

# Failure of the multiple peaking approximation for fast capture processes at milliradian scattering angles

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The first Born approximation is examined for different fast capture processes for the  $p + \text{He}$  system at incident energies of about 1 MeV. Calculations have been performed for the singly differential cross section (SDCS) for scattering angles 0–0.5 mrad in the laboratory frame. In the case of transfer ionization, we observe that the two-step-2 mechanism has a dominant contribution to the SDCS for the kinematics considered in this work. The present investigation demonstrates that the multiple peaking approximation is a very crude method which fails to describe the SDCS even at scattering angles below 0.5 mrad. We have also presented a doubly differential cross section for the fixed emission energy of 600 eV and compared our results with other theoretical calculations and experiments.

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## I. INTRODUCTION

The study of capture processes such as charge transfer, transfer excitation, and transfer ionization is of great interest in astrophysics, radiation physics, and plasmas. The history of these investigations is rather long and dates back more than 80 years. We can recommend to readers two rather full theoretical review articles devoted to this topic [1,2]. Nowadays, most of the theories are based on various time-dependent and time-independent distorted wave approaches (see, for example, a few recent articles [3–5]), and the focus of studies moves toward molecular targets.

In this respect, simple and physically clear first Born mechanisms, together with the kinematical domain of their validity, are rather relevant. In Ref. [6], the single-differential cross section (SDCS) for the charge-transfer  $p + \text{He} \rightarrow \text{H} + \text{He}^+$  (CT) and transfer-ionization  $p + \text{He} \rightarrow \text{H} + e + \text{He}^{2+}$  (TI) reactions was calculated for different trial helium wave functions (not only of the Slater type). The Oppenheimer-Brinkman-Kramers (OBK) [7] amplitude was used in the calculations. In the case of TI, a strong dependence of the SDCS on different helium ground-state wave functions was noticed in the scattering angular range 0–0.5 mrad, contrary to the case of CT reactions with the helium residual ion left in its ground state. It was found that the principal matrix element of the OBK amplitude is analogous to that for quasielastic ( $e, 3e$ ) reactions [8], which provide very important information on electron correlations in the target. This observation inspired us to think that a study of TI reactions at very small scattering angles would probably give valuable

information about the quantum structure of a target along with the electron momentum spectroscopy. Unfortunately, the agreement between the theory and the experiment was not satisfactory at that time.

Indeed, three terms can be attributed to the first Born approximation (FBA), and the OBK is only one of them. In a later article [9], the numerical FBA calculations for the TI reactions were accomplished for strongly and loosely correlated Slater-type helium wave functions and demonstrated some dependence on their choice. However, the authors did not consider the relative contribution of different terms to the FBA amplitude. Recently, it was shown [10,11] that the full FBA calculations for CT processes considerably improve the agreement with the experiment in the angular domain 0–0.5 mrad (i.e., the domain of the main SDCS peak).

For TI, we briefly recall the physical mechanisms in the three terms of the FBA which we call A1, A2, and A3 here (see diagrams in Fig. 1). The A1 (OBK) amplitude describes the hit of an electron by the proton, and then the capture of this electron by the projectile. Another electron is released due to a sudden rearrangement in the system. It is a typical shake-off (SO) mechanism, well-known in scattering theory [12].

The amplitude A3 describes the first interaction of the proton with the helium nucleus, followed by the capture of a target electron by the proton. Another target electron is released again due to a sudden rearrangement in the system. Both A1 and A3 processes are frequently considered in various applications.

The amplitude A2 describes a two-step process induced by the fast proton. In a first step, the proton hits a target electron and kicks it out, whereas in a second step, it picks up another active target electron. In the scattering theory, it is a so-called two-step-2 (TS2) mechanism usually attributed to the second Born approximation (SBA) [13], but in the

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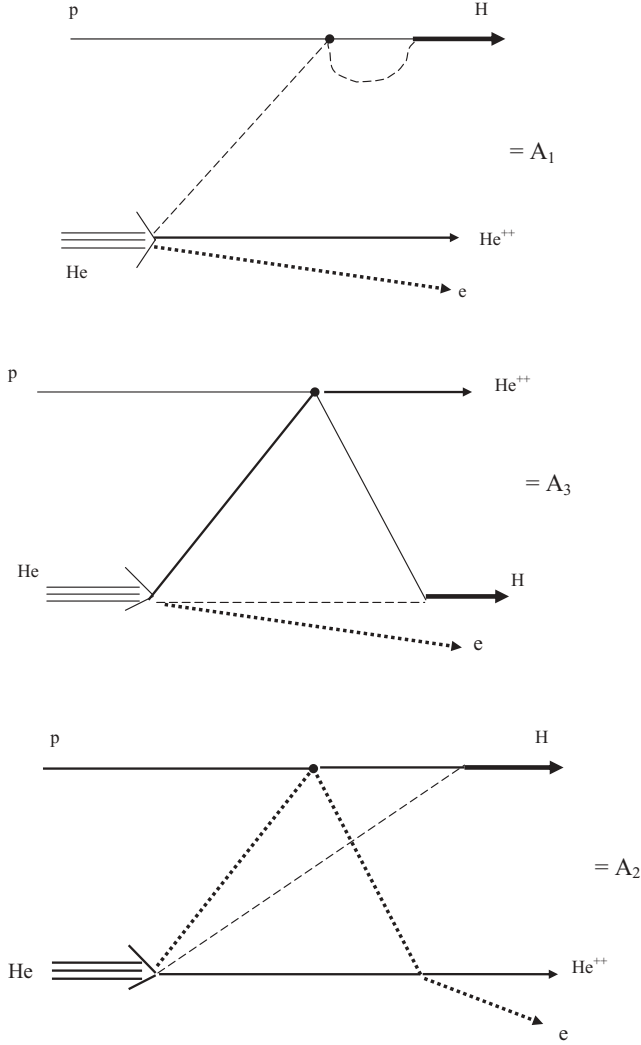


FIG. 1. FBA amplitudes, diagram representation.

capture processes it manifests itself like one of the first Born terms. The distinguishing feature of this mechanism is that it always contributes to the total amplitude, even in the absence of correlation between the electrons of the target atom. We shall see its role later in this article.

In this article, we compare the relative contributions of the amplitudes A1, A2, and A3 for both the TI and the CT reactions. Previously, in the CT processes [10] it was found that the terms A1 and A3 provide the main contributions to the SDCS, while the A2 term is a correction. However, this is not the case for TI.

The evaluation of the preceding amplitudes needs vigorous numerical calculations. It is worth mentioning that the first Born amplitudes for CT are expressed by three-dimensional (3D) integrals [6], and the SDCS for the TI reactions involves the evaluation of a 6D integration. In the case of molecules, we have to integrate the SDCS further over the three Euler angles, that is, three more integrations. If we want to take account of second Born terms (for example, [14,15]), we face an additional 3D integration. Such a situation demands reliable approximate computation of matrix elements.

The best known in this respect is the multiple peaking approximation (MPA) [16,17], which is employed for the reduction of the preceding multidimensional integrals to analytic expressions for fast projectiles. In a certain sense, this article is a continuation of the previous one [18], which examined the CT reaction  $p + H \rightarrow H + H^+$ . It was observed that the MPA was rather poor in comparison with numerical calculations of the SDCS even at very small scattering angles. Here we extend the examination to the case of the helium atom.

Atomic units are used throughout unless otherwise indicated.

## II. BASIC FORMULAS

As stated previously, we consider the He atom as a target for the TI reaction. Let us denote the projectile momentum by  $\vec{p}_p$ , the hydrogen momentum by  $\vec{p}_H$ , and the recoil-ion momentum by  $\vec{K}$ . We also define the transferred momentum by  $\vec{q} = \vec{p}_H - \vec{p}_p$ . We can deduce its approximate value using the momentum and energy conservation

$$\vec{q} + \vec{k} + \vec{k} = 0, \quad (1a)$$

$$\frac{p_p^2}{2m} + E_0^{\text{He}} = \frac{p_H^2}{2(m+1)} + \frac{K^2}{2M} + E^H + E^{\text{ion}}. \quad (1b)$$

Here  $\vec{k}$  is the electron momentum, the proton mass  $m = 1836.15$ , the ion mass  $M \approx 4m$ ,  $E_0^{\text{He}} \approx -2.903$ , and  $E^{\text{ion}} = k^2/2$ .

Now we choose very small scattering angles for the outgoing hydrogen ( $0 \leq \theta_p \lesssim 0.5$  mrad). It leads to a practically zero ion velocity  $K/M$  in the laboratory frame during the process, and we set its position as  $r_N = 0$ . The proton velocity  $\vec{v}_p = \vec{p}/m$  varies about 10 a.u. for its energy of several MeV. This fact allows one to neglect the values  $K^2/2M$  and  $q^2/2m$  after insertion of  $\vec{p}_H = \vec{q} + \vec{p}_p$  into Eq. (1b). As a result we obtain

$$\vec{v}_p \cdot \vec{q} = \frac{1}{2}v_p^2 + Q; \quad Q = E_0^{\text{He}} - E^H - E^{\text{ion}},$$

and choosing the vector  $\vec{v}_p$  as a  $z$  axis, there follows  $q_z = v_p/2 + Q/v_p$ . The perpendicular component of the vector  $\vec{q}$  is  $q_{\perp} \approx mv_p\theta_p$ .

The first Born amplitude for the TI (Fig. 1) follows from the matrix element

$$\mathcal{T}_{\text{FBA}} = \langle \Psi_f^-(\vec{p}_H, \vec{k}) | V_{p1} + V_{p2} + V_{pN} | \Psi_i^+(\vec{p}_p) \rangle,$$

where

$$\langle \vec{r}_p, \vec{r}_1, \vec{r}_2 | \Psi_i^+(\vec{p}_p) \rangle = e^{i\vec{p}_p \cdot \vec{r}_p} \Phi_0(\vec{r}_1, \vec{r}_2),$$

[ $\Phi_0(\vec{r}_1, \vec{r}_2)$  the helium wave function]

and

$$\langle \Psi_f^-(\vec{p}_H, \vec{k}) | \vec{r}_p, \vec{r}_1, \vec{r}_2 \rangle \approx \frac{1}{\sqrt{2}} [e^{-i\vec{p}_H \cdot \vec{r}_p} \phi_H(\vec{r}_p - \vec{r}_1) \varphi_c^{-*}(\vec{k}, \vec{r}_2) + (1 \leftrightarrow 2)],$$

with the well known Coulomb wave function

$$\varphi_c^{-*}(\vec{k}, \vec{r}) = e^{-\pi\xi/2} \Gamma(1 + i\xi) e^{-i\vec{k} \cdot \vec{r}} F_1(-i\xi, 1; ikr + i\vec{k} \cdot \vec{r});$$

$$\xi = -2/k.$$

Calculating the matrix element, we obtain

$$\begin{aligned} \mathcal{T}_{\text{FBA}} &= -4\pi\sqrt{2} \int \frac{d\vec{x}}{(2\pi)^3} \frac{\tilde{\phi}_{\text{H}}(x)}{|\vec{v}_p - \vec{q} - \vec{x}|^2} [F(\vec{q}; 0; \vec{k}) \\ &\quad + F(\vec{v}_p - \vec{x}; -\vec{v}_p + \vec{q} + \vec{x}; \vec{k}) - 2F(\vec{v}_p - \vec{x}; 0; \vec{k})] \\ &= \text{A1} + \text{A2} + \text{A3}, \end{aligned} \quad (2)$$

where

$$F(\vec{y}; \vec{\eta}; \vec{k}) = \int e^{-i\vec{y}\cdot\vec{r}_1 - i\vec{\eta}\cdot\vec{r}_2} \varphi_c^{-*}(\vec{k}, \vec{r}_2) \Phi_0(\vec{r}_1, \vec{r}_2) d\vec{r}_1 d\vec{r}_2 \quad (3)$$

and the hydrogen ground state in the momentum representation is

$$\tilde{\phi}_{\text{H}}(x) = \int e^{-i\vec{x}\cdot\vec{r}} \phi_{\text{H}}(\vec{r}) d\vec{r} = \frac{8\sqrt{\pi}}{(x^2 + 1)^2}.$$

The SDCS is expressed as the 3D integral,

$$\frac{d\sigma}{d\theta_p} = \frac{m^2\theta_p}{(2\pi)^4} \int |\mathcal{T}|^2 k dE_k d\Omega_k. \quad (4)$$

Only the term A1 in (2) can be expressed analytically,

$$\text{A1} = -\frac{4\sqrt{2\pi}}{1 + (\vec{v}_p - \vec{q})^2} F(\vec{q}, 0; \vec{k}),$$

and it is well known as the plane-wave OBK amplitude. The other two terms require numerical integration. It is supposed, of course, that the function  $F$  in (3) can be calculated analytically when the helium wave function is of the Slater type.

### A. Charge transfer reactions: A3

We begin by considering the CT reactions for the sake of comparison. The SDCS is then given by

$$\frac{d\sigma}{d\theta_p} = \frac{m^2\theta_p}{(2\pi)} |\mathcal{T}|^2.$$

To obtain the integral expression of the A3 term in this case, the final Coulomb wave function  $\varphi_c^{-*}(\vec{k}, \vec{r})$  in (3) should be replaced by the ground-state wave function  $\Phi_{\text{He}^+}(\vec{r})$  of the  $\text{He}^+$  ion, and  $E^{\text{ion}} = -2$  in (1b):

$$\text{A3} = 8\pi\sqrt{2} \int \frac{d\vec{x}}{(2\pi)^3} \frac{\tilde{\phi}_{\text{H}}(x)}{|\vec{v}_p - \vec{q} - \vec{x}|^2} F_0(\vec{v}_p - \vec{x}; 0), \quad (5)$$

where

$$F_0(\vec{y}; \vec{\eta}) = \int e^{-i\vec{y}\cdot\vec{r}_1 - i\vec{\eta}\cdot\vec{r}_2} \Phi_{\text{He}^+}(\vec{r}_2) \Phi_0(\vec{r}_1, \vec{r}_2) d\vec{r}_1 d\vec{r}_2. \quad (6)$$

Inserting (6) into (2), one obtains

$$\text{A3} = 2\sqrt{2} \int d\vec{r}_2 \Phi_{\text{He}^+}(\vec{r}_2) J(\vec{r}_2; \vec{q}, \vec{v}_p - \vec{q}),$$

with

$$\begin{aligned} J(\vec{r}_2; \vec{q}, \vec{v}_p - \vec{q}) \\ = \int \frac{d\vec{r}_0 d\vec{r}_1}{|\vec{r}_0 - \vec{r}_1|} e^{-i\vec{q}\cdot\vec{r}_1} e^{-i(\vec{v}_p - \vec{q})\cdot\vec{r}_0} \phi_{\text{H}}(\vec{r}_0) \Phi_0(\vec{r}_1, \vec{r}_2). \end{aligned} \quad (7)$$

A typical configuration interaction (CI) helium wave function takes the form

$$\Phi_0(\vec{r}_1, \vec{r}_2) = \sum_{l=0} \Psi_l(\vec{r}_1, \vec{r}_2), \quad (8)$$

where, for example,

$$\begin{aligned} \Psi_l(\vec{r}_1, \vec{r}_2) &= 4\pi \sum_{n \geq l+1} C_{nl} \psi_{nl}(r_1) \psi_{nl}(r_2) \\ &\quad \times \sum_{m=-l}^l \langle l, m; l, -m | 0, 0 \rangle Y_{l,m}(\vec{r}_1) Y_{l,-m}(\vec{r}_2); \\ \psi_{nl}(r) &= r^l \sum_i d_i^{nl} \sqrt{\frac{(\epsilon_i^{nl})^3}{\pi}} e^{-\epsilon_i^{nl} r}. \end{aligned} \quad (9)$$

In particular, the simplest  $1s^2$  Hylleraas (Hy) wave function is written as

$$\Phi_0(\vec{r}_1, \vec{r}_2) = \frac{Z^3}{\pi} e^{-Z(r_1+r_2)}.$$

Let us consider first this the simplest case. It follows from (6) and (9)

$$\begin{aligned} J(\vec{r}_2; \vec{q}, \vec{v}_p - \vec{q}) &= \sqrt{\frac{Z^3}{\pi}} e^{-Zr_2} \left[ \sqrt{\frac{Z^3}{\pi}} \sqrt{\frac{1}{\pi}} \int \frac{d\vec{r}_0 d\vec{r}_1}{|\vec{r}_0 - \vec{r}_1|} \right. \\ &\quad \left. \times e^{-i(\vec{v}_p - \vec{q})\cdot\vec{r}_0} e^{-r_0} e^{-i\vec{q}\cdot\vec{r}_1} e^{-Zr_1} \right]. \end{aligned} \quad (10)$$

The integral in the square brackets in (10),

$$\begin{aligned} [\dots] &= R(Z) \\ &= \frac{32\sqrt{Z^5}}{\pi} \int \frac{d\vec{x}}{x^2} \frac{1}{[(\vec{v}_p - \vec{q} - \vec{x})^2 + 1]^2 [(\vec{q} + \vec{x})^2 + Z^2]^2}, \end{aligned} \quad (11)$$

is connected to the well-known Lewis integral [19]

$$\begin{aligned} I(\lambda) &= \frac{1}{\pi^2} \int \frac{d^3x}{[x^2 + \lambda^2][\mu_1^2 + (\vec{x} - \vec{q}_1)^2][\mu_2^2 + (\vec{x} - \vec{q}_2)^2]} \\ &= \frac{\pi - 2 \arcsin(\beta/\gamma)}{\sqrt{\gamma^2 - \beta^2}}. \end{aligned} \quad (12)$$

In (12)

$$\begin{aligned} \beta &= \lambda[(\vec{q}_1 - \vec{q}_2)^2 + (\mu_1 + \mu_2)^2] + \mu_2(q_1^2 + \mu_1^2 + \lambda^2) \\ &\quad + \mu_1(q_2^2 + \mu_2^2 + \lambda^2), \\ \gamma^2 &= [(\vec{q}_1 - \vec{q}_2)^2 + (\mu_1 + \mu_2)^2][q_1^2 + (\mu_1 + \lambda)^2] \\ &\quad \times [q_2^2 + (\mu_2 + \lambda)^2], \end{aligned}$$

In particular,

$$R(Z) = 8\pi\sqrt{Z^3} \frac{\partial^2}{\partial\mu_1 \partial\mu_2} I(0), \quad (13)$$

with

$$\mu_1 = 1, \quad \mu_2 = Z, \quad \vec{q}_1 = \vec{v}_p - \vec{q}, \quad \vec{q}_2 = -\vec{q}.$$

In this case,

$$\text{A3}(Z) = 2\sqrt{2} R(Z) F_{1s}(Z), \quad (14)$$

with

$$F_{1s}(Z) = \sqrt{\frac{Z^3}{\pi}} \int d\vec{r}_2 \Phi_{\text{He}^+}(\vec{r}_2) e^{-Zr_2} = \frac{16\sqrt{2Z^3}}{(Z+2)^3}.$$

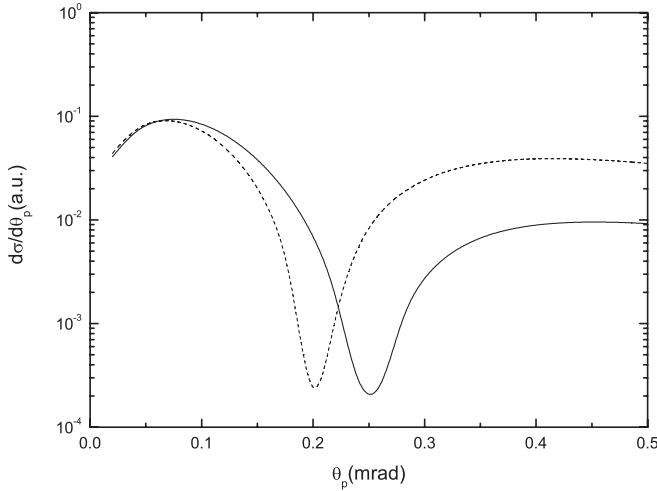


FIG. 2. SDCS (A1 + A3 amplitudes only) vs the hydrogen scattering angle  $\theta_p$  for the CT reaction  $\text{He} + p \rightarrow \text{He}^+ + \text{H}$  at proton energy  $E_p = 1.4$  MeV. The  $1s^2$  Hy wave function is used. Solid line, numerical calculations [fully coincident with Eq. (14)]; dashed line, the MPA Eq. (15).

Analytical calculations of A3 (14) can be done with MAPLE software, for instance.

MPA can be applied in (7) or (11). In this approximation, it is supposed that the main contribution to the integral (11) follows from the two domains:  $\vec{x} \sim -\vec{q}$  and  $\vec{x} \sim \vec{v}_p - \vec{q}$ . However, we evaluate the MPA from  $R(Z)$ , leaving the terms that are asymptotically proportional to  $v_p^{-6}$  [the leading asymptotic behavior in (13)]. We obtain

$$A3(Z)_{\text{MPA}} \approx 2\sqrt{2}R(Z)_{\text{MPA}}F_{1s}, \quad (15)$$

with

$$R(Z)_{\text{MPA}} = \frac{64\pi\sqrt{Z^3}}{[(Z+1)^2 + v_p^2]^2} \left[ \frac{Z}{(\vec{v}_p - \vec{q})^2 + 1} + \frac{1}{q^2 + Z^2} \right].$$

Of course, we obtain the same with the usual methods [16,17].

The comparison of SDCS calculating with (A1 + A3) and (A1 + A3<sub>MPA</sub>) is presented in Fig. 2. The proton energy is  $E_p = 1.4$  MeV. The coincidence of both expressions is rather poor except for a very small region of scattering angles  $\theta_p \sim 0-0.1$  mrad. The situation becomes even worse if we evaluate the asymptotical term proportional to  $v_p^{-7}$  from (13) in addition to the MPA. Calculations at  $E_p = 10$  MeV demonstrate practically the same effect, the convergence being very slow. This fact was already observed earlier [18].

$$A2 = -2^{10}\pi Z^4(Z+2) \left\{ \frac{1}{\pi^2} \int \frac{d\vec{y}}{y^2} \frac{1}{[(\vec{v}_p - \vec{q} - \vec{y})^2 + 1][(\vec{q} + \vec{y})^2 + Z^2][y^2 + (Z+2)^2]} \right\}. \quad (19)$$

The integral in the figure brackets can be reduced into two Lewis type integrals,

$$\{\dots\} = -\frac{1}{8\mu_1\mu_2\lambda} \frac{\partial^3}{\partial\mu_1\partial\mu_2\partial\lambda} \frac{1}{\lambda^2} [I(0) - I(\lambda)], \quad (20)$$

Of course, the numerical and analytical calculations of A3 fully coincide.

It is necessary to point out that the Gauss-Legendre and Gauss-Laguerre quadrature methods are very convenient for numerical calculations. A higher degree of accuracy can be reached by increasing the number of integration points.

The exact expression (11) and Eq. (7) allow one to formulate a proper approximation for A3 item in the case of CI trial wave function at high proton energies. The structure of the integral (7) also prompts one to assume that only  $1s^2$  item  $\Psi_0(\vec{r}_1, \vec{r}_2)$  in the sum (8) gives a leading contribution to A3 at big  $v_p$ ,  $q$ ,  $|\vec{v}_p - \vec{q}|$ . Defining

$$R_n(\text{CI}) = \sum_i d_i^{n0} R(\varepsilon_i^{n0}),$$

$$F_n(\text{CI}) = \sum_i d_i^{n0} F_{1s}(\varepsilon_i^{n0}),$$

we obtain

$$A3(\text{CI}) \approx 2\sqrt{2} \sum_{n \geq 1} C_{n0} R_n(\text{CI}) F_n(\text{CI}). \quad (16)$$

Analytical [Eq. (16)] and numerical calculations for the helium wave functions of Hylleraas (Hy), Roothaan-Hartree-Fock (RHF) [20], and Mitroy [21] are presented in Fig. 3. Coincidence is excellent, and it is a result of the dominance of the  $1s^2$  term in the He wave function. Of course, the application of the MPA to these calculations shows again a very poor result.

## B. Charge transfer reactions: A2

In accordance with definitions

$$A2 = -4\pi\sqrt{2} \int \frac{d\vec{x}}{(2\pi)^3} \frac{\tilde{\phi}_H(x)}{|\vec{v}_p - \vec{q} - \vec{x}|^2} \times F_0(\vec{v}_p - \vec{x}; -\vec{v}_p + \vec{q} + \vec{x})$$

$$= -\sqrt{2} \int \frac{d\vec{r}_0 d\vec{r}_1 d\vec{r}_2}{|\vec{r}_0 - \vec{r}_1 + \vec{r}_2|} e^{-i\vec{q}\cdot\vec{r}_1} \times e^{-i(\vec{v}_p - \vec{q})\cdot\vec{r}_0} \Phi_{\text{He}^+}(\vec{r}_2) \phi_H(\vec{r}_0) \Phi_0(\vec{r}_1, \vec{r}_2). \quad (17)$$

At the beginning, we consider again the Hy wave function and obtain from (3)

$$F_0(\vec{v}_p - \vec{x}; -\vec{v}_p + \vec{q} + \vec{x}) = \frac{128\sqrt{2}\pi Z^4(Z+2)}{[(\vec{v}_p - \vec{x})^2 + Z^2]^2 [(\vec{v}_p - \vec{q} - \vec{x})^2 + (Z+2)^2]^2}. \quad (18)$$

Insertion of (18) into (17) and exchange of variables gives

with  $\lambda = (Z+2)$ ,  $\mu_1 = 1$ ,  $\mu_2 = Z$ ,  $\vec{q}_1 = \vec{v}_p - \vec{q}$ ,  $\vec{q}_2 = -\vec{q}$ .

Finally,

$$A2 = 2^7\pi Z^3 \frac{\partial^3}{\partial\mu_1\partial\mu_2\partial\lambda} \left[ \frac{I(0) - I(\lambda)}{\lambda^2} \right]. \quad (21)$$

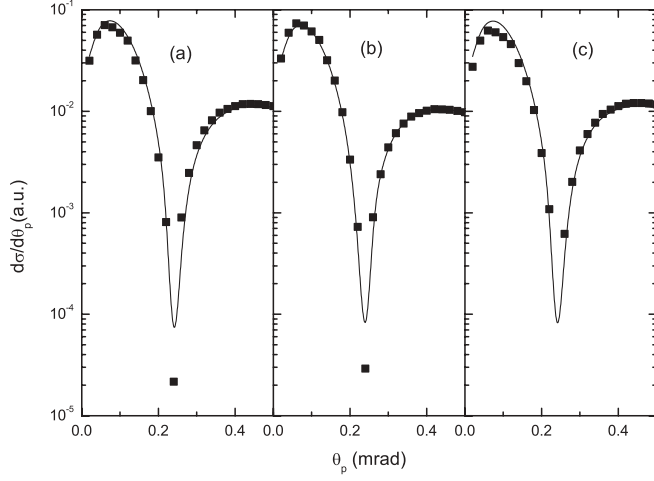


FIG. 3. The same as in Fig. 2. Solid line, numerical calculations; squares, Lewis approach with MAPLE Eq. (16). (a) Hy, (b) RHF, and (c) Mitroy wave functions.

It is a very bulky expression of analytical items calculated with MAPLE software, which can be converted to FORTRAN if necessary.

We again suppose that, according to (15), only the  $1s^2$  ( $l = 0$ ) state gives the leading contribution to A2 at big  $v_p$ ,  $q$ , and  $|\vec{v}_p - \vec{q}|$  in the case of CI wave functions. So we can write now

$$\begin{aligned}
 & F_0(\vec{v}_p - \vec{x}; -\vec{v}_p + \vec{q} + \vec{x}) \\
 &= \sum_{n \geq 1} C_{n0} \sum_{i,j} d_i^{n0} d_j^{n0} \\
 & \quad \times \frac{2^7 \sqrt{2\pi} \sqrt{(\varepsilon_i^{n0})^5 (\varepsilon_j^{n0})^3} [(\varepsilon_j^{n0}) + 2]}{[(\vec{v}_p - \vec{x})^2 + (\varepsilon_i^{n0})^2]^2 \{(\vec{v}_p - \vec{q} - \vec{x})^2 + [(\varepsilon_j^{n0}) + 2]^2\}^2}, \quad (22)
 \end{aligned}$$

and on the basis of the formulas presented previously, we obtain

$$\begin{aligned}
 A2 &\approx 2^7 \pi \sum_{n \geq 1} C_{n0} \sum_{i,j} d_i^{n0} d_j^{n0} \sqrt{(\varepsilon_i^{n0})^3 (\varepsilon_j^{n0})^3} \frac{\partial^3}{\partial \mu_1 \partial \mu_{2i} \partial \lambda_j} \\
 & \quad \times \left[ \frac{I_i(0) - I_i(\lambda_j)}{\lambda_j^2} \right], \quad (23)
 \end{aligned}$$

with

$$\begin{aligned}
 \lambda_j &= (\varepsilon_j^{n0} + 2), \quad \mu_1 = 1, \quad \mu_{2i} = \varepsilon_i^{n0}, \\
 \vec{q}_1 &= \vec{v}_p - \vec{q}, \quad \vec{q}_2 = -\vec{q}.
 \end{aligned}$$

We do not present a comparison of numerical and analytical results, because the coincidence is just as in Fig. 3.

On the other hand, an approximated formula can be derived from (17). We assume that the main contribution to the integral follows from the domains  $r_0 \sim 0$  and  $r_1 \sim 0$  because of large values of the momenta  $q$  and  $|\vec{v}_p - \vec{q}|$  in the exponential indexes in (17). Consequently, for the Hy wave function the

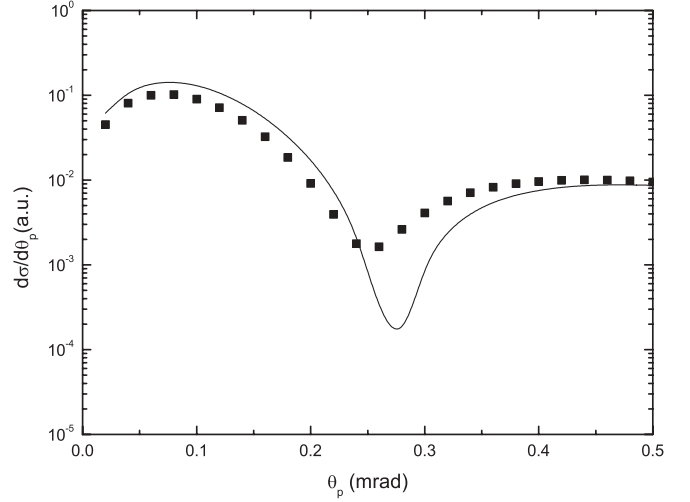


FIG. 4. The same as in Fig. 2, but the amplitude A2 is also included. Solid line, numerical calculation; squares, A1 + A3<sub>MAPLE</sub> + Eq. (24).

approximation can be written as

$$\begin{aligned}
 A2 &\approx -\sqrt{2} \int \frac{d\vec{r}_0 d\vec{r}_1 d\vec{r}_2}{r_2} e^{-i\vec{q} \cdot \vec{r}_1} e^{-i(\vec{v}_p - \vec{q}) \cdot \vec{r}_0} \\
 & \quad \times \frac{\Phi_{\text{He}^+}(\vec{r}_2) \phi_{\text{H}}(\vec{r}_0) \Phi_0(\vec{r}_1, \vec{r}_2)}{2^{10} \pi Z^4} \\
 &= -\frac{1}{(Z+2)^2 [(\vec{v}_p - \vec{q})^2 + 1]^2 [q^2 + Z^2]^2}. \quad (24)
 \end{aligned}$$

This expression is of the asymptotical order  $v_p^{-8}$  and should be much smaller than A1 and A3.

In Fig. 4, the numerical and approximate calculations of the SDCS are presented. Numerical calculations include all three items, whereas the approximate calculations take into account A1 + A3 analytically and A2 by Eq. (24). One easily sees that the contribution of A2 item is rather small in the case of CT, as it was marked in our previous publications [10,11]. That is why its approximate calculation does not differ from the numerical result considerably.

Concluding the part about CT reactions, one has to note that exact analytical formulas for all three FBA amplitudes can be written for any CI helium wave function, but they are very bulky. For example, the term  ${}^l Y_{l,m}(\vec{r}_i)$  in (8) can be presented like a finite linear combination of items  $x^\lambda y^\mu z^\nu$  ( $l = \lambda + \mu + \nu$ ). On insertion in the integrand of (10), this combination leads to an additional application of the differential operator  $(-i\partial/\partial q_{2x})^\lambda (-i\partial/\partial q_{2y})^\mu (-i\partial/\partial q_{2z})^\nu$  to the basic integral (13), etc. The analogous considerations are valid for Eqs. (17) and (20). MAPLE can be useful here. However, there is no sense in using analytical calculations for the integrals A2 and A3 because calculations by using the Gauss-Legendre numerical quadrature scheme give rather reliable and relatively fast results even for CT from molecules (7D integration) [11].

### C. Transfer ionization reactions: A3

By definition (2),

$$A3(\vec{k}) = 8\pi\sqrt{2} \int \frac{d\vec{x}}{(2\pi)^3} \frac{\tilde{\phi}_{\text{H}}(x)}{|\vec{v}_p - \vec{q} - \vec{x}|^2} F(\vec{v}_p - \vec{x}, 0; \vec{k}), \quad (25)$$

with  $F(\vec{y}, \vec{\eta}; \vec{k})$  given by Eq. (3). By analogy with (5), we write

$$A3(\vec{k}) = 2\sqrt{2} \int d\vec{r}_2 \varphi_c^{-*}(\vec{k}, \vec{r}_2) J(\vec{r}_2; \vec{q}, \vec{v}_p - \vec{q}),$$

with

$$J(\vec{r}_2; \vec{q}, \vec{v}_p - \vec{q}) = \int \frac{d\vec{r}_0 d\vec{r}_1}{|\vec{r}_0 - \vec{r}_1|} e^{-i\vec{q}\cdot\vec{r}_1} e^{-i(\vec{v}_p - \vec{q})\vec{r}_0} \times \phi_H(\vec{r}_0) \Phi_0(\vec{r}_1, \vec{r}_2). \quad (26)$$

Let us consider in the beginning the simplest Hy helium wave function. In this particular case,

$$A3(\vec{k}; Z) = 2\sqrt{2} R(Z) F(\vec{k}; Z), \quad (27)$$

where  $R(Z)$  is given by (11) (the same, like for CT), and

$$\begin{aligned} F(\vec{k}; Z) &= \sqrt{\frac{Z^3}{\pi}} \int d\vec{r}_2 \varphi_c^{-*}(\vec{k}, \vec{r}_2) e^{-Zr_2} \\ &= e^{-\pi\xi/2} \Gamma(1 + i\xi) \frac{8\sqrt{\pi Z^3} (Z + k\xi)}{(k^2 + Z^2)^2} e^{2\xi \arctan(k/Z)}. \end{aligned} \quad (28)$$

Correspondingly,

$$|F(\vec{k}; Z)|^2 = \frac{4\pi/k}{1 - \exp(-4\pi/k)} \frac{64\pi Z^3 (Z - 2)^2}{(k^2 + Z^2)^4} \times e^{(-8/k) \arctan(k/Z)}. \quad (29)$$

With the purpose of convenience, we write the analytical expression of the sum A1 + A3

$$A1 + A3 = 2\sqrt{2} \left\{ -\frac{16\pi\sqrt{Z^5}}{[1 + (\vec{v}_p - \vec{q})^2][Z^2 + q^2]^2} + R(Z) \right\} \times F(\vec{k}; Z). \quad (30)$$

Now we consider the CI wave functions. According to (26), we expect from the general rules of calculation of rapidly oscillating integrals that only  $1s^2$  ( $l = 0$ ) state gives the leading contribution to A3 at big  $v_p$ ,  $q$ , and  $|\vec{v}_p - \vec{q}|$ . Defining

$$\begin{aligned} R_n(\text{CI}) &= \sum_i d_i^{n0} R(\varepsilon_i^{n0}), \\ F_n(\text{CI}, \vec{k}) &= \sum_i d_i^{n0} F(\vec{k}; \varepsilon_i^{n0}), \end{aligned}$$

we obtain

$$A3(\vec{k}) \approx 2\sqrt{2} \sum_{n \geq 1} C_{n0} R_n(\text{CI}) F_n(\text{CI}, \vec{k}). \quad (31)$$

For the RHF  $1s^2$  wave function this formula is exact.

In Fig. 5, the SDCS is displayed for A1 + A3 amplitudes where the solid line represents the numerical calculations with

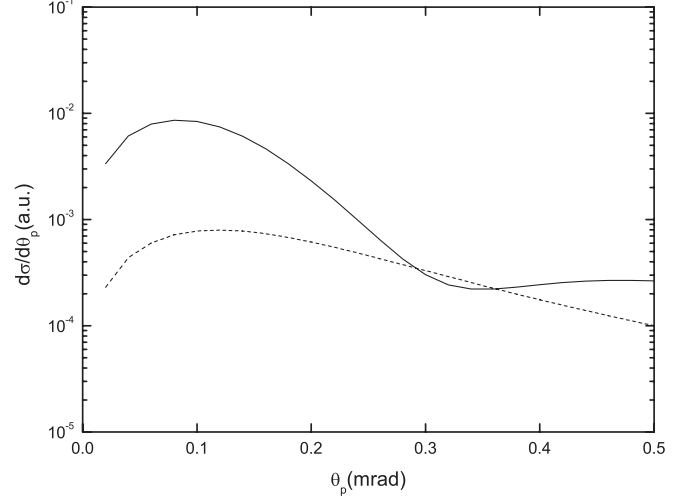


FIG. 5. SDCS (A1 + A3 amplitudes only) vs the hydrogen scattering angle  $\theta_p$  for the TI reaction  $\text{He} + p \rightarrow \text{He}^{2+} + e + \text{H}$  at proton energy  $E_p = 1.4$  MeV. The Mitroy wave function is used. Solid line, numerical calculations; dashed line, Eq. (31) (only  $1s^2$  part of the full wave function is taken into account).

the Mitroy wave function, whereas the dashed line takes into account only its  $1s^2$  part given by (31). We see that contrary to the CT case, the  $1s^2$  part of the correlated helium wave function is obviously not enough to reproduce full calculations. Higher angular momenta play a very important role for the TI.

#### D. Transfer ionization reactions: A2

This integral A2 cannot be reduced now to the Lewis type integral, and we consider its representation in the coordinate space

$$\begin{aligned} A2(\vec{k}) &= -\sqrt{2} \int \frac{d\vec{r}_0 d\vec{r}_1 d\vec{r}_2}{|\vec{r}_0 - \vec{r}_1 + \vec{r}_2|} e^{-i\vec{q}\cdot\vec{r}_1} e^{-i(\vec{v}_p - \vec{q})\vec{r}_0} \\ &\times \varphi_c^{-*}(\vec{k}, \vec{r}_2) \phi_H(\vec{r}_0) \Phi_0(\vec{r}_1, \vec{r}_2). \end{aligned} \quad (32)$$

The same considerations resulting in Eq. (24) make it possible to obtain the approximation like the MPA

$$\begin{aligned} A2(\vec{k}) &\approx -\sqrt{2} \int \frac{d\vec{r}_0 d\vec{r}_1 d\vec{r}_2}{r_2} e^{-i\vec{q}\cdot\vec{r}_1} e^{-i(\vec{v}_p - \vec{q})\vec{r}_0} \\ &\times \varphi_c^{-*}(\vec{k}, \vec{r}_2) \phi_H(\vec{r}_0) \Phi_0(\vec{r}_1, \vec{r}_2) \\ &= -\frac{8\sqrt{2}\pi}{[1 + (\vec{v}_p - \vec{q})^2]^2} \int \frac{d\vec{r}_1 d\vec{r}_2}{r_2} e^{-i\vec{q}\cdot\vec{r}_1} \\ &\times \varphi_c^{-*}(\vec{k}, \vec{r}_2) \Phi_0(\vec{r}_1, \vec{r}_2). \end{aligned} \quad (33)$$

For the Hy wave function, Eq. (33) gives

$$\begin{aligned} A2(\vec{k}) &\approx -\sqrt{2} \frac{2^8 \pi^2 \sqrt{Z^5} e^{-\pi\xi/2} \Gamma(1 + i\xi) e^{2\xi \arctan(k/Z)}}{[1 + (\vec{v}_p - \vec{q})^2]^2 [Z^2 + q^2]^2 (Z^2 + k^2)}; \\ \xi &= -\frac{2}{k}. \end{aligned} \quad (34)$$



For the sake of convenience, we write the approximate expression of the sum  $A1(\vec{k}) + A3(\vec{k}) + A2(\vec{k})$

$$A1(\vec{k}) + A3(\vec{k}) + A2(\vec{k}) \approx 2\sqrt{2} \left\{ -\frac{16\pi\sqrt{Z^5}}{[1 + (\vec{v}_p - \vec{q})^2][Z^2 + q^2]^2} + R(Z) - \frac{16\pi^{3/2}Z(Z^2 + k^2)}{(Z-2)[1 + (\vec{v}_p - \vec{q})^2][Z^2 + q^2]^2} \right\} F(\vec{k}; Z). \quad (35)$$

For comparison, in the case of CT

$$A1 + A3 + A2 \approx 2\sqrt{2} \left\{ -\frac{16\pi\sqrt{Z^5}}{[1 + (\vec{v}_p - \vec{q})^2][Z^2 + q^2]^2} + R(Z) - \frac{16\pi\sqrt{Z^5}(Z+2)}{[1 + (\vec{v}_p - \vec{q})^2][Z^2 + q^2]^2} \right\} F_{1s}(Z). \quad (36)$$

Even the approximate expression (35) shows that the contribution of the A2 item can be rather big in spite of its asymptotical smallness. Moreover, if we switch off for a moment the  $ee$  correlation in the helium ground wave function (put  $Z = 2$ ), only this item remains nonzero. In fact, this is the case, and the item A2 is bigger than A1 and A3 for the incoming energy of a few MeV. For comparison, the SDCS (4) for the Hy wave function is presented in Fig. 6.

In principle, by using the Lewis integrals instead of MPA, we can reduce 3D integration in A2 and A3 to 1D integration. For this, the Coulomb wave function  $\varphi_c^{-*}(\vec{k}, \vec{r})$  should be represented by the well-known 1D integral, and then the remaining part can be analytically calculated. Sometimes the reduction of two more integrations gives a huge profit. However, if we are limited with calculations of the SDCS and DDCS for fast TI reactions on atoms, 6D numerical integrations can be fulfilled.

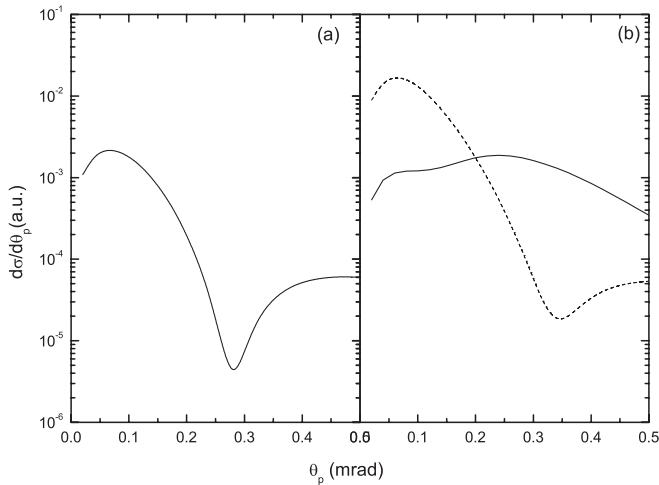


FIG. 6. The kinematical conditions are the same as in Fig. 5, but the Hy wave function is used. (a)  $(A1 + A3)$  numerical calculations; (b)  $(A1 + A2 + A3)$  numerical calculations (solid line) and  $(A1 + A2 + A3)$  Eq. (35) (dashed line).

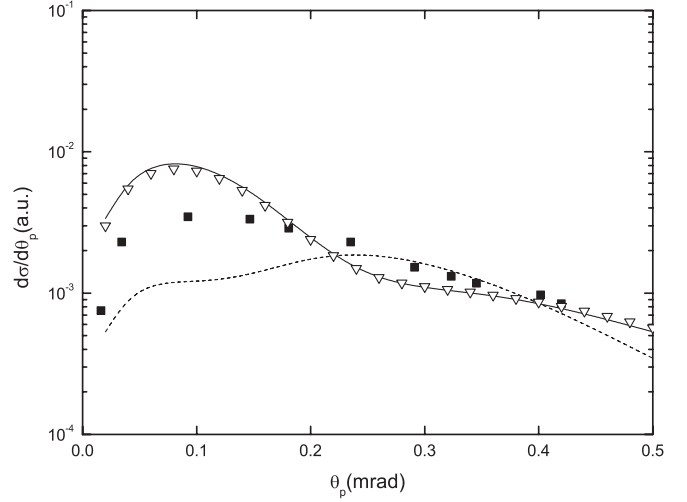


FIG. 7. FBA SDCS (4) vs the hydrogen scattering angle  $\theta_p$  for the TI reaction  $\text{He} + p \rightarrow \text{He}^{2+} + e + \text{H}$  at proton energy  $E_p = 1.4$  MeV. Solid line, Mitroy; open triangles, Nesbet, and dashed line, Hy wave functions. Solid squares, experiment [23].

### III. RESULTS AND DISCUSSION

Unfortunately, any analytical expression of the integral A2 in the case of TI is unknown. However, it is the leading amplitude in the sum  $(A1 + A2 + A3)$ . In this case, the SDCS for TI in atoms involves a 6D integration. In Fig. 7, our results are presented for Hy, Mitroy, and Nesbet [22] wave functions and compared with experiment [23]. One sees that just the broad tail of the term A2 agrees with the shape of the experimental distribution beyond  $\theta_p = 0.2$  mrad (see Fig. 2 in [6] for comparison), and the correlated CI wave function gives better agreement in this angular domain.

Another result is shown in Fig. 8, where we present our calculated DDCS

$$\frac{d^2\sigma}{dE_e d\Omega_e} = \frac{m^2 k}{(2\pi)^5} \int |A1 + A2 + A3|^2 d\Omega_p \quad (37)$$

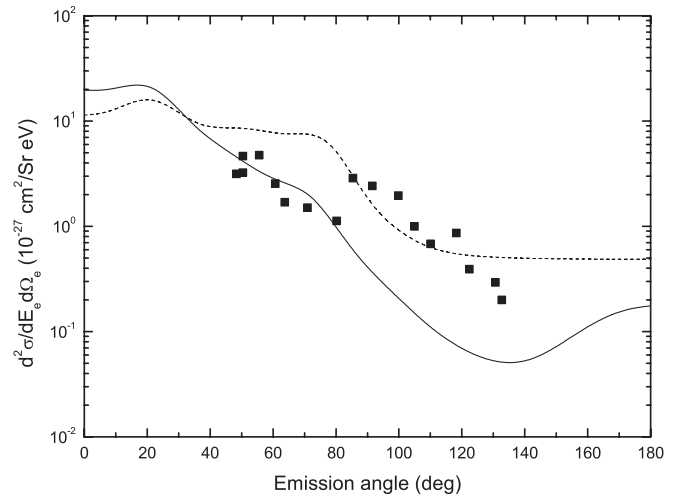


FIG. 8. FBA DDCS (37) vs the electron emission angle  $\theta_e$  for the TI reaction  $\text{He} + p \rightarrow \text{He}^{2+} + e + \text{H}$  at proton energy  $E_p = 1$  MeV. Solid line, Mitroy; dashed line, Hy wave functions, solid squares, experiment [26].

(see also Fig. 1 in [9] for comparison). One sees the distribution of the escaped electron vs its scattering angle at its emission energy  $E_e = 600$  eV and the proton energy  $E_p = 1$  MeV. The results are obtained with correlated and  $1s^2$  wave functions. Of course, we agree with a discussion on the role of the SBA amplitudes presented in [9]. However, the wave functions with different forms of  $ee$  correlations can describe different regions of the experimental distribution. However, this can lead in another cases to fallacious conclusions.

#### IV. CONCLUSIONS

We briefly enumerate the results of our studies of SDCS and DDCS for different capture processes for the ( $p$ -He) system at incident energies of about 1 MeV.

(i) The MPA is a very crude approximation which fails to describe the SDCS even for the scattering angles below 0.5 mrad. However, it can be avoided by the use of analytical Lewis-type integrals for most fast capture processes.

(ii) Any “simplifications” of the SBA amplitudes (for example, [4,24]) must be carefully examined. It is found that

the amplitudes for capture processes are very sensitive to such “simplifications.”

(iii) For TI reactions, the TS2 mechanism (item A2) mainly contributes to the SDCS at the proton energies of a few MeV and scattering angles below 0.5 mrad. We come out with a cautious suggestion that the same effect may also be observed for transfer excitation reactions. On the contrary, this scattering mechanism is quite small in this kinematical domain for CT reactions leaving a residual ion in its ground state.

(iv) The SDCS for TI reactions within the range of scattering angles 0–0.5 mrad seems to distinguish helium trial wave functions with different degrees of correlation. Here we see the same effect noted earlier for ( $e, 3e$ ) reactions in the kinematical regime of the electron momentum spectroscopy [25].

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