Energy sharing and angular distribution in the double photoionization of helium

A. K. Kazansky and V. N. Ostrovsky
Institute of Physics, The University of St. Petersburg, 198904 St. Petersburg, Russia
(Received 18 July 1994; revised manuscript received 20 January 1995)

The double photoionization of an atom is considered in the near-threshold domain. The angular correlation pattern is analyzed for an arbitrary sharing of the excess energy by the electrons. The motion over the hyperspherical radius R is treated semiclassically which casts the problem in a nonstationary form. For motion over the hyperspherical angle α the set of classical trajectories is considered. They converge to the same ($R \to \infty$) limit which corresponds to a chosen energy-sharing ratio. For each $\alpha(R)$ trajectory the quantum wave packet (over the correlation angle θ_{12}) is propagated from the inner zone to the region of free-electron motion. At the border of the reaction zone a realistic boundary condition is imposed. The cross sections exhibit a weak dependence on the energy-sharing ratio.

PACS number(s): 32.80.Fb, 34.80.Dp, 34.80.Kw

The description of strong electron-electron correlations is one of the most fundamental problems in atomic physics. The correlations can be observed most directly in the angular and energy-sharing distributions for three-body breakup processes, such as ionization by electron impact $(e,2e)$ and double photoionization $(\gamma,2e)$. The latter process is particularly convenient for the detailed analysis since the selection rules specify the quantum numbers of the final-state two-electron continuum. The recent breakthrough in experiments on angular distributions in the $(\gamma,2e)$ process [1–8] provides a challenge for theory, where two major approaches are now underway.

The key problem for the theory is the construction of the correlated final-state wave function for the two-electron continuum. Maulbetsch and Briggs [9] employ the method commonly referred to as Brauner-Briggs-Klar (BBK) [10], i.e., they use the Garibotti-Miraglia [11] wave function, which accounts on equal footing for all three two-particle Coulomb interactions but in an empirical way. This approach was applied recently in a broad range of energies for both $(e,2e)$ and $(\gamma,2e)$ processes.

The alternative theory developed by the authors [12–14] stems from ideas due to Wannier [15]. In its existing form it has been limited to the analysis of the angular distributions in the equal-energy-sharing case. As a manifestation of this fact, the calculations are confined to the so-called Wannier ridge, i.e., the region of configuration space where the electrons recede, being at equal distances from the atomic core ($r_1 = r_2$). Generally, the Wannier mechanism is operative in the near-threshold domain. However, in the case when the electrons share equally the energy excess E above the threshold, the extended Wannier-ridge theory reproduces well the experimental data even for E as high as 20 eV [14].

The object of the present paper is to put forward a broader scheme which allows us to calculate the angular distribution for the arbitrary sharing of the excess energy E between the electrons. Double-photoionization experiments of this type are known to be underway. The same approach can be extended to the calculation of the distribution differential in both variables. Previously, only the energy-sharing distributions integrated over the angles were calculated exclusively within the classical trajectory approach (see, e.g., the review by Read [16]).

In what follows collective coordinates are employed: the hyperradius $R = (r_1^2 + r_2^2)^{1/2}$, the hyperangle $\alpha \equiv \tan^{-1}(r_1/r_2)$, the angle θ_{12} between the electron vectors $\vec{r}_1, \vec{r}_2$, and the set of Euler angles $\Omega = \{\alpha_E, \beta, \gamma\}$. For the sake of brevity we consider here only the P^o state of the two-electron continuum which is populated by the dipole one-photon transition from the initial (ground) S^e state of the atom. In this case the wave function is represented exactly [13,17,18] as

$$\Psi_{1M}(R,\alpha,\theta_{12},\Omega) = R^{-5/2}(\sin 2\alpha)^{-1} \times [\phi_{11}^{+}(R,\alpha,\theta_{12}) D^{1+}_{-M1}(\Omega) + \phi_{11}^{-}(R,\alpha,\theta_{12}) D^{1-}_{-M1}(\Omega)] , \tag{1}$$

where the combinations of the Wigner functions $D^{L}_{MM'}(\Omega)$ are employed [17]:

$$D^{1+}_{M1}(\Omega) = 2^{-1/2}[D^{L}_{M1}(\Omega) - D^{L}_{M-1}(\Omega)] ,$$
$$D^{1-}_{M1}(\Omega) = 2^{-1/2}\frac{1}{i}[D^{L}_{M1}(\Omega) + D^{L}_{M-1}(\Omega)] . \tag{2}$$

The components ϕ_{11}^{+} and ϕ_{11}^{-} obey the coupled equations which are the particular case of the general system of equations presented by Bhatia and Temkin [[17], Eqs. (70)] and Nikitin and Ostrovsky [[18], Eqs. (2.9)]. The distinction appears exclusively due to the fact that we make an additional transformation to the hyperspherical coordinates R,α [that is expressed by the common factor before the brackets in the expression (1) which is related to the Jacobian of the transformation]. The explicit form of the exact equations in the hyperspherical representation is

$$H_{11}^{(0)}\phi_{11}^{\pm}\mp\frac{1}{R^2\sin^2 2\alpha}\frac{\cos\theta_{12}}{\sin^2\theta_{12}}\phi_{11}^{\pm}$$
$$\mp\frac{2}{R^2}\frac{\cos 2\alpha}{\sin^2 2\alpha}\left[\frac{\cos\theta_{12}\mp 1}{2\sin\theta_{12}}+\frac{\partial}{\partial\theta_{12}}\right]\phi_{11}^{\mp}=E\phi_{11}^{\pm}\ , \quad (3)$$

with

$$H_{LK}^{(0)}=-\frac{1}{2}\frac{\partial^2}{\partial R^2}-\frac{1}{2R^2}\frac{\partial^2}{\partial\alpha^2}$$
$$-\frac{2}{R^2\sin^2 2\alpha}\left[\frac{1}{\sin\theta_{12}}\frac{\partial}{\partial\theta_{12}}\sin\theta_{12}\frac{\partial}{\partial\theta_{12}}\right.$$
$$\left.-\frac{L(L+1)-K^2}{2\sin^2\theta_{12}}-\frac{K^2}{4}+\frac{1}{4}\right]+\frac{C}{R}\ , \quad (4)$$

$$C(\alpha,\theta_{12})=-Z/\cos\alpha-Z/\sin\alpha$$
$$+(1-\sin 2\alpha\cos\theta_{12})^{-1/2}\ . \quad (5)$$

Our first approximation is the semiclassical treatment of the motion along the coordinate R. In this case the Schrödinger equation for the two-electron system may be approximately transformed to the nonstationary form. We introduce the "mock" time τ by the relations

$$d\tau=\frac{dR}{p_R R}\ , \quad \tfrac{1}{2}p_R^2-\frac{Z_0}{R}=E\ , \quad Z_0=2^{3/2}(Z-\tfrac{1}{4})\ , \quad (6)$$

and new functions

$$\tilde{\phi}_{11}^{\pm}\equiv\phi_{11}^{\pm}[p_R(R)]^{1/2}\exp\left[-i\int^R p_R(R')dR'\right]\ .$$

Here Z is the charge of the nucleus; for the details, see Refs. [12,13]. Excluding also the first-order derivatives over θ_{12} by the transition to the functions $\chi_{11}^{\pm}\equiv\tilde{\phi}_{11}^{\pm}(\sin\theta_{12})^{1/2}$, one obtains for P^o states the set of two "time"-dependent coupled Schrödinger equations

$$i\frac{\partial\tilde{\chi}_{11}^{\pm}}{\partial\tau}=\mathcal{H}_{11}(R(\tau),\alpha)\tilde{\chi}_{11}^{\pm}\mp\frac{\cos\theta_{12}}{R(\tau)\sin^2 2\alpha\sin^2\theta_{12}}\tilde{\chi}_{11}^{\pm}$$
$$+\frac{\cos 2\alpha}{R(\tau)\sin^2 2\alpha}\left[-\frac{1}{\sin\theta_{12}}\mp 2\frac{\partial}{\partial\theta_{12}}\right]\tilde{\chi}_{11}^{\mp}\ , \quad (7)$$

$$\mathcal{H}_{LK}=-\frac{1}{2R(\tau)}\frac{\partial^2}{\partial\alpha^2}+[C(\alpha,\theta_{12})+Z_0]$$
$$-\frac{2}{R(\tau)\sin^2 2\alpha}\left[\frac{\partial^2}{\partial\theta_{12}^2}-\frac{2[L(L+1)-K^2]-1}{4\sin^2\theta_{12}}\right.$$
$$\left.-\frac{K^2}{4}+\frac{1}{2}\right]\ . \quad (8)$$

Equations (7) and (8) can be considered as a generalization of our extended Wannier-ridge model [13,14], which now is not confined to the Wannier ridge $\alpha=\frac{1}{4}\pi$. It should be stressed that the present development does not presume any model assumptions but results directly from the exact two-electron Schrödinger equation with the single approximation of the semiclassical motion over R.

The proper solution of Eqs. (7) is selected [12,13] by imposing the model initial condition at some time $\tau=\tau_0$

$$\chi_{11}^{\pm}(\alpha,\theta_{12},\tau_0)=g_{11}^{\pm}(\alpha,\theta_{12})\ . \quad (9)$$

The particular form of the functions $g_{11}^{\pm}(\alpha,\theta_{12})$ is discussed below. An alternative *ab initio* approach in terms of the wave source [14] can also be realized within the present scheme.

Thus the electron-correlation problem is reduced to the propagation of the two-dimensional (α,θ_{12}) two-component $(\tilde{\chi}_{11}^{+},\tilde{\chi}_{11}^{-})$ wave packet governed by the time-dependent Hamiltonian. Generally, the numerical solution for a two-dimensional problem of this type is accessible by modern computing facilities. The application of the fast-Fourier-transform technique is particularly effective for such purposes [19,20]. However, in the present particular case the situation is complicated by the attractive Coulomb singularities in the "effective charge" $C(\alpha,\theta_{12})$. Indeed, the exact solution of Eqs. (7)–(9) not only describes the double-ionization process but also incorporates single ionization with the population of any Rydberg state of the residual singly charged ion. Clearly, the solution of this broad problem implies serious extra efforts of a character beyond the scope of the present paper.

These difficulties are avoided by an additional approximation which is the key idea of the present study. It concerns the evolution over the hyperangle α and combines semiclassical, eikonal, and adiabatic elements. There is some analogy with studies of electron correlations in doubly excited states [21] which tentatively suggested the following hierarchy: the hyperradius R appears as the slowest variable, the next is the hyperangle α, and the other variables are considered as fast. In a very broad sense the present scheme could be considered as an elaboration of similar ideas for the two-electron continuum states. Note, however, that this is only a qualitative concatenation. The theoretical framework is substantially different from the schemes employed previously.

Bearing in mind that the Coulomb repulsion favors electron ejection in opposite directions ($\theta_{12}=\pi$), we introduce an auxiliary Hamiltonian H_α,

$$H_\alpha=\frac{\Pi_\alpha^2}{2R(\tau)}+[C(\alpha,\pi)+Z_0]\ , \quad (10)$$

$$C(\alpha,\pi)=-Z/\sin\alpha-Z/\cos\alpha+(1+\sin 2\alpha)^{-1/2}\ , \quad (11)$$

which does not depend on θ_{12}, but incorporates the most significant part of the interaction over the coordinate α. Consider the classical trajectory $\alpha(\tau)$ governed by the Hamiltonian (11):

$$\dot{\alpha}=\frac{\partial H_\alpha}{\partial\Pi_\alpha}\ , \quad \dot{\Pi}_\alpha=-\frac{\partial H_\alpha}{\partial\alpha}\ , \quad (12)$$

with Π_α being the momentum conjugate to the coordinate α in terms of the Hamiltonian H_α. We need the particular trajectory specified by the initial and final values of the coordinate: $\alpha(\tau=\tau_0)=\alpha_0$, $\alpha(\tau=T)=\alpha_1$ (in the numerical calculations T should correspond to sufficiently large R). Such a trajectory is the solution of the canoni-

cal two-point problem, the full (extended) notation being $\alpha(\tau)=\alpha(\alpha_1,T;\alpha_0,\tau_0;\tau)$.

The semiclassical propagator for the Hamiltonian H_α is expressed as a sum of the contributions related to various trajectories $\alpha_j(\alpha_1,T;\alpha_0,\tau_0;\tau)$ (enumerated by the index j) which start from the point α_0 and terminate at α_1:

$$K(\alpha_1,T;\alpha_0,\tau_0)=\sum_j D_j(\alpha_1,T;\alpha_0,\tau_0)\exp[iS_j(\alpha_1,T;\alpha_0,\tau_0)] . \quad (13)$$

Here S_j is the action calculated along the trajectory:

$$S_j(\alpha,T;\alpha_0,\tau_0)=\int_{(\alpha_0,\tau_0)}^{(\alpha_1,T)}(\Pi_\alpha d\alpha - H_\alpha d\tau) . \quad (14)$$

This formula is related to the well-known Feynman-trajectory representation of the quantum mechanics. A similar approach was employed, e.g., by Gutzwiller [22], but for time-independent Hamiltonians. The Maslov indices are not important in the present study; hence they are not written down explicitly (one can imply that they are incorporated in S_j). The integral in Eq. (14) is taken along the jth two-point trajectory.

The preexponential factor $D_j(\alpha,T;\alpha_0,\tau_0)$ ensures conservation of the flux in the vicinity of the jth trajectory. In order to define it, consider a small deviation $\{\delta\alpha_j(\tau),\delta\Pi_j(\tau)\}$ from the two-point trajectory $\alpha_j(\tau)$. The deviation is governed by the linearized equations of motion

$$\delta\dot{\alpha}_j=R(\tau)^{-1}\delta\Pi_j , \quad \delta\dot{\Pi}_j=-[\partial^2 H_\alpha/\partial\alpha^2]_{\alpha=\alpha_j(\tau)}\delta\alpha_j . \quad (15)$$

The linearized problem is equivalent to that of the harmonic oscillator with a time-dependent frequency where the Green function is known, due to Husimi [23]. Following this analogy in detail, one obtains $D_j=[\pi/\delta\alpha_j(T)]^{1/2}$, where the solution of Eqs. (15) is specified by the initial conditions

$$\delta\alpha_j(\tau=\tau_0)=0 , \quad \delta\dot{\alpha}_j(\tau=\tau_0)=1 . \quad (16)$$

We cite also an alternative expression for D_j (the integration is performed along the jth trajectory):

$$D_j(\alpha_1,T;\alpha_0,\tau_0)=\exp\left[-\int_{\tau_0}^{T}\frac{\partial\Pi_\alpha}{\partial\alpha}\frac{d\tau}{2R(\tau)}\right] . \quad (17)$$

The two-point trajectories $\alpha_j(\alpha_1,T;\alpha_0,\tau_0;\tau)$ serve as a base in our construction of the approximate solution of the full two-dimensional (α,θ_{12}) propagation problem. Namely, each trajectory generates the dependence $\alpha_j(\tau)$ which is used to reduce the two-dimensional propagation to the one-dimensional propagation over the coordinate θ_{12}. In this approximation the wave-function components are expressed as

$$\chi_{11}^{\pm}(\theta_{12},\alpha_1,R(T))=\sum_j\int d\alpha_0 D_j(\alpha_1,T;\alpha_0,\tau_0)\times\exp[iS_j(\alpha_1,T;\alpha_0,\tau_0)]\times\chi_{11}^{\pm}(\theta_{12},\{\alpha_j(\tau)\},\tau) . \quad (18)$$

The symbol $\{\alpha_j(t)\}$ in Eq. (18) indicates that $\chi_{11}^{\pm}$ is the functional of the two-point α trajectory $\alpha_j(\alpha,T;\alpha_0,\tau_0;\tau)$ which is unique for both wave-function components. Namely, the functions $\chi_{11}^{\pm}(\theta_{12},\{\alpha_j(\tau)\},\tau)$ obey a system of equations analogous to (7), but with the substitution $\alpha\Longrightarrow\alpha_j(\tau)$ and $\mathcal{H}_{LK}\Longrightarrow\tilde{\mathcal{H}}_{LK}$, where

$$\tilde{\mathcal{H}}_{LK}(\tau)=[1-\sin2\alpha_j(\tau)\cos\theta_{12}]^{-1/2}-[1+\sin2\alpha_j(\tau)]^{-1/2}-\frac{2}{R(t)\sin^2 2\alpha,(\tau)}\left[\frac{\partial^2}{\partial\theta_{12}^2}-\frac{2[L(L+1)-K^2]-1}{4\sin^2\theta_{12}}-\frac{K^2}{4}+\frac{1}{2}\right] . \quad (19)$$

The summation over j in the expressions (13) or (18) reflects the existence of the (infinite) set of two-point trajectories rebounding from the edges $r_1=0$ or (and) $r_2=0$ of the (r_1,r_2) quadrant. The existence of such trajectories is closely related to the unstable double-Rydberg resonances below the double-escape threshold [24] and to the population of the Rydberg series above the threshold [see the discussion below the formula (9)]. However, it is expected that for double-escape processes the principal contribution is given by Wannier-type trajectories which are free of the rebounding peculiarities. Only one trajectory of this type exists for each (α_0,α_1) that lifts the summation over j in (18) (Fig. 1). Note that high instability [25] of the classical Wannier trajectory (arising from the triple-collision point) is irrelevant here since only the trajectories outgoing from the region $R<R_0\equiv R(\tau_0)$ contribute.

For the final one-electron energies E_1,E_2 the final $(R\to\infty)$ value of the hyperangle is expressed via the energy-sharing ratio $\alpha_f=\tan^{-1}\sqrt{E_1/E_2}$. For fixed E_1/E_2 the angular correlation pattern contains the contributions from the trajectories starting from various α_0 and terminating at the same α_f. Figure 1 shows that such trajectories merge quite rapidly. With good precision one can assume that starting from $R=R_u\sim 50a_0$ a universal trajectory appears independent of the initial condition α_0. Hence the multitrajectory scheme can be reduced to the single-trajectory one for $R>R_u$, the latter being much simpler. This observation is extremely important for the numerical calculations which are quite time consuming when wave-packet propagation is concerned.

In the case of equal energy sharing ($E_1=E_2=\frac{1}{2}E$) the universal trajectory is trivial: $\alpha(\tau)\equiv\frac{1}{4}\pi$. Here the single-($\alpha=\frac{1}{4}\pi$) trajectory approximation coincides with the extended Wannier-ridge model developed by the authors

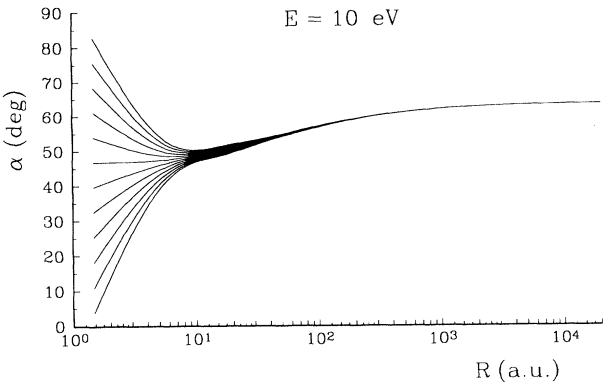

FIG. 1. The "classical trajectories" $\alpha(R)$, exposing variation of the hyperangle α with the hyperradius R as the electrons recede from the charged core ($Z=2$). The trajectories have various initial values α_0 but the same $R\to\infty$ asymptote $\alpha_f=\tan^{-1}2$, which corresponds to the energy-sharing ratio $E_1{:}E_2=4{:}1$. The excess energy is $E_1+E_2=10$ eV. Note that

[13,14].

The functions $\chi_{11}^{\pm}(\theta_{12},\{\alpha_j(\tau)\},\tau)$ should satisfy the initial (in terms of the "time" τ) or boundary (in terms of R) condition

$$\chi_{11}^{\pm}(\theta_{12},\{\alpha_j(\tau)\},\tau_0)=g_{11}^{\pm}(\theta_{12},\alpha_0)\ . \tag{20}$$

Below we carry out the concrete calculations for the double photoionization of the helium atom. In this case the initial conditions are specified as the product of the ground-state helium wave function ψ_0 and the transition operator in the dipole length form $\sim z_1+z_2=r_1\cos\theta_1+r_2\cos\theta_2$. For definiteness we assume here the linear polarization of the light wave [i.e., $M=0$ in Eq. (1)]. Huetz *et al.* [8] have shown that this is sufficient to describe the experimental data obtained by these authors for $E_1=E_2$. Following the scheme outlined by the authors [13] and accounting for the transformation between the conventional and hyperspherical representations one obtains

$$\begin{aligned} g_{11}^{+}(\theta_{12},\alpha_0)&=\cos(\tfrac{1}{2}\theta_{12})g_{+}\ ,\\ g_{11}^{-}(\theta_{12},\alpha_0)&=\sin(\tfrac{1}{2}\theta_{12})g_{-}\ , \end{aligned} \tag{21}$$

$$\begin{aligned} g_{\pm}=&N(\sin\theta_{12})^{1/2}(\cos\alpha_0\pm\sin\alpha_0)\\ &\times R_0^{7/2}\sin(2\alpha_0)\psi_0(R_0,\alpha_0,\theta_{12})\ . \end{aligned} \tag{22}$$

The value of the common normalization constant N is unessential since below we calculate only the relative angular distributions for various energy-sharing ratios E_1/E_2. Our experience [14] shows that the initial-state correlations in the He atom are of minor importance. Therefore in the first application of the theory we take the simplest uncorrelated wave function

$$\psi_0(\alpha,R)\simeq\exp[-\tfrac{27}{16}(\cos\alpha+\sin\alpha)R\ ]\ .$$

The boundary condition should be imposed on the border of the Wannier [15] reaction zone $R=R_0$ which is the empirical parameter of the theory. (Note that this parameter does not appear in the source formulation of the theory [14], where the numerical calculations are more time consuming and will be carried out in future.) Below, the value of R_0 is chosen to provide a maximum for $g_{11}^{+}(\theta_{12},\frac{1}{4}\pi)$ considered as a function of this parameter: $R_0=\frac{28}{27}2^{1/2}$.

The second term at the right-hand side of Eq. (7) differs in sign for χ^{+} and χ^{-}. As a result, the effective centrifugal repulsion inhibits penetration of the vicinity of the straight-line configuration $\theta_{12}=\pi$ for the component χ_{11}^{+}. For the function χ_{11}^{-} this effect is absent. More exactly, near the straight-line configuration one has $\tilde{\phi}_{11}^{+}\sim\sin\theta_{12}$, $\tilde{\phi}_{11}^{-}\sim$const. This implies that the value of the triple-differential cross section (TDCS) for $\theta_{12}=\pi$ directly reflects the weight of the $(-)$ component in the wave function (1).

In the boundary conditions (21) and (22) the functions $g_{11}^{+}(\alpha)$ and $g_{11}^{-}(\alpha)$ are, respectively, symmetric and antisymmetric under the reflection at the midpoint: $\alpha\Longrightarrow\frac{1}{2}\pi-\alpha$. This property is retained approximately for the function $\chi_{11}^{\pm}(\theta_{12},\{\alpha_j(\tau)\},\tau)$ for all R. For equal energy sharing ($\alpha_f=\frac{1}{4}\pi$), it holds exactly and leads to the exact cancellation of the contributions to $\chi_{11}^{-}(\alpha_f,R\to\infty)$ which come from the segments $0<\alpha_0<\frac{1}{4}\pi$ and $\frac{1}{4}\pi<\alpha_0<\pi$ (in particular, this implies zero TDCS for $\theta_{12}=\pi$). As α_f deviates from $\frac{1}{4}\pi$ the exact cancellation vanishes. However, the numerical calculations show that the contribution of χ_{11}^{-} to the TDCS remains very small. In this respect, the important circumstance is that the actions S_j gained on the different trajectories (see Fig. 1) are also almost symmetric under the reflection $\alpha\Longrightarrow\frac{1}{2}\pi-\alpha$ and do not vary much.

In the practical calculations an additional simplification was introduced: the quadratic approximation for the potential (11) in the vicinity of the saddle point $\alpha=\frac{1}{4}\pi$. The partial cross sections

$$\sigma^{\pm}(\theta_{12})\equiv|\tilde{\phi}_{11}^{\pm}(\theta_{12},\alpha_f,R\to\infty)|^2$$

were calculated for various excess energies E and the sharing ratios characterized by α_f. Figure 2 shows the results for the $\sigma^{+}(\theta_{12})$ cross sections. Although the cross sections are given in relative units, their ratios for different E and α_f are significant. The cross sections $\sigma^{-}(\theta_{12})$ at the maximum ($\theta_{12}=\pi$) are about 30 times less than their $(+)$ counterparts. Hence the related contributions to the observed TDCS's are far beyond the accuracy of the current experiments. Therefore we do not present them graphically.

The observed TDSC's are expressed as the squared modulus of the coherent sum of $\tilde{\phi}_{11}^{\pm}$ amplitudes. The concrete coefficients generally are functions of θ_{12} and depend on the experimental geometry. At present there are no published data for $E_1\neq E_2$ although the experiments are underway. The prominent qualitative feature of our results is the weak dependence of the cross-section shape on the energy-sharing ratio. The TDCS remains negligibly small at $\theta_{12}=\pi$ even for quite high excess energies. These conclusions could be verified directly in the forthcoming experiments. The value of the TDCS at $\theta_{12}=\pi$

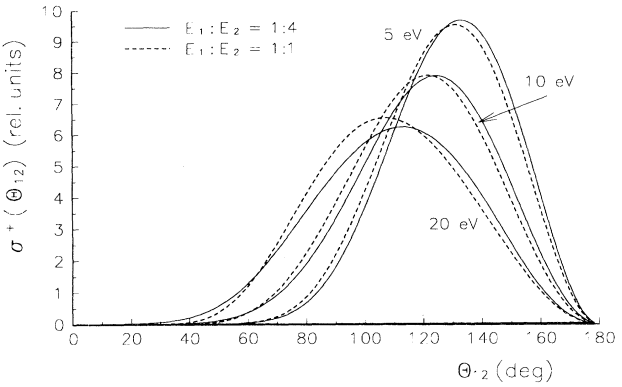

FIG. 2. The partial cross sections $\sigma^+(\theta_{12})$ for the double photoionization of the helium atom at various values of the excess energy $E=E_1+E_2$ indicated on the figure. The solid curves are for the energy-sharing ratio $E_1:E_2=1:4$ and the dashed curves are for $E_1:E_2=1:1$.

could be enhanced due to the contribution of the rebounding trajectories. This contribution could be expected to increase with E. Part of the trajectories could be included in future calculations within the present scheme.

We develop the scheme of calculations based on the hierarchy of three essential coordinates R, α, and θ_{12}. The hyperradius R is reduced to the effective time; the hyperangle α is treated semiclassically; due to these simplifications the quantum (wave-packet) treatment of θ_{12} becomes numerically tractable. The present scheme can be compared with that used by Bottcher [26], which also represents a combination of semiclassical and quantum elements. The latter calculations were restricted to a very few trajectories and eventually used the semiclassical approximation for the θ_{12} motion.

The important question is to what extent the interaction of θ_{12} and α motion is taken into account within the present scheme. In fact, the interaction is incorporated partially by using the accurate phase accommodated by the θ_{12} wave packets for the different trajectories. The situation is analogous to that in the eikonal approximation in scattering theory, where the straight-line classical trajectories are considered, but the phase for each trajectory depends on the impact parameter. This allows one to calculate the differential cross section, thus effectively lifting the initial approximation of the straight-line motion.

This work was greatly stimulated by the discussions with Dr. A. Huetz. One of the authors (A.K.K.) is thankful to Laboratoire de Dynamique Moléculaire et Atomique, Université Pierre et Marie Curie, Paris, France for hospitality. This work was supported by Grant. No. 93-02-1488 from the Russian Foundation for Fundamental Research and by Grant No. NX 20009 from the International Science Foundation.

[1] J. Mazeau, P. Selles, D. Waymel, and A. Huetz, Phys. Rev. Lett. **67**, 820 (1991).
[2] R. I. Hall, L. Avaldi, G. Dawber, M. Zubek, K. Ellis, and G. C. King, J. Phys. B **24**, 115 (1991); R. I. Hall, K. Ellis, A. G. McConkey, G. Dawber, L. Avaldi, M. A. McDonald, and G. C. King, *ibid.* **25**, 377 (1992); R. I. Hall, A. G. McConkey, L. Avaldi, K. Ellis, M. A. MacDonald, G. Dawber, and G. C. King, *ibid.* **25**, 1195 (1992); R. I. Hall, G. Dawber, A. G. McConkey, M. A. MacDonald, and G. C. King, *ibid.* **26**, L653 (1993).
[3] R. Wehlitz, F. Heiser, O. Hemmers, B. Langer, A. Menzel, and U. Becker, Phys. Rev. Lett. **67**, 3764 (1991).
[4] D. Waymel, L. Andric, J. Mazeau, P. Selles, and A. Huetz, J. Phys. B **26**, L123 (1993).
[5] O. Schwarzkopf, B. Krässig, J. Elmiger, and V. Schmidt, Phys. Rev. Lett. **70**, 3008 (1993).
[6] O. Schwarzkopf, B. Krassig, J. Elmiger, and V. Schmidt, J. Phys. (France) IV **3**, C6-169 (1993).
[7] B. Krässig, O. Schwarzkopf, and V. Schmidt, J. Phys. B **26**, 2589 (1993).
[8] A. Huetz, P. Lablanquie, L. Andric, P. Selles, and J. Mazeau, J. Phys. B **27**, L13 (1994).
[9] F. Maulbetsch and J. S. Briggs, Phys. Rev. Lett. **68**, 2004 (1992); J. Phys. B **26**, 1679 (1993); **26**, L647 (1993).
[10] M. Brauner, J. S. Briggs, and H. Klar, J. Phys. B **22**, 2265 (1989).
[11] C. R. Garibotti and J. E. Miraglia, Phys. Rev. A **21**, 572 (1980).
[12] A. K. Kazansky and V. N. Ostrovsky, J. Phys. B **26**, 2231 (1993); Phys. Rev. A **48**, 871 (1993).
[13] A. K. Kazansky and V. N. Ostrovsky, J. Phys. B **27**, 447 (1994); J. Phys. (France) IV **3**, C6-159 (1993).
[14] A. K. Kazansky and V. N. Ostrovsky, Phys. Rev. A **51**, 3712 (1995); J. Phys. B **28**, 1453 (1995).
[15] G. H. Wannier, Phys. Rev. **90**, 817 (1953).
[16] F. Read, in *Electron Impact Ionization,* edited by T. D. Märk, and G. H. Dunn (Springer, New York, 1985), pp. 43–87.
[17] A. K. Bhatia and A. Temkin, Rev. Mod. Phys. **36**, 1050 (1964).
[18] S. I. Nikitin and V. N. Ostrovsky, J. Phys. B **18**, 4349 (1985).
[19] R. Kosloff, J. Phys. Chem. **92**, 2087 (1988).
[20] A. K. Kazansky and L. Yu. Sergeeva, J. Phys. B **27**, 3217 (1994).
[21] J. Macek, J. Phys. B **1**, 831 (1968): U. Fano, Rep. Prog. Phys. **46**, 97 (1983); C. D. Lin, Adv. At. Mol. Phys. **22**, 77 (1986).
[22] M. Gutzwiller, J. Math. Phys. **8**, 1979 (1967).
[23] K. Husimi, Prog. Theor. Phys. **9**, 381 (1953).
[24] S. Watanabe, Phys. Rev. A **36**, 1566 (1987); G. S. Ezra, K. Richter, G. Tanner, and D. Wintgen, J. Phys. B **24**, L413 (1991).
[25] K. Richter and D. Wintgen, J. Phys. B **23**, L197 (1990).
[26] C. Bottcher, Adv. At. Mol. Phys. **25**, 303 (1988).