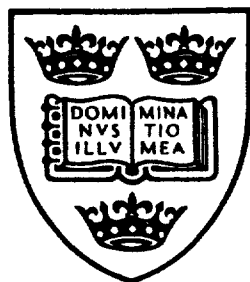


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PARTICLE AND NUCLEAR PHYSICS

**ONE-NUCLEON REMOVAL REACTIONS AS A TEST OF OVERLAP
FUNCTIONS FROM THE ONE-BODY DENSITY MATRIX
CALCULATIONS**

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ONE-NUCLEON REMOVAL REACTIONS AS A TEST OF OVERLAP FUNCTIONS FROM THE ONE-BODY DENSITY MATRIX CALCULATIONS

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Overlap functions and spectroscopic factors extracted from a model one-body density matrix (OBDM) accounting for short-range nucleon-nucleon correlations are used to calculate differential cross-sections of (p, d) reactions and the momentum distributions of transitions to single-particle states in ^{16}O and ^{40}Ca . A comparison between the experimental (p, d) and $(e, e'p)$ data, their DWBA and CDWIA analyses and the OBDM calculations is made. Our theoretical predictions for the spectroscopic factors are compared with the empirically extracted ones. It is shown that the overlap functions obtained within the Jastrow correlation method are applicable to the description of the quantities considered.

I. INTRODUCTION

One-nucleon transfer reactions have been extensively used to determine the quantum numbers and spectroscopic strengths of nuclear single-particle states. The usual method is to calculate the differential cross-section using the Distorted Wave Born Approximation (DWBA) (see e.g. [1]) with optical potentials obtained by analyzing the appropriate elastic scattering data. Normalizing the cross-sections to the data then gives the spectroscopic factor for each state. Frequently each single-particle state is split into several fragments by the residual interaction, and the total spectroscopic factor for all the states may be normalized to $(2j+1)$. The meaningfulness of the extracted spectroscopic information, however, depends on whether the shape of the calculated differential cross-section reproduces the experimental data or not which is not always easy to achieve, especially for light nuclei. Many analyses [2-8] of the (p, d) pick-up

reaction at low energies have been made using the standard DWBA method. The main disadvantage of this method is, however, that it is often possible to find several optical potentials that fit well the elastic scattering data, but give appreciably different spectroscopic factors from one-nucleon removal reactions. Thus it is desirable to extract the spectroscopic factors independently from the optical model potential used and, moreover, to calculate them within a given theoretical approach. Various theoretical methods have been applied to determine the formfactors which enter the expression of the DWBA transition amplitude. Usually they are taken as eigenfunctions of a single-particle equation with a Woods-Saxon potential.

There have been many efforts to improve the agreement between the theoretical results for the differential cross-sections of (p, d) reactions and the experimental data. On the one hand adiabatic deuteron optical model potentials were developed [9–11]. On the other hand, formfactors calculated as solutions of the exact formfactor equation [11,12] or using the surface peak method [13–15] (which takes into account the residual interaction by adding a peak at the Woods-Saxon potential at the surface region) were applied. However, the values of the spectroscopic factors extracted from the fit to the magnitude of the differential cross-section to the experimental data depend significantly on all components of the theoretical calculations.

Recently it has been shown that absolute spectroscopic factors and overlap functions for one-nucleon removal reactions can be extracted from the OBDM of the target nucleus [16]. The restoration procedure proposed was applied in [17] to OBDM obtained within the low order approximation of the Jastrow correlation method [18–21]. The overlap functions calculated are used in the present work within DWBA calculations of differential cross-sections of pick-up (p, d) reactions on ^{16}O and ^{40}Ca . This method allows some of the above difficulties to be avoided. These calculations thus give *absolute cross-sections, with no normalizing factors*. Due to the approximations inherent in the calculations of the OBDM we do not expect to reproduce the empirical data very well. Actually, the aim of this work is *to test in general the applicability of the theoretically calculated overlap functions* to the description of the one-nucleon removal reactions. We find an agreement between the calculations and the empirical cross-sections and we point out that acceptable spectroscopic factors are obtained with our method. This confirms the reliability of the overlap functions obtained from the OBDM.

Knock-out reactions initiated with electrons are also a powerful tool for studying single-particle properties of nuclei (e.g. [22–26]). In particular, the nucleon momentum distributions extracted from the electron

induced experiments for a variety of nuclei show unambiguously the existence of high-momentum components [27]. The larger values of the mean kinetic and removal energies which are obtained in comparison with their shell-model and Hartree-Fock values [28] are due to the short-range correlation (SRC) effects. They originate from the high-momentum and removal energy components in the realistic many-body spectral function. The knowledge of the spectral function makes it possible to determine the extent to which the single-particle description of the nucleus is valid, in particular for the most strongly bound nucleons, and it permits a test of the various correlation methods.

The general relationship which connects the asymptotic behaviour [29–32] of the one-body density matrix with the overlap functions of the $(A-1)$ -particle system eigenstates [16] is of significant importance because it enables one to obtain the overlap functions by means of the realistic OBDM of the ground state of the A -particle system. On this basis a theoretical method to calculate the hole spectral function in the discrete part of the spectrum has been developed [33] within the natural orbital representation (NOR) [34] of the OBDM. Properties of the overlap functions and the natural orbitals are considered in [18,19,29,35–37].

In this work we calculate some differential cross-sections of (p, d) reactions and momentum distributions of single-particle transition on ^{16}O and ^{40}Ca nuclei. It is instructive to compare the calculated differential cross-sections with the experimental data and the spectroscopic factors deduced from [17] with those obtained from the conventional calculations. In addition, the theoretical result for a single-particle momentum distribution is compared with available experimental data from $^{40}\text{Ca}(e, e'p)$ reaction.

A brief description of the theoretical method which determines the overlap functions and spectroscopic factors by means of the ground-state OBDM of the target A -particle system is given in Sec.2 of the paper. The results for the differential cross-sections of (p, d) pick-up reactions calculated within the DWBA with overlap functions as formfactors are presented in Sec.3. In Sec.4 a comparison of the theoretical estimations for a single-particle nucleon momentum distribution with available experimental data from $^{40}\text{Ca}(e, e'p)$ knock-out reaction is made. The conclusions are given in Sec.5.

II. THEORETICAL METHOD FOR CALCULATING OVERLAP FUNCTIONS

In the $(e, e'p)$ reactions the measured momentum distribution for a transition to a discrete state α in the residual nucleus $\rho_\alpha(\mathbf{p}_m)$ is expressed by the bound-state wave function which is the Fourier transform of the overlap wave function $\phi_\alpha(\mathbf{r})$ between the ground state wave function of the target $\Psi^{(A)}$ and the

wave function of the final state of the residual nucleus $\Psi^{(A-1)}$. In the coordinate space $\phi_\alpha(\mathbf{r})$ is defined as

$$\phi_\alpha(\mathbf{r}) = \langle \Psi_\alpha^{(A-1)} | a(\mathbf{r}) | \Psi^{(A)} \rangle, \quad (1)$$

where $a^\dagger(\mathbf{r})$ and $a(\mathbf{r})$ are creation and annihilation operators for a nucleon with spatial coordinate \mathbf{r} (spin and isospin coordinates are implied). In the mean-field approximation (MFA) $\Psi^{(A)}$ and $\Psi^{(A-1)}$ are Slater determinants and the overlap wave function is identified with a single-particle wave function in a mean-field potential. This is not the case when N-N correlations are explicitly included in the many-body wave function. Therefore, the growing interest in the interpretation of the recent (p, d) and $(e, e'p)$ experimental data is motivated by the possibility to clarify the limitation of the nuclear mean-field picture and to investigate the influence of the N-N correlations on the nuclear structure characteristics.

The overlap functions (1) are not orthonormalized. Their norm defines the spectroscopic factor $S_\alpha = \langle \phi_\alpha | \phi_\alpha \rangle$ of the level α and the normalized overlap function is:

$$\tilde{\phi}_\alpha(\mathbf{r}) = S_\alpha^{-1/2} \phi_\alpha(\mathbf{r}). \quad (2)$$

The method [16] is based on the knowledge of the ground-state OBDM of the target nucleus and makes it possible to calculate the overlap functions, spectroscopic factors and separation energies of the bound $(A-1)$ -particle eigenstates. In [17] the recipe [16] was applied within the model OBDM for ^{16}O and ^{40}Ca nuclei which takes into account the short-range nucleon correlations obtained within the lowest-order approximation to the Jastrow correlation method [18–21]. Although the resulting density matrix has a simple analytical form, it is physically significant since it incorporates to a large extent the SRC in the nuclei considered. In addition, its natural orbital representation is well investigated [18–20]. In [17] acceptable quantitative results are obtained for the spectroscopic factors and the overlap functions by this method which is supplemental to the more sophisticated approaches [29]. Thus the use of the overlap functions as formfactors in the DWBA calculations of one-nucleon removal processes such as (p, d) - and $(e, e'p)$ reactions is justified.

III. OVERLAP FUNCTIONS AS REALISTIC FORMFACTORS IN THE PICK-UP REACTIONS

It has been shown [18,19] that the nucleon-nucleon short-range correlations affect the one-body characteristics of both hole and particle states in the nuclei. They lead to a depletion of the Fermi sea and to a

population of the states above the Fermi level. The comparison between the shell-model wave functions, the natural orbitals and the overlap functions shows that they differ from each other especially in the surface region [17].

In order to test the role of the overlap functions as realistic formfactors we consider the $^{16}\text{O}(p, d)$ reaction at incident proton energy of 45.34 MeV [3] to the $1/2^-$ ground state in the residual ^{15}O nucleus as well as the $^{40}\text{Ca}(p, d)$ reaction at $E_p = 65 \text{ MeV}$ [8] and at $E_p = 27.5 \text{ MeV}$ [2] to the $3/2^+$ ground state of ^{39}Ca . The DWBA calculations of these pick-up reactions were performed using the DWUCK4 code [38].

The overlap function for the one-neutron removal from the $1p$ state in ^{16}O obtained in [17] is compared in Fig.1 with the formfactor calculated using the separation energy prescription (SEP). The latter suggests the replacement of the true neutron formfactor by an eigenfunction of a single-particle wave equation with a Woods-Saxon potential whose depth is adjusted so that the eigenfunction satisfies the asymptotic boundary condition. The Woods-Saxon wave functions used in this paper are calculated with the geometrical parameters: $r_0 = 1.16 \text{ fm}$ and $a = 0.69 \text{ fm}$ for ^{16}O and $r_0 = 1.27 \text{ fm}$ and $a = 0.70 \text{ fm}$ for ^{40}Ca .

Since in the Jastrow-type nuclear structure calculations [18,19] harmonic-oscillator single-particle wave functions have been used, the corresponding overlap functions have a unrealistic asymptotic behaviour: they fall off too rapidly at large distances. The consequences of this will be discussed later in this paper. In our calculations the parameters C_{nlj} and k_{nlj} are those obtained within the restoration procedure [17].

It is seen from Fig.1 that for the hole state $1p_{1/2}$ in ^{16}O the overlap function is peaked at larger distance in the surface region of the nucleus compared with the Woods-Saxon wave function. A similar behaviour of the formfactor is achieved with the surface-peaked model [14,15], where the residual interaction is phenomenologically taken into account by adding a derivative term to the Woods-Saxon potential. The same is valid for the case of ^{40}Ca .

The differential cross-sections for the (p, d) pick-up transitions are calculated within the DWBA approach using a zero-range interaction. It can be written in the form [38]:

$$\frac{d\sigma_{pd}^{lsj}(\theta)}{d\Omega} = \frac{3}{2} \frac{S_{lsj}}{2j+1} \frac{D_0^2}{10^4} \sigma_{DW}^{lsj}(\theta), \quad (3)$$

where S_{lsj} is the spectroscopic amplitude, j is the total angular momentum of the final state, $D_0^2 \approx 1.5 \times 10^4 \text{ MeV} \cdot \text{fm}^3$ and $\sigma_{DW}^{lsj}(\theta)$ is the cross-section calculated by the DWUCK4.

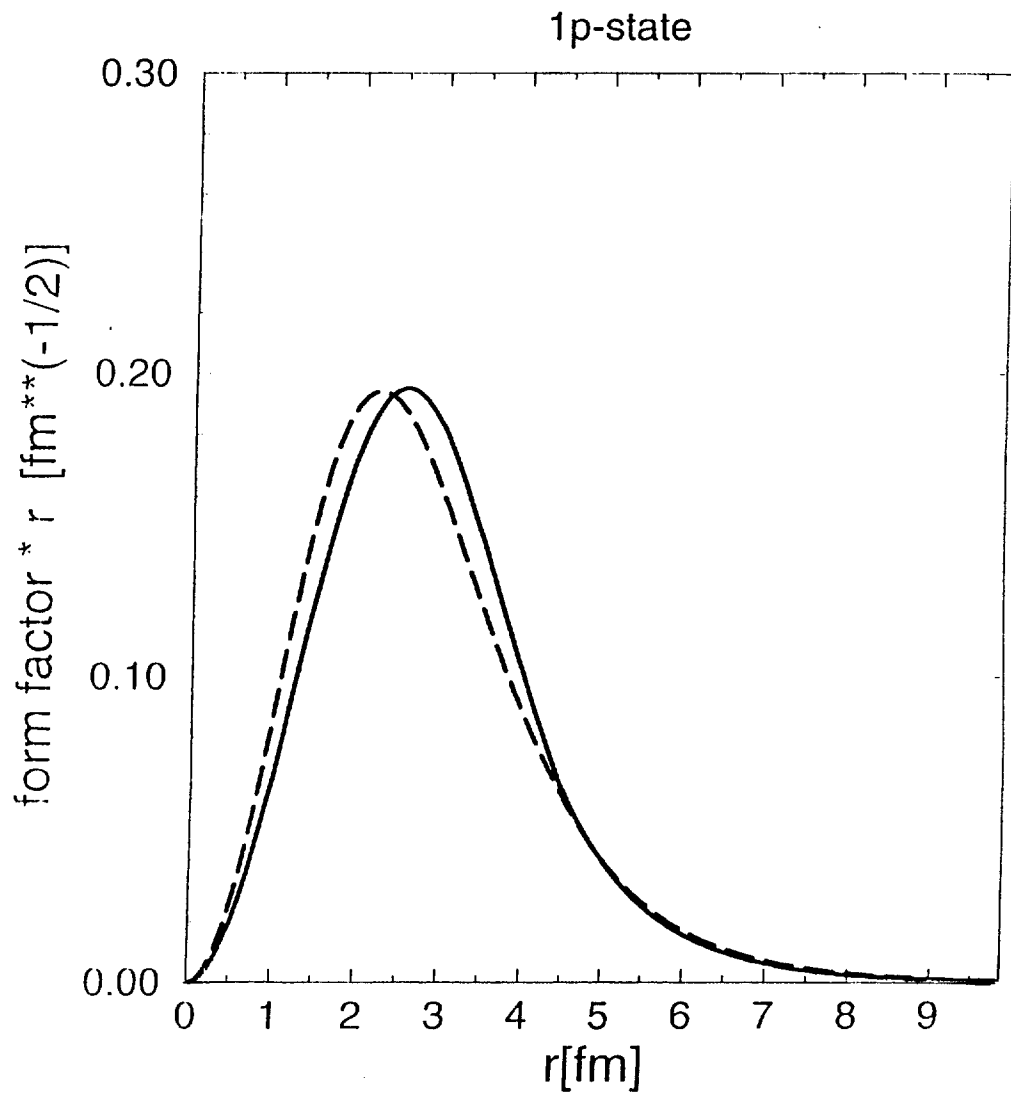


Figure 1. One-neutron removal overlap function [17] (solid line) and formfactor obtained within the SEP (dashed line) for the transition to the $1/2^-$ ground state in ^{15}O . The functions are normalized to unity.

The standard DWUCK4 procedure is performed by calculating the bound-neutron wave function using the SEP and different sets of proton and deuteron optical model parameters. The optical potential is defined to be

$$V_{opt} = -V f(x_0) - i \left(W - 4W_D \frac{d}{dx_D} \right) f(x_D) - \left(\frac{\hbar}{m\pi c} \right)^2 V_{s.o.}(\mathbf{L}\cdot\boldsymbol{\sigma}) \frac{1}{r} \frac{d}{dr} f(x_{s.o.}) + V_c, \quad (4)$$

where

$$f(x_i) = [1 + \exp(x_i)]^{-1}, \quad x_i = (r - r_i A^{1/3})/a_i, \quad (5)$$

and V_c is the Coulomb potential of a uniformly charged sphere of radius $r_c A^{1/3}$. The proton optical model parameters we use are those of Snelgrove and Kashy [39] for ^{16}O at $E_p = 45.34 \text{ MeV}$ incident energy and for ^{40}Ca those of Ridley and Turner cited in [2] at $E_p = 27.5 \text{ MeV}$ and of Menet et al. [40] at $E_p = 65 \text{ MeV}$. As suggested in [8] an adiabatic potential [9] constructed with the proton and neutron optical potential parameters of Becchetti and Greenlees [41] was used for the deuterons from ^{16}O and ^{40}Ca at 65 MeV incident energy. The applicability of the adiabatic potential has been intensively discussed but this problem is out of the scope of the present investigation. The differential cross-sections for ^{40}Ca at $E_p = 27.5 \text{ MeV}$ incident energy are calculated using the deuteron optical model parameters of Perey and Perey [42] derived from elastic scattering analyses.

For our purposes the standard DWBA formfactor was replaced by that obtained in the framework of the one-body density matrix calculations and the spectroscopic factor S_{lsj} in **(3)** was taken to be equal to unity, since our overlap functions "contain" the spectroscopic factors. Their normalization is:

$$4\pi \int |\phi_{lsj}(r)|^2 r^2 dr = S_{lsj}. \quad (6)$$

The results for the differential cross-sections calculated with overlap functions obtained from the OBDM in the Jastrow correlation method [17] and with standard formfactors are given in Figs.2 and 3. They are compared with the experimental data from [2,3,8]. As can be seen the use of our overlap functions for the transitions to the ground state leads to a qualitative agreement with the experimental data. This means that the residual interaction is taken into account to some extent. Moreover, the spectroscopic factors deduced from the restoration procedure [17] which are "contained" in the overlap functions reproduce the amplitude of the first maximum of the differential cross-section. We emphasize that in Figs.2 and 3 we give our results without any normalization while the SEP curves are already multiplied by the fitting parameter (i.e. they are normalized by the spectroscopic factor). The results of the calculations carried

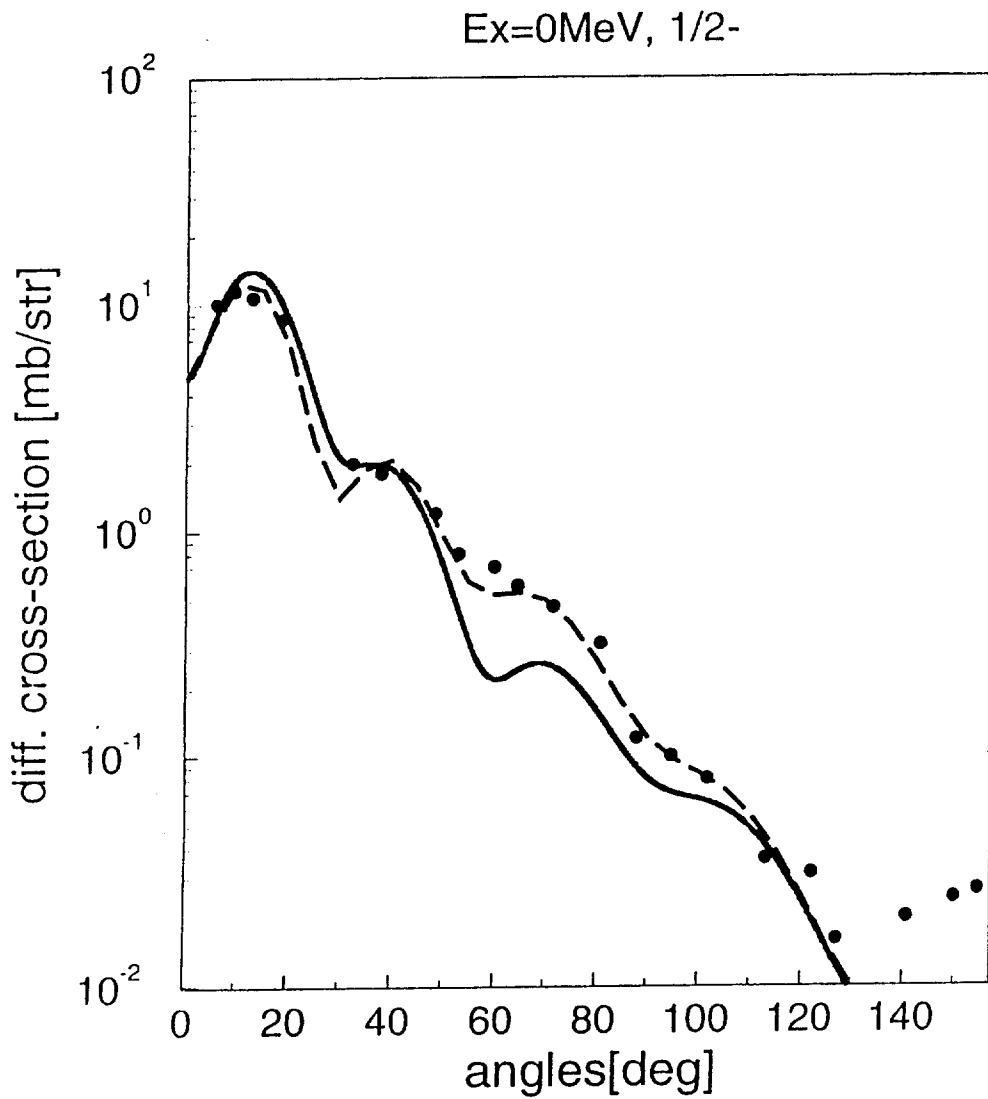


Figure 2. Differential cross-section (solid line) for the $^{16}\text{O}(p,d)$ reaction at $E_p = 45.34 \text{ MeV}$ incident energy to the $1/2^-$ ground state in ^{15}O . The DWBA result within the SEP (dashed line) is also shown. The experimental data are given by the solid circles.

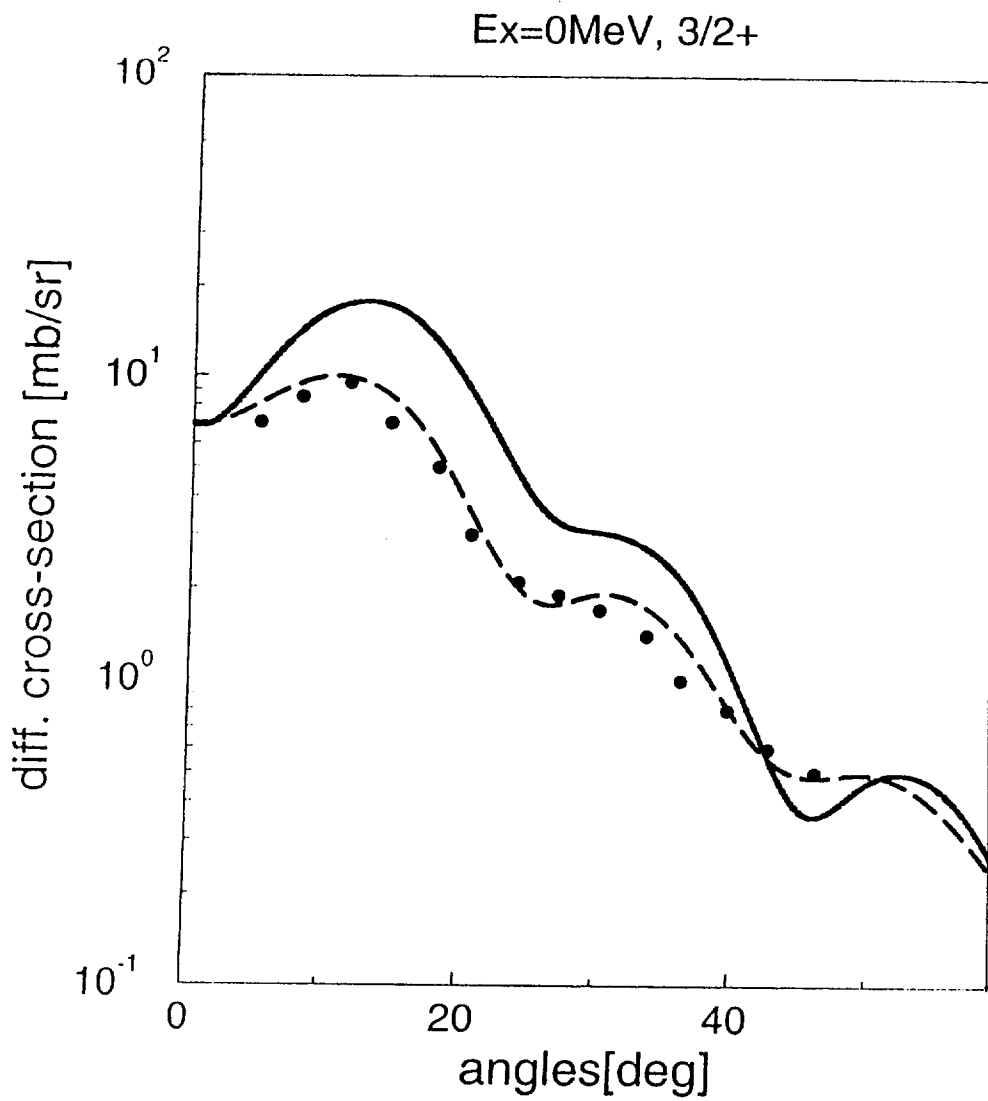


Figure 3. Differential cross-section for the $^{40}\text{Ca}(p,d)$ reaction at $E_p = 65 \text{ MeV}$ to the $3/2^+$ ground state in ^{39}Ca . The notations are the same as in Fig.2.

out additionally for the transitions to the excited states are less satisfactory. One of the reasons for this is that the population of the particle states in ^{16}O and ^{40}Ca cannot be realistically described by the simple central pair-correlations included in our OBDM. Another reason already mentioned above is the unrealistic asymptotic behaviour of the Jastrow type OBDM [18,19] which has been used to calculate the overlap functions [17] following the method described in Section II. It turned out that the overlap functions for the particle states are much more sensitive to the asymptotic behaviour of the OBDM than the overlap functions of the hole states. We should note that as it is known the tensor correlations play important role as well [43]. The coupling of single-particle states to collective modes of the target nucleus is also not taken into account, though this mechanism causes an additional reduction of the spectroscopic factors near the Fermi-energy (see e.g. [29]).

In Table 1 we give the values of the spectroscopic factors of the transitions to the ground states in ^{16}O and ^{40}Ca . A comparison is made between the spectroscopic factors extracted from the OBDM [17] and those from the experimental data applying DWBA. Let us consider the spectroscopic factors of the transitions to the ground state, especially in ^{16}O . The problem of obtaining reasonable values for the spectroscopic factors in ^{16}O is well known and intensively studied [11,39]. The DWBA calculations with optical model parameters obtained from the elastic scattering analysis fail to reproduce the shape of the differential cross-section [11]. By adopting the adiabatical deuteron optical model the shape of the cross-section is well reproduced but the value of the spectroscopic factor exceeds the maximum allowed value of 2 (see Table 1). An acceptable agreement with the experimental data can be achieved using the overlap function from [17] which has a reasonable norm (spectroscopic factor) of 1.86. Considering the transition to the ground state in ^{40}Ca it is seen that the DWUCK4 calculations with the overlap function extracted from the OBDM reproduce qualitatively the experimental cross-sections for both incident energies (see Figs.3 and 4). We would like to mention that the spectroscopic factors extracted from one-nucleon removal reactions by the standard procedure depend on the incident energy of the projectile (as can be seen in Table 1) which is a significant disadvantage of this procedure.

In the conclusion of this Section we would like to emphasize that in the standard SEP procedure the overlap function is replaced by a single-particle wave function corresponding to a given mean-field potential. In such calculations the nucleon correlations are included approximately by adjusting the mean-field potentials. The essence of our work is to show in the cases of removal reactions that *it is necessary in principle and possible in practice* to account for the short-range nucleon-nucleon forces using overlap

TABLE I. Spectroscopic factors for the ground states in ^{15}O and ^{39}Ca .

^{15}O		^{39}Ca	
	$1/2^-(g.s.)$		$3/2^+(g.s.)$
OVF [17]	1.86	OVF [17]	3.60
$SEP(E_p = 45 \text{ MeV})$	3.40	$SEP(E_p = 27.5 \text{ MeV})$	3.20
		$SEP(E_p = 65 \text{ MeV})$	3.70

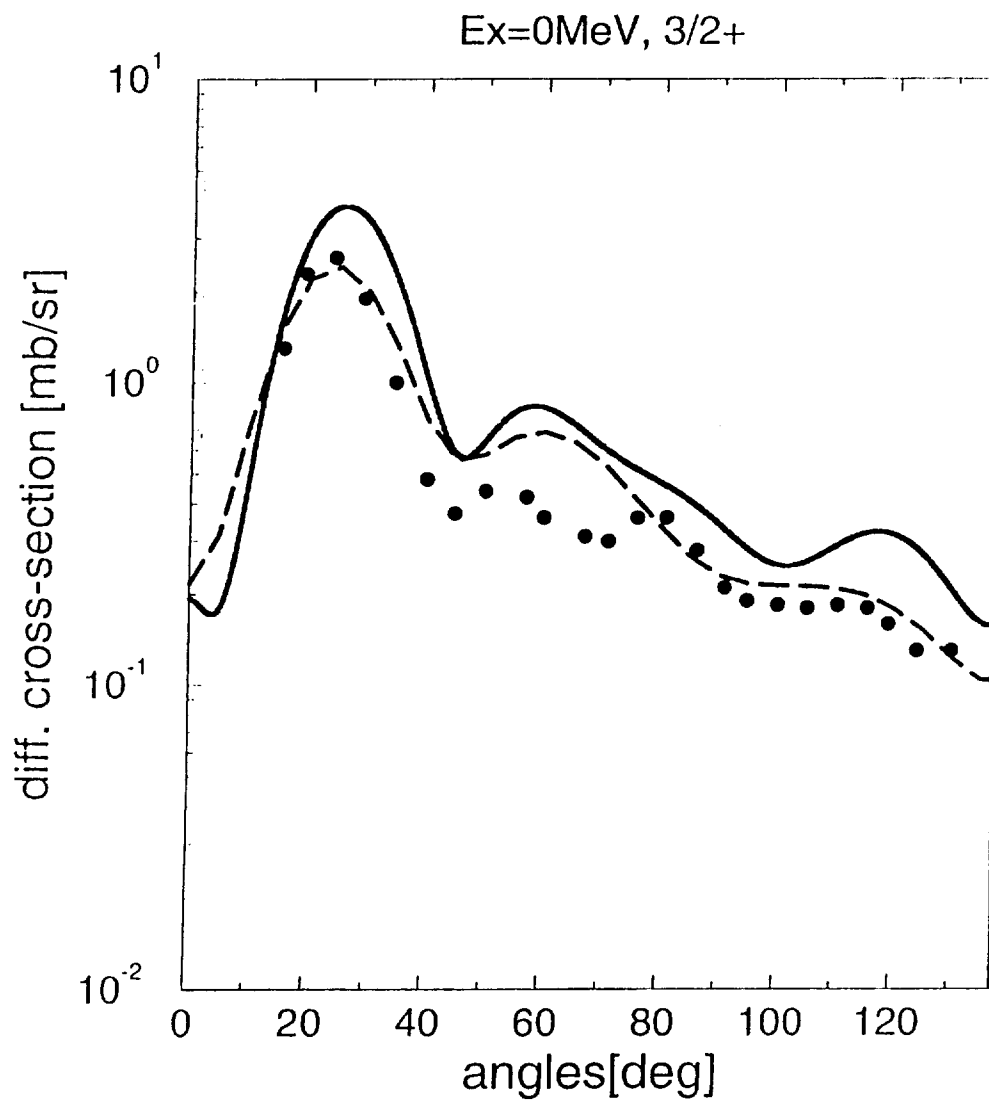


Figure 4. The same as in Fig.3 for $E_p = 27.5$ MeV.

functions (which contain the spectroscopic factors) obtained on the basis of a correlated OBDM. Thus our calculations are *absolute in contrast to the standard DWBA results* which are adjusted to give the correct magnitude of the differential cross-section. We would like to add that it is worthwhile to investigate the differential cross-sections of pick-up reactions using absolute formfactors which are extracted from more sophisticated one-body density matrices, as for example the ones obtained by variational Monte Carlo calculations [44].

IV. MOMENTUM DISTRIBUTIONS OF TRANSITIONS TO SINGLE-PARTICLE STATES FROM $(E, E'P)$ -REACTIONS

The most direct way to get information on the single-particle wave functions is to study the one-nucleon knock-out reactions. In this Section we present as an example the results of the calculations of the single-particle momentum distribution corresponding to a transition to a given single-particle state in comparison with the empirical data from the $^{40}\text{Ca}(e, e'p)$ reaction. In the Plane-Wave Impulse Approximation (PWIA) the energy ω and the momentum \mathbf{q} lost by the electron are transferred to a proton with missing energy E_m and missing momentum \mathbf{p}_m . From the energy and momentum conservation laws the latter are determined by

$$E_m = \omega - E_p - T_{A-1}, \quad \mathbf{p}_m = \mathbf{k}_p - \mathbf{q}, \quad (7)$$

where \mathbf{k}_p and E_p are the momentum and the energy of the knocked-out proton, respectively, and T_{A-1} is the kinetic energy of the residual nucleus. The $(e, e'p)$ cross-section in the PWIA can be written in the form:

$$\frac{d^6\sigma}{dk_e' dk_p} = K \sigma_{ep} S(\mathbf{p}_m, E_m), \quad (8)$$

where K is a kinematical factor and σ_{ep} is the elementary electron-proton cross-section [45]. The spectral function $S(\mathbf{p}_m, E_m)$ is the joint probability of finding a proton with separation energy E_m and momentum \mathbf{p}_m inside the nucleus. For the transition to a discrete state α one can write

$$S(\mathbf{p}_m, E_m) = \rho_\alpha(\mathbf{p}_m) \delta(E_m - E_\alpha), \quad (9)$$

where the single-particle momentum distribution

$$\rho_\alpha(\mathbf{p}_m) = |\phi_\alpha(\mathbf{p}_m)|^2 \quad (10)$$

is the Fourier transform squared of the overlap (1) between the initial and final nuclear state. In the analyses of the experimental data the integration of the empirical data over the interval that covers the peak of the transition under study gives the single-particle momentum distribution $\rho_\alpha(\mathbf{p}_m)$. The spectroscopic factor S_α for a given α -state is determined by scaling the theoretical predictions for $\rho_\alpha(\mathbf{p}_m)$ to the experimental data.

In order to obtain the momentum distribution over a large range of \mathbf{p}_m one has to vary the kinematics [23,25,26]. We consider experimental data on the $^{40}\text{Ca}(e, e'p)$ reaction measured in different kinematics up to momentum $p_m \approx 300 \text{ MeV}/c$ and compare them with the theoretical results for $\rho_\alpha(\mathbf{p}_m)$ (Eq.(23)) obtained by using the overlap functions from the restoration procedure [17]. The comparison between the experimental data and the theoretical calculations for the single-particle momentum distribution for the $2s$ hole state knockout deduced from the $^{40}\text{Ca}(e, e'p)$ reaction is given Fig.5. In the same Figure the experimental data are given together with the results from the Coulomb Distorted Wave Impulse Approximation (CDWIA) analysis [23] which is used to obtain spectroscopic factors for discrete transitions and rms radii for the various orbitals. The CDWIA calculations are performed employing different wave functions so that their rms radii are fitted to describe the data. *In our method the necessity to use such parameters is avoided* and we would like to emphasize the possibility to obtain the momentum distributions in a consistent way on the basis of the OBDM corresponding to a correlated system. At the same time it is important to note the fact that the overlap functions from [17] are for neutron bound states. In the case of proton bound states some modifications due to the Coulomb asymptotic behaviour of the overlap functions have to be taken into account. In addition, in our calculations we cannot distinguish between overlap functions for states with different values of the quantum number j and a given value of l . Nevertheless, the calculated results for the momentum distribution are close to the experimental data. As an example, we give in Fig.5 the momentum distribution for the transition leading to the excited $1/2^+$ state in the ^{39}K nucleus. Our calculations for this and other examples show that generally the shape of the momentum distributions can be adequately described by mean-field wave functions for momenta up to the Fermi momentum $k_F (\approx 250 \text{ MeV}/c)$. Generally, measurements over a more extended range of momenta and with better accuracy are necessary to test the various bound-state wave functions. Due to the short-range correlation effects accounted for in the OBDM used in our calculations one can expect that the deduced overlap functions will describe correctly the shape of the single-particle momentum distributions of the transitions to single-particle nuclear states. This will be especially true when more

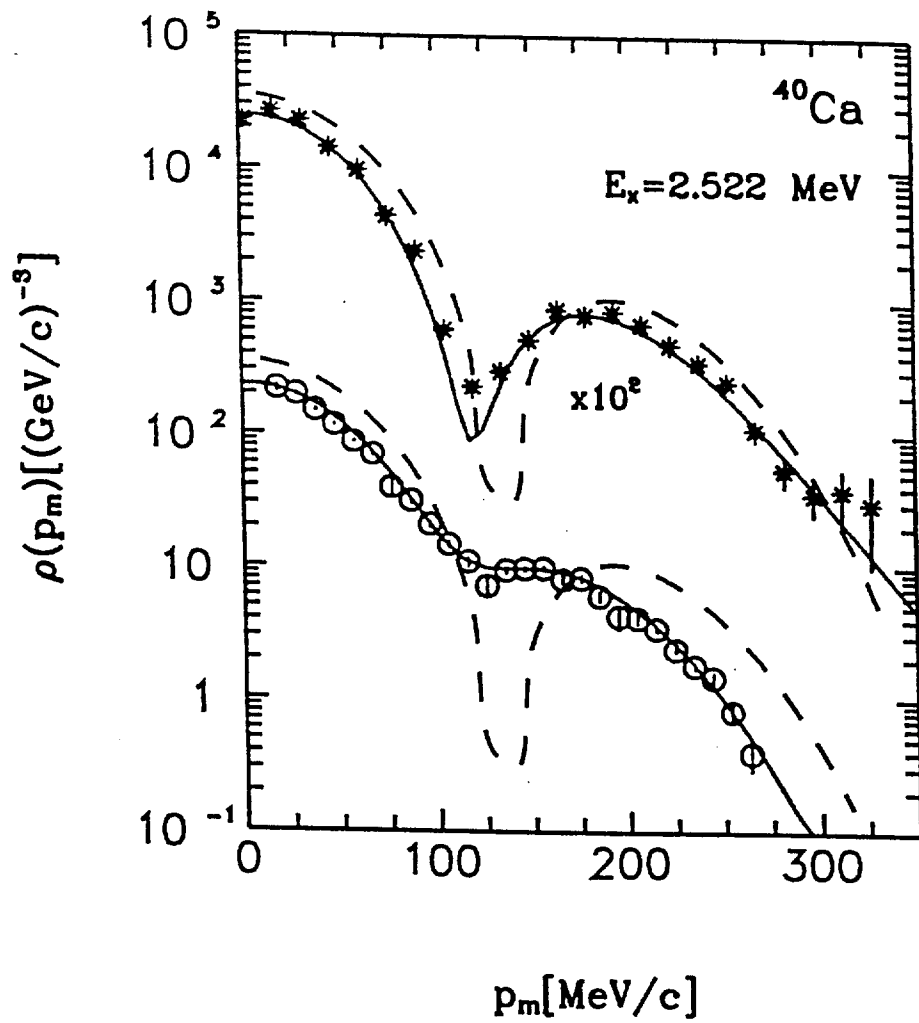


Figure 5. Momentum distribution for the transition to the $1/2^+$ excited state in ^{39}K from $^{40}\text{Ca}(e, e'p)$ reaction. The calculations by using $2s$ -overlap functions from [17] are presented by the dashed line. The stars and circles represent the empirical data measured in different kinematics [23]. The CDWIA calculations [23] are shown by solid lines.

realistic OBDM are used in order to obtain correct proton overlap functions and spectroscopic factors.

V. CONCLUSIONS

In the present work we show that it is possible to include the short-range nucleon correlations using a realistic OBDM and hence to obtain and apply both the overlap functions and the spectroscopic factors in a consistent way. This is in contrast to the methods such as SEP, CDWIA and others which use mean-field single-particle wave functions instead of overlap functions and take the nucleon correlations into account by modifying the mean-field potentials. The new theoretical method is applied to study one-nucleon removal processes. It is shown that the overlap functions of the $(A-1)$ -particle system eigenstates obtained in [17] by using the general relationship [16] which connects them with the OBDM can be applied as realistic formfactors to calculate the differential cross-sections of $^{16}\text{O}(p, d)$ and $^{40}\text{Ca}(p, d)$ pick-up reactions at various incident energies. We emphasize that the angular distributions obtained *have not been normalized by spectroscopic factors* because the latter are already included in the overlap functions. The angular distributions obtained are in qualitative agreement with the experimental cross-sections of the transitions to the ground states of the residual nuclei.

Our calculations of the single-particle momentum distribution describe qualitatively the empirical data obtained by the $^{40}\text{Ca}(e, e'p)$ knock-out reaction at momenta below the Fermi momentum. The results are close to the CDWIA calculations using bound-state wave functions corresponding to a mean-field potential. New measurements should be made at higher momenta where the SRC effects on the momentum distribution can be sizable. Using the correct asymptotic behaviour of the proton overlap function in a procedure similar to that from [17] as well as more realistic OBDM, one can expect that the resulting overlap functions will be able to describe more accurately the experimental single-particle momentum distributions and the cross-sections of the reactions considered.

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