obtain $\sigma_{pm}=26.1\pm2.5$ b. This value is to be compared with a value of 23.5 b for the neighboring element Ho, obtained[28] from the experimental angular distribution of scattered neutrons, and a value of 27 b calculated by Zimmerman *et al.*[29] for natural erbium, using neutron scattering form factors calculated by Blume *et al.*[30] Finally, if we use $\sigma_{pm}=26.1\pm2.5$ b for Er^{164}, we get an absorption cross section for this isotope equal to 13 ± 9 b. Since the contribution of the positive energy resonances to the thermal absorption of Er^{164} is only 2 b, this indicates that Er^{164} has a bound level which contributes significantly to the thermal absorption cross section.

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One- and Three-Quasiparticle States of Odd-Mass Ni Isotopes*

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The modified Tamm-Dancoff approximation has been used to study the states of odd-mass Ni isotopes as the superposition of one- and three-quasiparticle states. The three-quasiparticle basic states are classified according to the well-known seniority scheme and are expressed in an equivalent second-quantized form. These three-quasiparticle states form an orthonormal and nonredundant set. The effect of the spurious 0^+ two-quasiparticle state has also been removed from these basis wave functions. Several different kinds of two-body residual interaction have been used in the calculation. Fairly decent agreement is obtained in the energy spectra between our results and the exact shell-model results, using the effective interaction of Cohen *et al.* Various approximate methods, such as the perturbation theory and a phonon approximation, are discussed in the context of the present method. The effect of the ground-state correlation is also studied. The admixture of the three-quasiparticle states in the lowest few levels causes very little change in the magnetic moment, and the $M1$ transition rates calculated on the basis of a single-quasiparticle structure of these states. The $E2$ transition rate is fairly sensitive to the admixture and the type of interaction used.

1. INTRODUCTION

THE nuclear shell model has been successfully applied to the description of nuclei having few nucleons in the unfilled major shell. This line of approach becomes very complicated with the increase of number of nucleons due to the large number of near degenerate configurations involved. Such calculations are made possible by the development of the superconductivity (BCS) model[1,2] of the nucleus, which takes into account the strong "pairing interaction" between nucleons by the Bogoliubov-Valatin transformation resulting in quasiparticles. In the lowest approximation, the model interprets the first few low-lying states of odd-A nuclei as independent one-quasiparticle excitations. The first 2^+ state of spherical even nuclei, the so-called one-phonon state, is described as a superposition of quasiparticle pair states in the framework of Tamm-Dancoff approximation (TDA) and as a superposition of quasiparticle pair and quasihole pair states in the framework of random-phase approximation (RPA). A better approximation for odd-mass nuclei, then, is to mix the independent quasiparticle states with the states obtained by coupling single quasiparticles to this phonon state. Hereafter, this will be referred to as the phonon approximation (PA).

A more rigorous procedure is to do the configuration-mixing calculation of quasiparticle residual interaction in an enlarged space of all the one- and three-quasiparticle states. Such calculations involve technical difficulty in the construction of three-quasiparticle basic states when all the three-quasiparticles are in the same level.

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In the work of Ref. 3 we considered the case of even nuclei and discussed the method of doing a quasiparticle calculation in the space of two- and four-quasiparticle states using the correct set for the latter. The types of problems associated with the construction of a nonredundant and orthogonal set of four-quasiparticles states were discussed there, and the solution to the problem was laid down in terms of states classified by the well-known shell-model seniority scheme. In the present paper the three-quasiparticle basic states are constructed according to the same scheme. In this sense the present work is an extension to odd nuclei of the modified TDA method (henceforth MTDA), already proposed in our earlier work[3] on even nuclei.

The seniority classified three-quasiparticle states, together with the tabulated values of their fractional parentage coefficients, are very convenient in evaluating the matrix elements contained in the three-quasiparticle subspace. The equivalent second-quantized versions of these states are also given in this paper. They are necessary for the evaluation of matrix elements between one- and three-quasiparticle subspaces.

The spurious effects arising because of the nonconservation of the number of particles in the quasiparticle method have been removed following the procedure of Ref. 3.

The main aim of this paper is to test first the accuracy of our formalism by comparing the results on energy levels with the exact shell-model results for phenomenological interactions. Apart from this, the reliability of various approximations, used by earlier workers, such as the perturbation theory (PT) in which the quasiparticle interaction is treated by the perturbation method and the PA, described above, have also been investigated in a quantitative manner. Various two-body interactions have been used and detailed results presented on level energies, magnetic moments, and transition rates.

2. MODIFIED TAMM-DANCOFF APPROXIMATION

The quasiparticle method of treating the Hamiltonian has been described by many authors.[1,2] The important aspects of this theory that are required in our work are summarized in Sec. 2 of Ref. 3. All the notations used in the present paper are defined there. We would like to add here only one statement concerning the solution of Eqs. (2.5) and (2.6) of Ref. 3. The latter equation giving the number of particles, applies to an even nucleus, the right-hand side being the expectation value of the number operator for the vacuum state of quasiparticles. For an odd-mass nucleus, the expectation value has to be taken for a single quasiparticle state, say $|jm\rangle$. As a result we should now, strictly speaking, add a term $(\epsilon_j-\lambda)/E_j$ to the right-hand side of the above-mentioned equation. We, however, checked by actual numerical computation that the addition of such a term makes a very small difference in the solutions of the chemical potential λ and the energy-gap parameters Δ_a. The maximum discrepancy occurs for Ni^{59}, where the values of the quasiparticle energies E_a and transformation coefficients V_a, that are calculated with λ and Δ_a, change by about 5 and 20%, respectively. We have therefore ignored the extra term of the number equation in solving our quasiparticle quantities for odd-mass nuclei. The slight error that this procedure entails for Ni^{59} is not considered to be serious because the number of particles in unfilled levels being only three, the quasiparticle method is not expected to yield very good quantitative results for this nucleus anyway.

Having obtained the quasiparticle transformation coefficients U_a and V_a, and energies E_a with the help of formulas of Ref. 3, the task that remains is to use these quasiparticle quantities and set up the matrix for the residual quasiparticle interaction $\bar{H}_{\text{int}}$. We now proceed to quote the necessary formulas for computing these matrix elements.

A. Basis States

The one-quasiparticle state $|\alpha\rangle$ is just the quasiparticle operator $a_\alpha^\dagger$ operating on $|0\rangle$, viz.,

$$|\alpha\rangle=a_\alpha^\dagger|0\rangle. \tag{2.1}$$

In the second-quantized notation, a normalized three-quasiparticle state of angular momentum J with projection M can be written as

$$\Psi(abJ_1,c;JM)=N(abc,J_1J)[A^\dagger(abJ_1),a_c^\dagger]_M{}^J|0\rangle, \tag{2.2}$$

where $N(abc,J_1J)$ is the normalization constant and J_1 is the intermediate angular momentum of two quasiparticles (a,b). These wave functions Ψ form an orthonormal set except when all the three indices (a,b,c) are equal. In this case

$$\Psi(aaJ',a;JM) \quad \text{and} \quad \Psi(aaJ_1',a;JM) \tag{2.3}$$

are not generally independent; in other words, they are redundant and nonorthonormal. Therefore, this case requires special treatment. Here we follow the procedure of Ref. 3 and classify the three-quasiparticle states according to the well-known seniority scheme[4] which automatically ensures an independent, orthogonal, and nonredundant basis. The following are the possible three-quasiparticle configurations.

$$\begin{aligned}&(1)\ |a^3J\nu\rangle \quad (2)\ |a_1{}^2J_1,a_2;J\rangle\\ &(3)\ |a_1a_2J_{12},a_3;J\rangle.\end{aligned} \tag{2.4}$$

Here J is the total angular momentum, ν is the seniority,

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and a subscripted J is the intermediate angular momentum of a quasiparticle pair. The superscript on a and a_1 denotes the number of quasiparticles present in that particular state.

For configuration (1), the antisymmetric normalized state $|a^3J\rangle$ can easily be written with the help of coefficients of fractional parentage,[4] while for the types (2) and (3), the antisymmetric normalized state can be obtained by using the relation (4.6) of Ref. 3.

These shell-model forms are very well suited for the calculation of matrix elements connecting any two three-quasiparticle basis states. But it is essential to write these states in their second quantized form for the evaluation of the matrix elements between one- and three-quasiparticle states. The second-quantized version of these states is given below (cf. Ref. 3):

Configuration (1): $|j^3J\nu M\rangle$

$$=\{(3!)^{1/2}\langle j^2(J_1),j,J||j^3J\rangle\}^{-1}\times[A^\dagger(jjJ_1),a_j^\dagger]_M{}^J|0\rangle \quad (2.5)$$

Configurations (2) and (3): $|j_1j_2J_{12},j_3;JM\rangle$

$$=[\mathfrak{A}^\dagger(j_1j_2J_{12}),a_{j_3}^\dagger]_M{}^J|0\rangle. \quad (2.6)$$

$\mathfrak{A}^\dagger$ and $A^\dagger$ are the normalized and unnormalized creation operators for a quasiparticle pair state.

B. Matrix Elements in Three-Quasiparticle Subspace

In this case, only the H_{22} part (which conserves the number of quasiparticles) of $\bar{H}_{\rm int}$ will contribute and the various expressions for the matrix elements are given below. A typical matrix element connecting a type-(1) state with another type-(1) state is given by

$$\langle a_1^3J\nu|\bar{H}_{\rm int}|a_2^3J\nu'\rangle=\tfrac{3}{2}\sum_{J_1}\langle a_1^2(J_1),a_1,J||a_1^3J\nu\rangle\langle a_2^2(J_1),a_2,J||a_2^3J\nu'\rangle\bar{Y}(a_1a_1a_2a_2J_1)\delta a_1a_2. \quad (2.7)$$

A matrix element connecting a state of type (1) with another of type (2) or (3) is given by the expression

$$\langle a_1^3J\nu|\bar{H}_{\rm int}|a_2a_3J_{23},a_4;J\rangle=N(a_2a_3)(\tfrac{3}{2})^{1/2}\{\langle a_1^2(J_{23}),a_1,J||a_1^3J\nu\rangle\bar{Y}(a_1a_1a_2a_3J_{23})\delta a_1a_4+\bar{P}(a_2a_3J_{23})\times\sum_{J_1}\langle a_1^2(J_1),a_1,J||a_1^3J\nu\rangle[J_1J_{23}]^{1/2}W(a_2a_3Ja_4;J_{23}J_1)(-1)^{a_1+J_1-J}\delta a_1a_2\bar{Y}(a_1a_1a_3a_4J_1)\}. \quad (2.8)$$

The matrix element between any two states of types (2) and (3) is given by the following expression:

$$\langle a_1a_2J_{12},a_3;J|\bar{H}_{\rm int}|a_4a_5J_{45},a_6;J\rangle=N(a_1a_2)N(a_4a_5)\{\delta a_3a_6\delta J_{12}J_{45}\bar{Y}(a_1a_2a_4a_5J_{45})+\bar{P}(a_1a_2J_{12})[J_{12}J_{45}]^{1/2}\times W(a_1a_2Ja_3;J_{12}J_{45})(-1)^{a_6+J_{45}-J}\delta a_1a_6\bar{Y}(a_2a_3a_4a_5J_{45})+\bar{P}(a_4a_5J_{45})[J_{12}J_{45}]^{1/2}W(a_4a_5Ja_6;J_{45}J_{12})\times\delta a_3a_4(-1)^{a_3+J_{12}-J}\bar{Y}(a_1a_2a_5a_6J_{12})+\bar{P}(a_1a_2J_{12})\bar{P}(a_4a_5J_{45})\sum_{J_{23}}[J_{23}][J_{12}J_{45}]^{1/2}W(a_1a_2Ja_3;J_{12}J_{23})\times W(a_4a_5Ja_6;J_{45}J_{23})\delta a_1a_4\bar{Y}(a_2a_3a_5a_6J_{23})\}. \quad (2.9)$$

Here $\langle a^2(J_1),a,J||a^3J\nu\rangle$ is the one-particle-type fractional parentage coefficient, and $\bar{P}(abJ)=1-(-1)^{a+b-J}\times P(a\leftrightarrow b)$, where the operator $P(a\leftrightarrow b)$ interchanges a and b. $\bar{Y}$ is the matrix element of H_{22} between two-quasiparticle states defined by

$$\bar{Y}(abcdJ)=\langle 0|A(abJM)H_{22}A^\dagger(cdJM)|0\rangle=\{(U_aU_bU_cU_d+V_aV_bV_cV_d)G(abcdJ)+\bar{P}(cdJ)(U_aV_bU_cV_d+V_aU_bV_cU_d)F(abcdJ)\}. \quad (2.10)$$

The notations $[a]=2a+1$ and $[ab\cdots]=(2a+1)(2b+1)\cdots$. For the notations F, G, U, V, and W, see Ref. 3.

C. Matrix Elements Between One- and Three-Quasiparticle Subspaces

A typical matrix element of this kind is given by

$$\langle\Psi|H_{31}a_\alpha^\dagger|0\rangle, \quad (2.11)$$

where Ψ is any of the three-quasiparticle states of (2.4). To evaluate it, we first express $H_{31}a_\alpha^\dagger|0\rangle$ as a sum of three-quasiparticle basis states and then pick up the coefficient of Ψ in the expansion. In this way we obtain

$$\langle a^3J\nu M|H_{31}a_\beta^\dagger|0\rangle=\tfrac{1}{2}\sum_{J_1}(U_a{}^2U_bV_a-V_a{}^2V_bU_a)(3!)^{1/2}\langle a^2(J_1),a,J||a^3J\nu\rangle\{[J_1]/[b]\}^{1/2}G(aaabJ_1)\delta_{bJ}\delta_{\beta M}. \quad (2.12)$$

For the states Ψ of types (2) and (3) of (2.4), the single general expression, given below, is adequate;

$$\langle 0|[\mathfrak{A}^\dagger(abJ_{12}),a_c^\dagger]_M{}^{J\dagger}H_{31}a_\delta^\dagger|0\rangle=\bar{N}(ab)\{[J_{12}]/[d]\}^{1/2}\{(U_aU_bU_dV_c-V_aV_bV_dU_c)G(abcdJ_{12})-\bar{P}(abJ_{12})(U_bU_cU_dV_a-V_bV_cV_dU_a)F(abcdJ_{12})\}\delta_{dJ}\delta_{\delta M}. \quad (2.13)$$

D. Ground-State Correlation

To derive the equation of motion for the correlated ground state, one has to retain in the commutators of H with one- and three-quasiparticle operators only those terms containing single and triple quasiparticle and quasihole operators. These commutators can be written as

$$[H,a_{JM}^{\dagger}]=E_J a_{JM}^{\dagger}+\sum_{bcdJ_{12}} S(J|bcJ_{12},d;J)\Psi^{\dagger}(bcJ_{12},d;JM) + \sum_{bcdJ_{12}} R(J|bcJ_{12},d;J)(-1)^{J-M}\Psi(bcJ_{12},d;J-M), \quad (2.14)$$

and

$$[H,\Psi^{\dagger}(abJ_{12},c;JM)]=(E_a+E_b+E_c)\Psi^{\dagger}(abJ_{12},c;JM)+\sum_{defJ_{12}'} L(abJ_{12},c|deJ_{12}',f;J)\Psi^{\dagger}(deJ_{12}',f;JM) + S(J|abJ_{12},c;J)a_{JM}^{\dagger}-R(J|abJ_{12},c;J)(-1)^{J-M}a_{J-M}. \quad (2.15)$$

Here $\Psi^{\dagger}$ and Ψ are, respectively, the creation and annihilation operators for a three-quasiparticle state, designated by the quantum numbers inside parentheses. S stands for the matrix element between one- and three-quasiparticle states denoted inside the parentheses wherein a vertical line has been used to separate the two states. L denotes the matrix elements between three-quasiparticle states defined by Eqs. (2.7)–(2.9), and R is given by

$$R(a|bcJ_{12},d;a)=N(bc)\{[J_{12}]/[a]\}^{1/2}\{(U_bU_cV_dV_a+V_bV_cU_dU_a)G(bcdaJ_{12}) -\bar{P}(bcJ_{12})(U_cU_dV_bV_a+V_cV_dU_bU_a)F(bcdaJ_{12})\} \quad (2.16)$$

except for the case of $b=c=d$. In this case it is expressed by

$$R(a|bbJ_{12},b;a)=\tfrac{1}{2}(U_b^2V_bV_a+V_b^2U_bU_a)(3!)^{1/2}\langle b^2(J_{12}),b;a||b^3a\nu\rangle\{[J_{12}]/[a]\}^{1/2}G(bbbaJ_{12}). \quad (2.17)$$

The corresponding commutators of one- and three-quasihole operators with H will be obtained by taking the Hermitian conjugate of Eqs. (2.14) and (2.15) and then reversing the sign.

E. The Energy Matrix

The energy matrix in the space of one- and three-quasiparticles and one- and three-quasiholes is given by

$$\begin{pmatrix} E & S & 0 & R \\ S & L+E' & -R & 0 \\ 0 & -R & -E & -S \\ R & 0 & -S & -L-E' \end{pmatrix}, \quad (2.18)$$

where E' is a diagonal matrix with elements equal to the unperturbed energies of three-quasiparticle states. Note that the above RPA matrix for odd-A nuclei is symmetric. The energy matrix without ground-state correlations (MTDA) will be just

$$\begin{pmatrix} E & S \\ S & L+E' \end{pmatrix}. \quad (2.19)$$

F. The Spurious Effects

The effect of the spurious 0^+ pair states has been removed by the method described in Sec. 4.1 of Ref. 3. Instead of using n three-quasiparticle states of the type $|a_i^2 0,j;jm\rangle$, $i=1, 2, \cdots, n$, we use $(n-1)$ states of the type $|\phi_i,j;jm\rangle$, $i=1, 2, \cdots, n-1$. The states $|\phi_i\rangle$ are defined in Ref. 3, Eq. (4.4). The quantum numbers after the semicolon denote the final angular momentum and its projection, while the quantum numbers separated by the comma denote the two angular momenta that have been coupled to each other to produce the final value. In practice, an orthogonalized set, obtained by suitable linear combination, is used.

3. APPROXIMATE METHODS

A. Perturbation Theory (PT)

The independent quasiparticle excitation energies can be improved upon by treating the $\bar{H}_{\rm int}$ as a perturbation. Second-order perturbation theory is expected to yield good results for the first few low-lying states if all the three-quasiparticle states are quite high and if the collective effects are not important. The lowest eigenvalues in this case are given by

$$\omega_a=E_a-\sum_{bcdJ_{12}} \frac{\{S(a|bcJ_{12},d;a)\}^2}{E_b+E_c+E_d-E_a}. \quad (3.1)$$

B. Phonon Approximation (PA)

The first 2^+ state of a spherical even nucleus is described as a one-phonon state in the quasiparticle theory.[1,2] The state of projection M is created by an operator $Q_M^{\dagger}$ given by

$$Q_M^{\dagger}=\sum_{(ab)} x(ab)\mathcal{A}^{\dagger}(ab2M) + \sum_{(ab)} \bar{x}(ab)(-1)^M\mathcal{A}(ab2-M). \quad (3.2)$$

The coefficients x and $\bar{x}$ appearing in this expression

denote, respectively, the amplitudes of the quasiparticle and quasihole pair states. Here (ab) stands for the restricted sum over the distinct quasiparticle (hole) pairs $(a \leqslant b)$. In the framework of TDA the amplitudes $\bar{x}$ are neglected.

The low-lying states of the next odd-mass nucleus, in the phonon approximation, are obtained by mixing the single quasiparticle states with the states arising from the coupling of single quasiparticles to the phonon state. The matrix elements between the one-quasiparticle state and the states resulting from the coupling of a quasiparticle to the phonon are just combinations of the "S" and "R" matrix elements given by Eqs. (2.12), (2.13), (2.16), and (2.17). The matrix element between any two quasiparticle plus phonon states is zero, except for the diagonal case which is given by the sum of energy of the first 2^+ state of the even nucleus and the coupled quasiparticle state. This is because only the H_{22} part of $\bar{H}_{\text{int}}$ can contribute to this type of matrix element; but H_{22} in the phonon approximation is a pure phonon operator and has already been diagonalized in obtaining the lowest quadrupole phonon.

4. ELECTROMAGNETIC MOMENTS AND TRANSITION RATES

General expressions for the reduced transition probability have been given in Sec. 6 of Ref. 3, Eqs. (6.1)–(6.7). The static moments are given by the same kind of matrix elements, the only difference being that the nuclear states on the two sides of the operator Ω^L are identical. The operator for the quadrupole moment is $(16\pi/5)^{1/2}$ times the zero projection component of the $E2$ transition operator, while the magnetic moment operator is obtained from the z component of the $M1$ transition operator by omitting the multiplying factor of $(3/4\pi)^{1/2}$.

The matrix elements necessary for the computation of these quantities are given below.

(i) Matrix elements connecting one- and three-quasiparticle states: type-(1) three-quasiparticle state:

$$\langle a^3 J\nu||\Omega^L||b\rangle=(-1)^{L+b-J}R^L(a,a)(3!)^{1/2}\langle a^2(L),a,J||a^3 J\nu\rangle\delta_{ab}. \tag{4.1}$$

Type-(2) or -(3) three-quasiparticle state:

$$\langle a_1a_2J_{12},a_3;J||\Omega^L||b\rangle=N(a_1a_2)\bar{P}(a_1a_2J_{12})\{(-1)^{L+b-J}R^L(a_1,a_2)\delta_{a_3b}\delta_{LJ_{12}}+\delta_{a_1b}[J_{12}L]^{1/2}$$
$$\times W(ba_2Ja_3;J_{12}L)[R^L(a_2,a_3)-(-1)^{a_2+a_3-L}R^L(a_3,a_2)]\}. \tag{4.2}$$

(ii) Matrix elements between states in the three-quasiparticle subspace: type (1) three-quasiparticle states:

$$\langle a_1^3J_1\nu_1||\Omega^L||a_2^3J_2\nu_2\rangle=6\sum_{J_1'}\langle a_1^2(J_1'),a_1,J_1||a_1^3J_1\nu_1\rangle\langle a_2^2(J_1'),a_2,J_2||a_2^2J_2\nu_2\rangle$$
$$\times\delta_{a_1a_2}[LJ_2]^{1/2}W(J_1'a_1J_1L;J_2a_1)\bar{R}^L(a_1,a_1). \tag{4.3}$$

Type-(1), type-(2), or type-(3) three-quasiparticle states:

$$\langle a_1^3J_1\nu_1||\Omega^L||a_2a_3J_{23},a_4;J_2\rangle=2\sqrt{3}\delta_{a_2a_3}\delta_{a_1a_2}\langle a_1^2(J_{23}),a_1,J_1||a_1^3J_1\nu_1\rangle\bar{R}^L(a_1,a_4)[J_2L]^{1/2}W(J_{23}a_4J_1L;J_2a_1). \tag{4.4}$$

Type-(2) or type-(3) states:

$$\langle a_1a_2J_{12},a_3;J_1||\Omega^L||a_4a_5J_{45},a_6;J_2\rangle=2N(a_1a_2)N(a_4a_5)\{\bar{P}(a_1a_2J_{12})\delta_{a_1a_4}\delta_{a_2a_5}\delta_{J_{12}J_{45}}\bar{R}^L(a_3,a_6)[LJ_2]^{1/2}$$
$$\times W(J_{45}a_6J_1L;J_2a_3)+\bar{P}(a_1a_2J_{12})\bar{P}(a_4a_5J_{45})[J_{12}J_{45}J_2L]^{1/2}[\delta_{a_1a_5}\delta_{a_2a_6}\bar{R}^L(a_3,a_4)W(a_4a_5J_2a_6;J_{45}J_{12})$$
$$\times W(J_{12}a_4J_1L;J_2a_3)+\delta_{a_2a_4}\delta_{a_3a_5}\bar{R}^L(a_1,a_6)W(a_1a_2J_2a_3;J_{12}J_{45})W(J_{45}a_6J_1L;J_2a_1)+\sum_{J_{23}}\bar{R}^L(a_1,a_4)[J_{23}]$$
$$\times W(a_1a_2J_1a_3;J_{12}J_{23})W(a_4a_5J_2a_6;J_{45}J_{23})W(J_{23}a_4J_1L;J_2a_1)(\delta_{a_2a_5}\delta_{a_3a_6}-(-1)^{a_2+a_3-J_{23}}\delta_{a_2a_6}\delta_{a_3a_5})]\}. \tag{4.5}$$

5. NUMERICAL CALCULATIONS, RESULTS, AND DISCUSSIONS

For the explicit numerical calculation, the protons in the Ni isotopes are assumed to form an inert core corresponding to the semimagic number 28, while the neutrons in excess of 28 are assumed to be distributed in all possible ways among the close-lying $2p_{3/2}$, $1f_{5/2}$, and $2p_{1/2}$ orbitals. The unperturbed single-particle energies for $2p_{3/2}$, $1f_{5/2}$, and $2p_{1/2}$ were taken to be 0.0, 0.78, and 1.08 MeV, respectively, from the Ni^{57} spectrum, and in agreement with other authors.[5,6]

The following different effective two-body interactions have been used:

[5] R. D. Lawson, M. H. MacFarlane, and T. T. S. Kuo, Phys. Letters **22**, 168 (1966).

[6] S. Cohen, R. D. Lawson, M. H. MacFarlane, S. P. Pandya, and M. Soga, Phys. Rev. (to be published).

TABLE I. For each nucleus the first row gives the single-quasiparticle energy (E) in MeV, the second row gives the same quantity corrected by perturbation theory (see Sec. 3 A), and the third row gives the transformation coefficient (V). The pairing matrix elements of EIC have been used in obtaining these values.

	J^π		
A	$\frac{1}{2}^-$	$\frac{3}{2}^-$	$\frac{5}{2}^-$
59	1.80	1.26	1.51
	1.77	1.21	1.48
	0.379	0.647	0.416
61	1.58	1.45	1.40
	1.54	1.37	1.37
	0.512	0.783	0.581
63	1.38	1.65	1.34
	1.36	1.55	1.32
	0.644	0.870	0.724
65	1.21	1.85	1.32
	1.20	1.78	1.31
	0.783	0.931	0.847

(1) effective interaction of Cohen *et al.*[6] (EIC) and Auerbach[7] (EIA);

(2) the pairing plus quadrupole interaction;[1,8] the pairing interaction of Kisslinger and Sorensen is used in determining the quasiparticle quantities E_a, U_a, V_a, etc., while the residual interaction is taken to be of the quadrupole type:

$$H_{QQ}=-Xr_1^2r_2^2Y^2(1)Y^2(2), \qquad (5.1)$$

with the strength parameter X given by $\pi b^{-4}X=0.097$ MeV, where $b=(\hbar/M\omega)^{1/2}$ is the oscillator well parameter.

(3) Surface-delta (S-δ) interaction of Green and Moszkowski,[9] for which the required matrix elements were calculated using expression (7) of Gambhir and Ram Raj,[10] and a strength g equal to 0.50 MeV determined by the inverse-gap-equation method.[11]

(4) A potential[12] similar to Rosenfeld mixture (RM) with the following strength parameters (in MeV):

$$\text{odd singlet}=41.5,$$
$$\text{even singlet}=-34.4,$$
$$\text{odd triplet}=19.4,$$
$$\text{even triplet}=-46.9,$$

having Yakawa radial dependence and range=1.4 F.

Matrix elements between three-*particle* shell-model configurations are given by the same expressions for the three-quasiparticle states, namely, Eqs. (3.7)–(3.9), provided that $\bar{Y}$ in these expressions is replaced by G. The various matrices were first generated by feeding G in place of $\bar{Y}$ for EIC, and then diagonalized. The energy eigenvalues thus obtained reproduce the numbers for Ni^{59} reported in Ref. 6, reflecting the correctness of our code written for CDC 3600.

In Table I, we present the single quasiparticle energies (E) and transformation coefficients (V) using the pairing matrix elements of the EIC two-body interaction. The perturbation theory (see Sec. 3 A) values of the quasiparticle energies are also shown; the perturbation in each case is seen to be very small.

To test the importance of eliminating spurious effects from the three-quasiparticle states, we next diagonalize the residual interaction using these states alone (i.e., without mixing the one- and three-quasiparticle states).

The calculations in three-quasiparticle subspace are made for all the interactions with and without elimination of the spurious effects. The results of EIC, EIA, and QQ interactions show the same trend, while the results of S-δ and RM interactions are very similar. We present in Table II these results for S-δ and EIC interactions for the first two energy eigenvalues of $\frac{1}{2}^-$, $\frac{3}{2}^-$, and $\frac{5}{2}^-$ states. The results for the S-δ interaction show that there appears one three-quasiparticle state very near the energy of the one-quasiparticle state, and that the former is spurious. On the other hand, this spurious effect is not so obvious in the case of the EIC interaction. Therefore, it is essential to remove the spurious effects consistently before the diagonalization of the energy matrix, and before comparing the results for different interactions.

Table III presents, for the EIC interaction, a comparison between the various methods of calculation-phonon approximation (PA), TDA, and MTDA. PA has been explained in Sec. 3 B. In the TDA method, the diagonalization is done in the three-quasiparticle subspace alone; the predicted spectra then consist of the single-quasiparticle levels of Table I and the three-quasiparticle eigenstates resulting from the diagonaliz-

TABLE II. Energy levels (MeV) calculated in three-quasiparticle space (a) with and (b) without eliminating spurious 0^+ effects. (See Sec. 2 F.) The subscripts on the level quantum numbers denote the number of the particular J^π level in order of increasing energy.

Interaction	J^π	59 a	59 b	61 a	61 b	63 a	63 b	65 a	65 b
	$(\frac{1}{2})_1^-$	1.81	2.09	1.71	2.11	1.55	2.17	1.41	2.26
	$(\frac{1}{2})_2^-$	2.12	4.27	2.11	4.42	2.19	4.54	2.30	4.63
	$(\frac{3}{2})_1^-$	1.46	2.12	1.60	2.07	1.72	1.97	1.81	1.87
S-δ	$(\frac{3}{2})_2^-$	2.14	2.79	2.07	2.69	1.97	2.72	1.89	2.79
	$(\frac{5}{2})_1^-$	1.68	2.62	1.63	2.63	1.57	2.59	1.50	2.51
	$(\frac{5}{2})_2^-$	2.60	2.83	2.62	2.72	2.58	2.73	2.45	2.82
	$(\frac{1}{2})_1^-$	2.18	2.19	1.97	1.97	2.06	2.07	2.36	2.44
	$(\frac{1}{2})_2^-$	3.50	3.87	3.45	3.48	3.12	3.49	2.79	3.81
	$(\frac{3}{2})_1^-$	1.78	1.85	1.87	1.87	1.82	1.82	1.91	1.92
EIC	$(\frac{3}{2})_2^-$	2.69	2.77	2.18	2.18	2.08	2.09	2.44	2.47
	$(\frac{5}{2})_1^-$	2.41	2.43	2.05	2.05	1.94	1.97	2.09	2.18
	$(\frac{5}{2})_2^-$	2.82	2.81	2.70	2.70	2.73	2.76	2.81	3.08

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ation. MTDA consists of diagonalizing in the complete space of one- and three-quasiparticle states. It is clear from the table that the first $\frac{1}{2}^-$, $\frac{3}{2}^-$, and $\frac{5}{2}^-$ states have very nearly the same energy in all the cases. However, the energies of second $\frac{1}{2}^-$, $\frac{3}{2}^-$, and $\frac{5}{2}^-$ states obtained in the case of PA are somewhat higher (except in Ni^{59} and Ni^{65}) and occur nearly at the same energy. The effect of the mixing of one- and three-quasiparticle subspaces (MTDA) is to slightly lower the first state and to push up the second state relative to the TDA results. We also did the calculation based on RPA using the creation and annihilation operators for all our MTDA states. The results of including the effect of the ground-state correlation in this way, however, produce energy eigenvalues which are practically identical with the MTDA results. For this reason we have not shown the RPA results in the table. A similar trend is expected in the results for the other interactions and therefore only the MTDA results will be presented.

Although we did both TDA and MTDA calculations with all the different effective interactions listed in the beginning of this section, we present only the MTDA results for a few selected interactions in Table IV. About the TDA results we make only one general remark: Although these results are quite satisfactory, the goodness of fit to the data (included in the same table) definitely improves for all interactions as we go from TDA to MTDA. For example, the χ^2 value for the fit to all the known levels from $A=59$ to 65 changes from $0.092 \rightarrow 0.068$ for EIC, $0.057 \rightarrow 0.029$ for QQ, and $0.208 \rightarrow 0.193$ for RM. The MTDA results display a great deal of similarity in the cases of (i) EIC and EIA and (ii) QQ and S-δ. Hence, we present only the results for one each of the two groups, i.e., EIC and QQ. The results for RM have a significantly larger χ^2 value compared with other interactions, and hence they are not listed. Similar remarks hold for the results obtained by using the separable nonlocal potential of Tabakin,[13] which was used by Kuo *et al.*[14] Exact shell-model results are available[6] for the EIC interaction for which the value of χ^2 is 0.052. This shows that, although our prediction on particular energy levels differs somewhat from the exact results (also shown in Table IV), the over-all fit we have achieved is nearly of the same quality as that of Ref. 6.

TABLE III. Energies (MeV) obtained with EIC interaction and various methods of calculation. The three lines for each nucleus corresponds, respectively, to phonon approximation (PA), no mixing between one- and three-quasiparticle states (TDA), and mixing between these states (MTDA). The results for MTDA with ground-state correlation differs negligibly from MTDA, and hence is not presented separately. The subscripts on the level quantum numbers denote the number of the particular J^π level in order of increasing energy.

	J^π					
A	$(\frac{1}{2})_1^-$	$(\frac{1}{2})_2^-$	$(\frac{3}{2})_1^-$	$(\frac{3}{2})_2^-$	$(\frac{5}{2})_1^-$	$(\frac{5}{2})_2^-$
59	1.78	2.37	1.20	2.41	1.50	2.37
	1.80	2.19	1.26	1.85	1.51	2.43
	1.70	2.26	1.19	2.44	1.45	2.47
61	1.58	2.52	1.44	2.52	1.38	2.52
	1.58	1.87	1.45	1.87	1.40	2.05
	1.46	2.05	1.34	2.05	1.34	2.08
63	1.35	2.44	1.57	2.44	1.34	2.44
	1.38	2.07	1.65	1.82	1.34	1.97
	1.31	2.13	1.53	1.98	1.31	1.98
65	1.15	2.43	1.81	2.36	1.31	2.33
	1.21	2.44	1.85	1.92	1.32	2.18
	1.18	2.46	1.75	2.20	1.30	2.18

TABLE IV. Energy levels (MeV) of odd Ni isotopes by the MTDA-method. All the levels of a given nucleus have been calculated with respect to the lowest of them. The numbers labeled 1_{qp} denote the percentage of the one-quasiparticle state. The line "Exact" for EIC gives the energies calculated in Cohen *et al.*[a]

		J^π						
Interaction		$(\frac{1}{2})_1^-$	$(\frac{1}{2})_2^-$	$(\frac{3}{2})_1^-$	$(\frac{3}{2})_2^-$	$(\frac{5}{2})_1^-$	$(\frac{5}{2})_2^-$	A
EIC	Exact	0.29	1.10	0.0	0.82	0.21	1.47	
	MTDA	0.51	1.07	0.0	1.25	0.26	1.28	
	1_{qp}	85.9	4.21	96.6	0.03	95.7	0.95	
QQ	MTDA	0.51	1.06	0.0	0.95	0.31	1.40	59
	1_{qp}	80.7	2.22	96.6	0.33	94.5	0.51	
Expt. energy		0.47	1.32	0.0	0.89	0.34		
EIC	Exact	0.02		0.0		0.0	0.90	
	MTDA	0.12	0.73	0.01	0.71	0.0	0.75	
	1_{qp}	83.2	5.46	95.0	0.78	94.4	1.48	
QQ	MTDA	0.15	0.82	0.0	0.68	0.10	1.13	61
	1_{qp}	80.3	3.19	89.8	2.09	97.6	0.19	
Expt. energy		0.28		0.0		0.07	0.91	
EIC	Exact	0.0	1.18	0.24	0.90	0.01	0.95	
	MTDA	0.0	0.83	0.23	0.67	0.0	0.67	
	1_{qp}	92.2	3.03	93.1	4.23	97.3	0.65	
QQ	MTDA	0.0	0.87	0.18	0.54	0.06	1.15	63
	1_{qp}	87.0	2.72	88.0	1.92	99.0	0.0	
Expt. energy		0.0	1.01	0.16	0.53	0.09		
EIC	Exact	0.05		0.53	0.76	0.0	1.01	
	MTDA	0.0	1.28	0.57	1.02	0.12	1.00	
	1_{qp}	98.1	0.82	91.6	6.12	99.3	0.07	
QQ	MTDA	0.0	1.21	0.49	0.74	0.12	1.41	65
	1_{qp}	94.2	1.54	92.2	0.91	98.6	0.11	
Expt. energy		0.06		0.32	0.70	0.0		

[a] See Reference 6.

The percentage of one-quasiparticle states in each of the eigenstates of Table III shows the following systematic features: The first state of any given angular momentum is predominantly one-quasiparticle type, while in the second state three-quasiparticle states invariably predominate. The intermixture of one- and three-quasiparticle states, although small, accounts for the improvement in the χ^2 value from TDA to MTDA, as mentioned above.

The calculated magnetic moments are presented in Table V. As is well known, the correction to the magnetic moment operator itself due to velocity-dependent forces, meson-exchange current, etc., gives a contribution of roughly 0.2 nuclear magneton (nm). The values that we calculate using the various interactions, on the other hand, differ from each other by less than 0.1 nm. Hence we present only the results for EIC interaction and the one-quasiparticle (the same as the one-particle) values of the magnetic moments for comparison. The admixture of the three-quasiparticle states

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TABLE V. Quasiparticle contribution to the magnetic moment in nuclear magneton. 1_{qp} denotes the value for a single-quasiparticle state, and μ is the value calculated with our quasiparticle wave functions having three-quasiparticle admixture.

		μ			
J^π	1_{qp}	$A=59$	$A=61$	$A=63$	$A=65$
$\frac{1}{2}^-$	0.64	0.74	0.75	0.68	0.65
$\frac{3}{2}^-$	−1.91	−2.14	−2.22	−2.12	−1.97
$\frac{5}{2}^-$	1.36	1.35	1.36	1.38	1.38

in our calculation does produce a departure in some cases from single-quasiparticle values, but this once again is of the order of the basic uncertainty of 0.2 nm mentioned above. We make no attempt at fitting any observed data because it is well known that the core-polarization effect is a big contribution to the magnetic moment of these nuclei, and estimates of this effect already exist (see Ref. 8).

The same kind of observation holds for the $M1$ transition strengths of Table VI. The small admixture of the three-quasiparticle states affects the results to a very minor extent; consequently, the $M1$ strength connecting $f_{5/2}$ with $p_{3/2}$, which is strictly forbidden without the three-quasiparticle admixture, is still found to be negligibly small, and hence is not shown in the table.

The $E2$ transition strengths, shown in Table VII, on the other hand, display a more sensitive dependence on the interaction used, and the admixture of three-quasiparticle states. One must remember, however, that in this case the detailed form of the radial wave function plays an important role. We used harmonic oscillator radial functions; the use of more realistic functions seems to be necessary before the sensitive dependence of the $E2$ transition strengths may be utilized to arrive at definite conclusions. Experimental data are also rather scarce at the present time.

TABLE VI. $M1$ transition strength $B(M1)$ in units of squared nuclear magneton.

		$B(M1)$	
Transition	Nucleus	MTDA	1_{qp}
$\frac{1}{2}^- \rightarrow \frac{3}{2}^-$	59	0.91	1.05
	61	0.88	1.02
$\frac{3}{2}^- \rightarrow \frac{1}{2}^-$	63	2.00	2.05
	65	2.16	2.13

TABLE VII. E2 transition strength in units of e_{eff}^2 F^4 where F$=10^{-13}$ cm and e_{eff} is the effective charge of the neutron.

		$A=59$		$A=61$	
Transition	Interaction	1_{qp}	MTDA	1_{qp}	MTDA
$\frac{1}{2}^- \rightarrow \frac{3}{2}^-$	EIC	6.1	10.8	0.53	3.5
	EIA	6.2	12.9	0.50	6.6
	QQ	6.9	12.4	0.77	2.9
	S-δ	6.6	3.6	0.59	0.19
$\frac{5}{2}^- \rightarrow \frac{3}{2}^-$	EIC	1.5	0.46	0.02	0.32
	EIA	1.6	0.98	0.03	0.16
	QQ	1.6	0.05	0.03	1.55
	S-δ	1.5	3.9	0.02	1.2
		$A=63$		$A=65$	
$\frac{3}{2}^- \rightarrow \frac{1}{2}^-$	EIC	2.0	1.1	15.5	20.2
	EIA	2.2	0.38	15.6	8.0
	QQ	1.4	0.03	13.3	5.1
	S-δ	2.1	1.9	15.9	2.4
$\frac{3}{2}^- \rightarrow \frac{5}{2}^-$	EIC	0.50	0.87	2.2	1.8
	EIA	0.50	1.7	2.2	3.9
	QQ	0.44	2.9	2.0	3.2
	S-δ	0.49	0.09	2.2	0.78

We also calculated the spectroscopic factors for (d,p) and (d,t) reactions on even Ni targets leading to the odd isotopes as the final nucleus. The observed values are fairly well reproduced by pure single-quasiparticle states, and, hence, the small admixture of three-quasiparticle states we obtained left the quality of fit more or less unchanged.

The main point of this paper is to show how to do the quasiparticle calculation for odd nuclei using the correct set of three-quasiparticle states. A single quasiparticle coupled to a phonon gives rise to a state that has certain objectionable features, mentioned in the Introduction. The difference between the quasiparticle-phonon predictions and results predicted by the present formalism, which treats the three-quasiparticle states exactly, will make itself felt as experimental data on more and more excited levels start coming in.

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