Semimicroscopic description of neutron inelastic scattering by nuclei of medium mass

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In the framework of the quasiparticle-phonon model (QPM) of the nucleus a formalism for the semimicroscopic description of scattering of low-energy neutrons by spherical nuclei is developed. The potential of the neutron-nucleus interaction is constructed as a folding of the QPM nuclear transition densities and the M3Y effective nucleon-nucleon interaction. Calculations of the direct and compound cross sections for elastic and inelastic scattering of 1.5 to 3.0 MeV neutrons by $^{58}$Ni are performed. Satisfactory agreement with the experimental data is obtained.

1. INTRODUCTION

The standard coupled-channel method (CCM) has a series of drawbacks. Among them are a large number of adjustable parameters (the parameters of the optical potential, the deformation parameters, etc.), noninclusion of antisymmetrization, and lack of connection with the semimicroscopic nuclear models.

On the other hand, semimicroscopic approaches to the description of nuclear structure are undergoing an intensive development. Such approaches include the self-consistent theory of finite Fermi systems, the quasiparticle-phonon model (QPM), microscopic versions of the model of interacting bosons and fermions, etc. These models are, as a rule, used in the analysis of inelastic nuclear transitions associated with electromagnetic interactions. It is interesting to apply the semimicroscopic nuclear models to description of the inelastic scattering of neutrons by nuclei. In the standard version of the CCM such a possibility is absent. Semimicroscopic methods in the theory of nuclear reactions (the resonating group method, the method of the energy density functional, the folding model, etc.) have been widely developed; these methods are, on the one hand, free from the drawbacks associated with a macroscopic analysis of the scattering data, and, on the other hand, allow one to apply semimicroscopic nuclear models to analysis of the mechanism of nuclear reactions.

The simplest and most universal of these approaches is the folding model. This model is based on the construction of the optical potential and the form factors of the inelastic transitions using effective nucleon-nucleon forces and the nuclear transition densities calculated in a corresponding microscopic model.

Such an approach was used successfully in Ref. 12 and 13 on the basis of the folding model and the density matrix formalism, taking into account the many-particle and exchange nucleon-nucleon correlations in the case of strong channel coupling. In Refs. 14 and 15 this approach was applied to analysis of the inelastic scattering of $\alpha$ particles and protons using the QPM wave functions.

Recently great interest was attracted by the problem of inelastic scattering of low-energy electrons in the energy interval where equal contributions are given by processes of different nature: direct reactions and reactions through the compound nucleus stage. Therefore, microscopic study of inelastic neutron cross sections at these energies is a pressing issue.

In the present paper we develop a microscopic approach to the description of inelastic scattering of neutrons in spherical nuclei on the basis of the QPM of the nucleus. All the nuclear transition densities for the coupling scheme of the three lowest levels of $^{58}$Ni are calculated, including those for the elastic transitions responsible for the spin-flip effects. Calculations of the cross sections for elastic and inelastic scattering of neutrons with energies in the range 1–3 MeV are performed. The calculated results are compared with the experimental data.

2. BASIC ASSUMPTIONS

In the folding model the potential of the nucleon-nucleus interaction is defined in the following way:

$$U_{r}(r) = \int \rho(r') V(r-r') dr', \quad (1)$$

where $\rho(r')$ are the nuclear transition densities and $V(r)$ is the potential of the effective nucleon-nucleon interaction.

In order to find the folding potential (1), we first construct the nuclear transition densities in the framework of the QPM. In that model the general form of the Hamiltonian is

$$H = H_{sp} + H_{pro} + H_{n} + H_{SM}, \quad (2)$$

where $H_{sp}$ is the mean field of the neutron and proton systems, $H_{pro}$ is the interaction leading to pair correlations of the superconductivity type, and $H_{n}$ and $H_{SM}$ are separable multipole and spin-multipole forces generating the nuclear excitations.

This Hamiltonian can be transformed into the quasiparticle representation by means of the Bogolyubov transformation

$$a_{jm} = u_{jm} a_{jm} + (-1)^{j-m} v_{jm} a_{jm}, \quad (3)$$

where $a_{jm}^{+}$ and $a_{jm}^{+}$ ($a_{jm}$ and $a_{jm}$) are, respectively, the creation (annihilation) operators of the quasiparticles and particles, and $u_{jm}$ and $v_{jm}$ are the coefficients of the Bogolyubov transformation.

The phonon operator describing the elementary collective excitations of the nucleus has the form
\[ Q_{\omega i} = \frac{1}{2} \sum_{j=1}^{\infty} \left\{ \Psi_{\lambda i}^{\dagger}(\alpha_{i,n}^{\dagger} \alpha_{j,m}) \delta_{\omega i} - \left( -1 \right)^{\lambda - \mu} \phi_{\lambda i}^{\dagger}(\alpha_{i,n}^{\dagger} \alpha_{j,m}) \delta_{\omega i} \right\}, \]

where \( i \) is the number of the state with a given \( \lambda \mu \).

Next, the wave functions of a one-phonon state are constructed as
\[ Q_{\omega i} |0\rangle, \]

where the wave function \( |0\rangle \) of the ground state of an even-even nucleus describes the phonon vacuum. The energy \( \omega_{\lambda i} \) of the one-phonon state (5) and the amplitudes \( \Psi_{\lambda i} \) and \( \phi_{\lambda i} \) are calculated by solving the secular equation in the random phase approximation.\(^2\) The approximation in which the phonon excitations are assumed to be noninteracting is often inadequate and, therefore, one writes the wave function of an excited state of an even-even nucleus in a more complicated form:
\[ \Psi_{\lambda} (J M) = \sum_{\lambda i} \bar{\mathcal{R}}_{\lambda i} (J \nu) Q_{\omega i} + \sum_{\lambda \lambda' \lambda''} \mathcal{P}_{\lambda \lambda'}^{\dagger} (J \nu) \left[ Q_{\omega i} Q_{\omega i}^{\dagger} |J_M\rangle \right] |0\rangle, \]

where \( \bar{\mathcal{R}}_{\lambda i} (J \nu) \) and \( \mathcal{P}_{\lambda \lambda'}^{\dagger} (J \nu) \) are, respectively, the mixing coefficients of the one- and two-phonon excitations.

In the general case the wave function (6) is normalized:
\[ \sum_{\lambda i} \left[ \bar{\mathcal{R}}_{\lambda i} (J \nu) \right]^{\dagger} \bar{\mathcal{R}}_{\lambda i} (J \nu) + 2 \sum_{\lambda \lambda' \lambda''} \left[ \mathcal{P}_{\lambda \lambda'}^{\dagger} (J \nu) \mathcal{P}_{\lambda \lambda'} (J \nu) \right] = 1. \]

(7)

The function \( K^{\lambda} (\lambda', \lambda \mid \lambda', \lambda) \) appears because of the Pauli principle.\(^1\) In the present paper the calculations are performed in the quasiboson approximation without taking into account the Pauli principle. For collective excitations in even-even spherical nuclei it has been shown\(^1\) that the inclusion of the Pauli principle changes the result insignificantly. In this case the system of basic equations has the form
\[ (\omega_{\lambda i} - \eta_{\lambda i}) \bar{\mathcal{R}}_{\lambda i} (J \nu) + \sum_{\lambda \lambda'} U_{\lambda \lambda'}^{\dagger} (J \nu) \left[ \mathcal{P}_{\lambda \lambda'} (J \nu) \right] = 0, \]

\[ 2 (\omega_{\lambda i} + \omega_{\lambda'' i} - \eta_{\lambda i}) \mathcal{P}_{\lambda \lambda'}^{\dagger} (J \nu) + \sum_{\lambda \lambda'} U_{\lambda \lambda'}^{\dagger} (J \nu) \bar{\mathcal{R}}_{\lambda i} (J \nu) = 0, \]

where \( U_{\lambda \lambda'}^{\dagger} (J \nu) \) are the interaction matrix elements of the one- and two-phonon states.\(^3\) From the condition of existence of a nontrivial solution of the system of equations (8) we obtain the secular equation for determination of the energy \( \eta_{\lambda i} \) of a state with the wave function (6):
\[ F (\eta_{\lambda i}) = \det \left[ (\omega_{\lambda i} - \eta_{\lambda i}) \delta_{\omega i} - \frac{1}{2} \sum_{\lambda \lambda'} U_{\lambda \lambda'}^{\dagger} (J \nu) U_{\lambda \lambda'} (J \nu) \right] = 0. \]

(9)

Thus, substituting the solutions of the equation (9) into the system (8) one can find the respective values of the structure coefficients \( \bar{\mathcal{R}}_{\lambda i} (J \nu) \) and \( \mathcal{P}_{\lambda \lambda'}^{\dagger} (J \nu) \) of the one- and two-phonon parts of the wave function (6).

Next, we define the transition density of the nucleus
\[ \rho (r) = \left\langle \frac{1}{2} \sum_{\lambda} \delta (\tau - \tau_{\lambda}) \right| \bar{\mathcal{R}}_{\lambda i} (J \nu) \right\rangle. \]

(10)

To this end we expand the \( \delta \) function in spherical harmonics. Then the nuclear transition densities take the form
\[ \rho (r) = \sum_{\lambda \mu} c_{\lambda \mu} \langle \bar{\mathcal{R}}_{\lambda i} (J \nu) \mid J \nu \rangle \langle r | \delta (r - r_{\lambda i}) | \theta, \varphi \rangle, \]

(11)

where
\[ c_{\lambda \mu} = \sqrt{\frac{4}{\pi}} \text{ and } c_{\lambda \mu} = 1 \text{ (for } \lambda \neq 0) \]

are the normalization coefficients. Let us denote the single-particle operator contained in the matrix element (12) by
\[ T_{\lambda i} = \sum_{\lambda} \delta^{\lambda} (r - r_{\lambda}) \delta Y_{\lambda i} (0, \theta, \varphi), \]

(13)

which in the second quantization representation has the form
\[ T_{\lambda i} = \sum_{j} \langle j || \bar{\mathcal{R}}_{\lambda i} || j \rangle \sum_{m} \delta (j \nu - m \nu) \delta \left( \lambda | \lambda \right) a_{j m}^{\dagger} a_{j m}, \]

(14)

The reduced matrix element \( \langle j || \bar{\mathcal{R}}_{\lambda i} || j \rangle \) can be calculated by representing the single-particle wave function in the form
\[ |j \rangle = \sum_{m} \langle m | j \rangle a_{m}^{\dagger} | m \rangle, \]

(15)

where \( \bar{\mathcal{R}}_{\lambda i} (r) \) are the radial single-particle functions. Thus, one arrives at the following expression
\[ \langle j || \bar{\mathcal{R}}_{\lambda i} || j \rangle = \sum_{j} \delta (j \nu - j \nu) \delta \left( \lambda | \lambda \right) \left[ a_{j m}^{\dagger} a_{j m} \right] \left[ \delta \left( \lambda | \lambda \right) \right] \times \left[ \delta (j \nu - j \nu) \delta \left( \lambda | \lambda \right) \right] a_{j m}^{\dagger} a_{j m}, \]

(16)

Here and below we use the notation \( \bar{\mathcal{I}} = (2j + 1)^{1/2} \). Going over first to the quasiparticle representation by means of the transformation (3) and then to the phonon representation, we obtain the following expression for the operator (13):
\[ T_{\lambda i} = \sum_{j} \left\langle j || \bar{\mathcal{R}}_{\lambda i} || j \rangle \right\rangle \]

\[ \left\{ \frac{1}{2} \delta_{\nu j} \sum_{\lambda \mu} \left[ \Psi_{\lambda i}^{\dagger} (J \nu) \phi_{\lambda i}^{\dagger} (J \nu) \right] \frac{Q_{\omega i} - \left( -1 \right)^{\nu} \omega_{\lambda i}}{\delta_{\nu j}} + \frac{1}{2} \delta_{\nu j} \left[ \delta \left( j \nu - j \nu \right) \right] \left[ \delta (j \nu - j \nu) \right] \left[ \delta \left( \lambda | \lambda \right) \right] \left[ \delta \left( \lambda | \lambda \right) \right] \left[ \delta (j \nu - j \nu) \right] \right\} \]

(17)

where
\[ \delta \left( j \nu - j \nu \right) \delta \left( \lambda | \lambda \right) \left[ \delta \left( \lambda | \lambda \right) \right] \left[ \delta (j \nu - j \nu) \right], \]

(18)

Substituting (17) into (12), we arrive at the expressions for the nuclear transition density for the following transitions\(^1\): (a) the ground state
\[ p_{0} (r) = \frac{1}{4} \sum_{\lambda \mu} \left\langle J \nu \mid \bar{\mathcal{R}}_{\lambda i} (J \nu) \right| \delta_{\nu j} \right\rangle; \]

(19)
(b) ground state—one-phonon state
\[ \rho_0(r) = \sum_{\lambda} \langle J_1 \| T_x \| I \rangle \frac{1}{2} \left( \Psi_{\lambda}^{I+} + \psi_{\lambda}^{I-} \right); \]  

(20)

(c) one-phonon—one-phonon state
\[ c_{I} \rho_0 (r) = \rho_0 (r) \delta_{\lambda \lambda_1} V_{\lambda \lambda_1} \]
\[ - \sum_{J_{12} \lambda_{12}} \langle J_1 \| T_x \| J_2 \rangle \psi_{\lambda_1}^{J_1} \lambda_1 \lambda_2 \left( \frac{1}{2} \right) \left( \Psi_{\lambda_2}^{J_2} + \psi_{\lambda_2}^{J_2} \right); \]  

(21)

(d) ground state—state (7) (a mixture of the one- and two-phonon configurations)
\[ \rho_0 (r) = \sum_{J_{12} \lambda_{12}} \langle J_1 \| T_x \| J_2 \rangle \left[ \frac{1}{2} \left( \Psi_{\lambda_1}^{J_1} + \psi_{\lambda_1}^{J_1} \right) \right] \left( \Psi_{\lambda_2}^{J_2} + \psi_{\lambda_2}^{J_2} \right); \]  

(22)

(e) one-phonon state—state (7) (a mixture of the one- and two-phonon configurations)
\[ \rho_0 (r) = \sum_{J_{12} \lambda_{12}} \langle J_1 \| T_x \| J_2 \rangle \left[ \frac{1}{2} \left( \Psi_{\lambda_1}^{J_1} + \psi_{\lambda_1}^{J_1} \right) \right] \left( \Psi_{\lambda_2}^{J_2} + \psi_{\lambda_2}^{J_2} \right); \]  

(23)

(f) a state of the type (7)—state of the type (7)
\[ c_{I} \rho_0 (r) = \sum_{J_{12} \lambda_{12}} \langle J_1 \| T_x \| J_2 \rangle \left( \Psi_{\lambda_1}^{J_1} + \psi_{\lambda_1}^{J_1} \right) \left( \Psi_{\lambda_2}^{J_2} + \psi_{\lambda_2}^{J_2} \right); \]
\[ + \sum_{J_{12} \lambda_{12}} \langle J_1 \| T_x \| J_2 \rangle \left( \Psi_{\lambda_1}^{J_1} + \psi_{\lambda_1}^{J_1} \right) \left( \Psi_{\lambda_2}^{J_2} + \psi_{\lambda_2}^{J_2} \right); \]  

(24)

For a numerical calculation of the transition densities we have used the same computer code as in Ref. 15, modified so as to take into account the reorientation effect.

With the help of the microscopically calculated nuclear densities (19)–(24) and the chosen nucleon-nucleon interaction one can construct the form factors of the inelastic transitions, which are proportional to the corresponding folding potentials. Thus, the expression (1) for the folding potential reads
\[ U(r) = \sum_{\nu \mu} \langle J, M \| \omega \| J, M \rangle c_{\nu} U_{\nu} (r) \left[ r^2 Y_{\alpha} (\Omega) \right]^* \]  

(25)

where
\[ U_{\nu} (r) = \frac{1}{2\pi} \int k^2 dk \tilde{p} (k) \tilde{P} (k); \]
\[ \tilde{p} (k) = 4\pi \int r^2 dr \tilde{j}_3 (kr) \rho_0 (r); \]
\[ \tilde{P} (k) = 4\pi \int r^2 dr \tilde{j}_3 (kr) \nu (r). \]

For the effective nucleon-nucleon interaction we shall take the so-called M3Y Reid-type interaction on the basis of the fact that the elements of the G matrix of nucleon scattering by a nucleon bound in the nucleus are very close to the matrix elements of the NN interaction between bound nucleons, where the latter are calculated in the oscillator basis.

In this approximation the M3Y interaction is approximated by a sum of Yukawa terms. The direct part of the interaction is
\[ V_{\text{Yuk}} (r) = 7999 \frac{(e^{-r}/4r)}{2134 \frac{(e^{-r}/2.5r})} \]

In the calculations using this type of interaction the exchange term, which is responsible for the antisymmetrization between the incident nucleon and the nucleons of the target nucleus, is usually taken in the form of a zero-range pseudopotential:
\[ V_{\text{ex}} (r) = -276 \frac{(1 - 0.005E)}{\delta (r)} \]

where E is the energy of the incident nucleon in MeV.

3. SCATTERING OF NEUTRONS IN 58Ni

Let us consider the scattering of neutrons by the nucleus 58Ni at energies in the interval 1.5–3 MeV. At these energies it is possible to excite up to six levels of the target nucleus: 0\(^+\) (2.942 MeV), 1\(^+\) (2.902 MeV), 2\(^-\) (2.776 MeV), 4\(^+\) (2.459 MeV), 2\(^+\) (1.454 MeV), and 0\(^-\). The central part of the optical potential is chosen on the microscopic level in the form of the folding potential defined by the equation (25). In considering the nuclear transition densities, all possible transitions between the first three bound states are taken into account. By solving the system of equations (8) for the multipolarities 2\(^-\) and 4\(^+\), we find that in 58Ni the 2\(^-\) state is almost purely one-phonon, whereas the 4\(^+\) state contains approximately equal contributions of the one- and two-phonon configurations. We have taken the 2\(^-\) state to be purely one-phonon and the 4\(^+\) state to be a mixture of the one- and two-phonon states. The imaginary potential of surface absorption and the spin-orbit potential were taken in a phenomenological form. The imaginary part of the potential was assumed to be deformed with the value

<table>
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<th>$E_{\text{MeV}}$</th>
<th>$W_s, \text{MeV}$</th>
<th>$N_0^L_{\alpha=0,2}$</th>
<th>$N^L_{\gamma=2}$</th>
<th>$x^L$</th>
<th>$E_{\text{MeV}}$</th>
<th>$W_s, \text{MeV}$</th>
<th>$N_0^L_{\alpha=0}$</th>
<th>$N^L_{\gamma=2}$</th>
<th>$x^L$</th>
</tr>
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<tr>
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<td>1.093</td>
<td>1.418</td>
<td>11.72</td>
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<tr>
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<td>1.418</td>
<td>15.71</td>
<td>3.0</td>
<td>5.250</td>
<td>1.444</td>
<td>1.213</td>
<td>21.37</td>
</tr>
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</table>
of the dynamical deformation parameter $\beta_2$ determined from the experimental values of $\beta(E2)$ (Ref. 20).

As the starting values of the optical parameters we have taken the values that lead to best agreement with experiment in the phenomenological calculations.\(^\text{23}\) In the calculations of the compound cross sections we made use of the experimental spectrum of $^{68}\text{Ni}$. The compound cross sections were calculated in accordance with the Hauser-Feshbach statistical theory with the Moldauer corrections for the correlations associated with the presence of direct transitions.\(^\text{23}\)

One has to note that in the calculation of the compound cross sections for the state $0^+$, $2^+_1$, and $4^+_2$ we have used the same sticking coefficients as in the direct transitions with channel coupling, which, in turn, contain microscopic information on the nuclear structure embedded in the folding potential. Therefore, in this respect one can regard our calculations as self-consistent: The direct and compound cross sections are calculated using the same potential.

However, this approach contains also a certain inconsistency associated with the fact that the imaginary and spin-orbit parts of the potential are phenomenological. In principle, one could construct the spin-orbit folding potential using the Bertsch effective $NN$ spin-orbit interaction,\(^\text{16}\) but this would complicate the calculations considerably. Our main goal is to study the central part of the potential since it plays an important role in inelastic scattering of neutrons.

It is clear that with the addition of a realistic folding potential the values of the optical parameters cease to be optimal; therefore, we have refitted them to the experiment.

The procedure of adjustment of the parameters was performed in several steps. First, for the energy 1.5 MeV, at which the elastic scattering dominates, we varied the parameters of the spin-orbit potential $V_{so}$, $R_{so}$, and $a_{so}$; then, after reaching the optimum, we adjusted the parameters of the imaginary part of the potential $W_{so}$, $R_{w}$, and $a_{w}$. The resulting optimal set of the parameters $V_{so} = 7.5$ MeV, $R_{so} = 1.27$ fm, $a_{so} = 0.65$ fm, $R_{w} = 1.14$ fm, and $a_{w} = 0.85$ fm with $N_{2-1}^0 = 0.1$, $N_{2-1}^1 = 1.0$, and $N_{1-2}^1 = 0.0$ was used in the calculations at other energies. Then we adjusted the normalization coefficients $N_{I-1}$ of the form factors of various transitions. Here we have noted that in the fitting procedure the coefficients $N_{0-1}^0$, $N_{1-2}^1$, and $N_{1-2}^0$ change little; therefore, at the last stage we made a

![](image1.png)

**FIG. 1.** Elastic differential cross sections in $^{68}\text{Ni}$. The solid curves are the microscopic calculations, and the dashed curves are the phenomenological calculations. The experimental data are taken from Ref. 22.

![](image2.png)

**FIG. 2.** The sum of the elastic cross section and the inelastic cross section for excitation of the $2^+$ level in $^{68}\text{Ni}$. The curve is the microscopic calculation. The experimental data are taken from Ref. 22.

![](image3.png)

**FIG. 3.** Differential cross section for excitation of the $2^+$ level in $^{68}\text{Ni}$. The solid curves are the microscopic calculation, and the dashed curves are the phenomenological calculation. The experimental data are taken from Ref. 22.

![](image4.png)

**FIG. 4.** The microscopic form factors for the elastic transition (curve 1) and the following inelastic transitions: curve 2 $\rightarrow 2^+$ ($\lambda = 0$), curve 3 $\rightarrow 2^+$ ($\lambda = 2$), curve 4 $\rightarrow 2^+$ ($\lambda = 2$), and curve 5 $\rightarrow 2^+$ ($\lambda = 4$).
final adjustment of the values of $N_{0, -2}$, $N_{2, -2}$, and $W_d$ for different energies.

The obtained values of the parameters and of $\chi^2$ for the elastic channel are presented in Table I. As the table shows, in all the cases the values of the normalization coefficients are close to unity. This points to correctness of the model chosen.

The result of the calculation of the elastic differential and integrated cross sections and their comparison with the experimental data are shown in, respectively, Figs. 1 and 2. In general, good agreement with experiment is achieved at the energies 1.5, 2, and 2.5 MeV. At the energy 3 MeV the calculated values are too low at large angles. This discrepancy may be caused by the fact that at this energy the number of open channels is already large (up to six) and this was not taken into account in the fit. Fig. 3 shows the calculated results for the inelastic differential cross sections. Even though the theoretical curves describe the experiment qualitatively, they lie above the experimental points by 10–20%. Adjustment of the optical parameters and variation of the normalization coefficients of the form factors in reasonable limits do not allow one to reach a good agreement. Similar results are also obtained in phenomenological calculations.

Fig. 4 shows the behavior of the elastic and inelastic microscopic form factors for different transitions of definite multipolarity.

4. CONCLUSION

The mechanism of inelastic scattering of low-energy neutrons can be described in a satisfactory way in the framework of the presented microscopic approach, which consists in the construction of the folding potential on the basis of the effective nucleon-nucleon forces and the transition densities calculated using the QPM.

Such an approach is more consistent than the phenomenological one since it contains more extensive information on the structure of the nucleus.

20. S. Raman et al., AtOMIC DATA AND NUCLEI, Date Tables 36, 1 (1987).

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