm-Dancoff eigenvalues and eigenvectors. These problems are now being investigated. Calculations are now projected for the exact nucleon-number conserving projected qp second Tamm-Dancoff (PQSTD) theory, which is an extension of the PTD method described by MacFarlane.[12] In this method, the qp vacuum ($|0\rangle$) vector is replaced by the number-projected vector called the projected BCS (PBCS)

[22] E. Bodenstaedt *et al.*, Nucl. Phys. **89**, 305 (1966); Z. Physik. **168**, 370 (1962).

[23] Through an unfortunate trivial arithmetic error the values of g_{5_1}- of Ref. 3 must be corrected to read: for the Gaussian ($t=1$) force $g_{5_1}\text{-}(116) = -0.233$ (QTD) and $= -0.258$ (QSTD) if $e_{\text{eff}}^{(M1)} = 0$ and $g_{5_1}\text{-}(120) = -0.373$ for the same.

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ground state. The number-conserving PQTD and PQSTD excitation operators are then applied to PBCS and orthonormalized by a Schmidt procedure. The final exactly spurion-free solution of the secular problem represents mixing of shell-model configurations of seniority $v=0$, 2, and 4 in a Hilbert space spanned on QTD and QSTD modes, thus of dimensions reduced enormously with respect to the original "exact" shell model. The dimensions are, in fact, independent of the number of nucleons; only the matrix elements depend on a given isotope (or isotone). The PQSTD model should clear up the question of the role played by the higher-order spurions not projected out in QSTD.

ACKNOWLEDGMENTS

We are happy to acknowledge a number of useful discussions with and critical remarks from J. Hendekovič. Some of our computer codes are due to P. L. Ottaviani. All our numerical computations were performed on the IBM 7044 computer of the Centro di Calcolo della Università di Trieste, and the cooperation of its staff is gratefully acknowledged. Two of us (M. G. and J. S.) wish to thank Professor Abdus Salam and Professor P. Budini for their hospitality at the International Centre for Theoretical Physics, Trieste.

Financial support from UNESCO to one of us (M. G.) is greatly appreciated.

PHYSICAL REVIEW VOLUME 173, NUMBER 4 20 SEPTEMBER 1968

Overlapping Compound-Nucleus Resonances

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(Received 22 August 1967; revised manuscript received 29 April 1968)

A simple model to study two overlapping compound-nucleus resonances is constructed. Expressions have been derived for the joint probability distribution of the spacing and the widths of the collision matrix for the elastic and inelastic scattering. In the inelastic case, we have considered only a two-channel problem. It is shown that the unitarity gives rise to the statistical correlation between the width and the spacing of the collision matrix. The model is also used to check which of the relations between the averages of the parameters of the statistical collision matrix, obtained using the ensemble of random complex orthogonal matrices, are consistent with the constraint of unitarity.

I. INTRODUCTION

THE statistical properties of the resonance parameters of the low-energy collision matrix have been fairly well studied for the case of well-separated resonances.[1] During the last couple of years, there has been much interest in the study of the fluctuations of nuclear cross sections,[2] which occur in the region of overlapping resonances. In the derivation of the expressions for various average cross sections and their fluctuations we need the statistical properties of the resonance parameters in the region of overlapping resonances. Only a few attempts have been made for such a study.[3,4]

In Ref. 3 it was shown that the random-matrix hypothesis can be used to study the statistical properties of the statistical collision matrix introduced by Moldauer.[5] It was shown[3] that a number of relations between the parameters of the statistical collision matrix can be obtained without a complete knowledge of the weight function, which had to be introduced to make the normalization integral converge. Since the collision matrix must be unitary, there must be relations among the parameters of the collision matrix. The question we raise now is as follows: Which of the relations obtained using the ensemble of random complex orthogonal-matrices are consistent with the constraint of unitarity?

The statistical properties of the resonance parameters in Ref. 4 are obtained in two ways: (a) use of large-scale numerical computations. The numerical values of the parameters of the statistical collision matrix are obtained by diagonalizing a complex symmetric-level matrix, which is constructed using the parameters of the real-boundary-value problem. These numerical calculations are helpful in indicating certain trends in the behavior of the parameters only. (b) construction of unitary models. Some unitary models are constructed starting from R-matrix theory of nuclear reactions.[6] In most of these models the usual statistical distribution of the R-matrix parameters cannot be used.

A formulation using the ensemble of random unitary symmetric matrices is also developed by Krieger[7] to calculate the averages and the fluctuations of the cross sections. This formulation does not attempt to study the

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