Electron-impact excitation of helium at 26.5 eV

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We present convergent close-coupling (CCC) calculations and measurements of 26.5 eV electron-impact excitation of the ground state of helium. The present measurements extend the experimental information at this energy to include 3^3D excitation. The CCC theory is compared with all of the available 2^1P,3^1P,3^1D,3^3D measurements, the agreement with which is very satisfactory and comparable to that at higher impact energies. [S1050-2947(97)06110-6]

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I. INTRODUCTION

The convergent close-coupling (CCC) method, introduced by Bray and Stelbovics [1], has recently been applied to inelastic scattering from the ground state of helium over an extensive energy range from 30 eV upwards by Fursa and Bray [2]. It was found that discrepancies between previous theories and experiment were primarily due to an inadequate treatment of the scattering aspects of the calculation. It was shown that the frozen-core treatment of the helium atom was sufficiently accurate, but that inclusion of the target continuum was essential in order to obtain agreement with experiment. These conclusions are applicable to the energy range studied, and were confirmed subsequently by the R matrix with pseudostates (RMPS) calculations of Bartschat *et al.* [3]. However, given that the frozen-core model yields an error in the ground-state energy of approximately 0.8 eV it is less clear that this conclusion will still hold at energies approaching excitation thresholds.

The purpose of the present paper is to present new measurements (3^3D excitation) and to thoroughly test the CCC theory against the full available set of experimental data, 2^1P,3^1P,3^1D,3^3D states, at an energy that is only a few eV above the excitation thresholds.

II. EXPERIMENT

The apparatus is of the crossed electron-atom beams type. A parallel beam of electrons (10^{-6} A; energy resolution, full width at half maximum, ≤ 0.5 eV) crosses a beam of helium atoms from a long narrow capillary. The intensity and focussing of the incident electron beam are continuously monitored by a Faraday cup. Scattered electrons emitted into a small solid angle in a certain direction are transported to the entrance of an electrostatic hemispherical analyzer. Those electrons that have excited the $n=3$ states of helium are transmitted by the analyzer and detected using a channel electron multiplier. The analyzer is rotatable about the collision center over a wide range of scattering angles. Photons emitted into a small solid angle perpendicular to the scattering plane formed by the incident and scattered electron momenta are collected by a plano-convex lens with its focus at the interaction region. The Stokes parameters, as defined by Andersen *et al.* [4], P_1 and P_2 are determined using a linear polarizer and the circular polarization P_3 by a linear polarizer–quarter-wave-plate combination. Following polarization analysis, the appropriate transition is selected using a narrow band interference filter. For the new 3^3D experimental data presented here, 587.5-nm photons are selected corresponding to the 3^3D-2^3P transition. The transmitted photons are detected using a fast linear focused photomultiplier tube.

Following amplification and discrimination, the electron pulses are fed to the start input of a time-to-amplitude converter (TAC) and the photon pulses to the stop input. The TAC output is fed to a PC based pulse height analyzer, the true coincidence signal being extracted from the resulting time spectrum. The Stokes parameter P_4 is determined using a similar linear polarization analyzer for photons emitted in the scattering plane, perpendicular to the incident electron beam direction.

A full schematic representation of the apparatus has been given recently [5]. Details of alignment of the polarization components and of data correction for the effect of finite solid angles of the photon detectors are given in [6]. It should also be noted that the 2^1P [7] and 3^1P [8] angular correlation data measured in this laboratory and compared with the CCC calculations here were obtained with an angular correlation version of this same apparatus [9].

III. THEORY

Details of the CCC theory for electron-impact excitation of helium have been given by Fursa and Bray [2]. A review of applications to scattering and ionization from the ground and metastable states has also been given [10]. Briefly, the three-electron total wave function is expanded in a set of explicitly antisymmetric (two-electron) target states. These states are obtained by diagonalizing the target Hamiltonian in a set of configurations constructed from an orthogonal Laguerre basis. In each of these configurations we restrict one of the electrons to be described by the He^+ $1s$ orbital. This is the frozen-core approximation. This approximation may be relaxed, as was the case for a more complicated

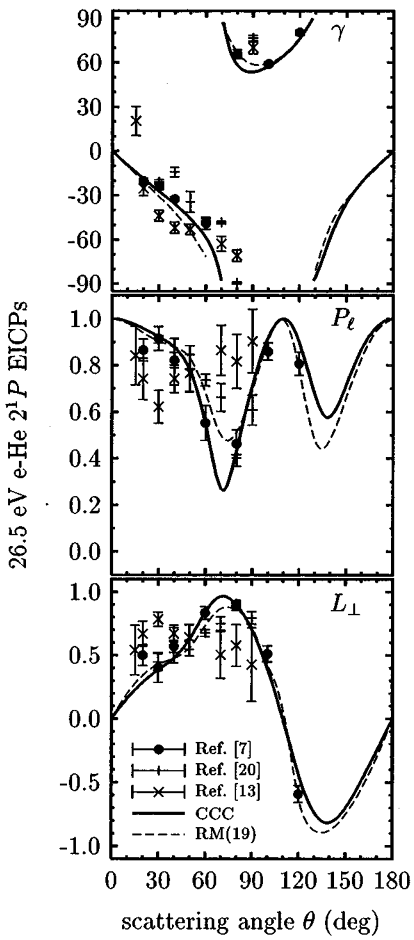

FIG. 1. Electron-impact coherence parameters for 2^1P excitation of the ground state of helium by 26.5-eV electrons. The present convergent close-coupling calculations are denoted by CCC. The 19-state R-matrix calculations are due to Fon *et al.* [21]. The measurements are from the stated references.

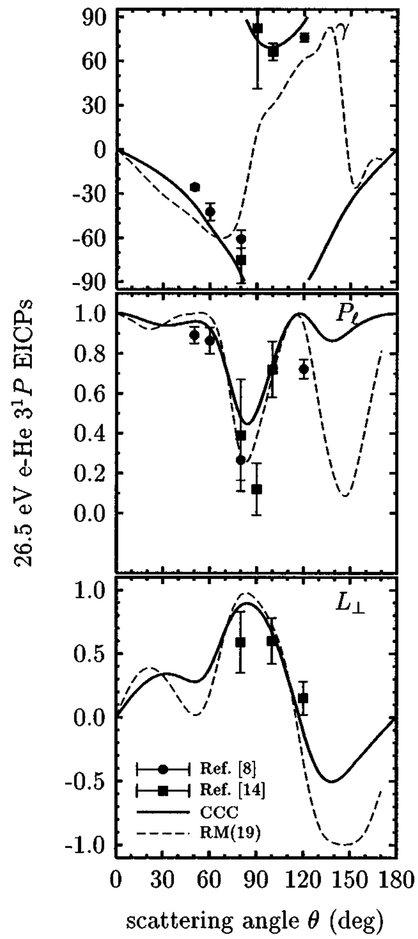

FIG. 2. As for previous caption, except for the 3^1P state.

target such as Be [11], but we keep it here for the sake of simplicity. The great strength of the frozen-core model is that convergence studies may be done as simply as in the case of quasi one-electron targets. Relaxing the frozen-core approximation results in too many states for present numerical implementation, requiring careful truncation.

In the present calculation a total of 89 states were used. These consist of 13 ^1S, 12 ^3S and $^{1,3}P$, 11 $^{1,3}D$, and 9 $^{1,3}F$ states. To reduce the problem of a 0.8 eV error in the ground state and therefore the total energy, we reduce the incident energy by 0.8 eV, thereby ensuring that the total energy is the same in both theory and experiment. This has the effect of having accurate outgoing electron energy.

IV. DISCUSSION

One of the great strengths of the close-coupling approaches is that a single calculation yields transition amplitudes between all of the states included in the expansion of the total wave function. So, for example, a CCC calculation at a total energy E may be simultaneously tested against available experiment for elastic, excitation, and ionization (total or fully differential) processes from the ground or any excited state. In practice it is rare to have such a diversity of measurements at the same total energy, but we suggest that new measurements should be performed at the same total energies as existing ones, whenever possible.

In the case of 26.5-eV excitation of the ground state of helium we have a number of measurements with which to compare the CCC calculation. We begin with 2^1P excitation, presented in Fig. 1. The data are presented in terms of the parameters γ and P_l describing the shape of the excited state and $L_\perp$, the expectation value of the angular momentum transfer [4]. There are three sets of measurements available, which show some discrepancy with each other. However, the present CCC calculation agrees very well with the 19-state R-matrix results and the data set due to Crowe and Nogueira [7]. It has previously been suggested [12] that the 27-eV data of Steph and Golden [13] may suffer from resonance radiation trapping effects.

Comparison of the CCC theory with the 19-state R-matrix calculations and angular [8] and polarization [14] correlation data for the 3^1P excitation is given in Fig. 2. Unlike in the 2^1P case there is now a substantial discrepancy between the CCC and R-matrix results. At intermediate angles, the measurements of γ support the CCC theory. The large discrepancies between the two theories for all parameters at back-

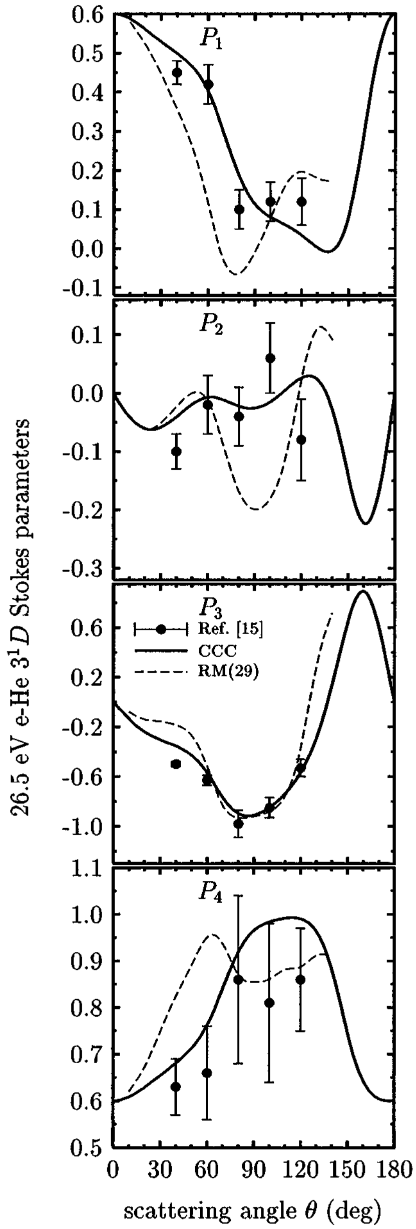

FIG. 3. Observed Stokes parameters for 3^1D excitation of the ground state of helium by 26.5-eV electrons. The 29-state R-matrix calculation is due to Ratnavelu *et al.* [16]. The measurements are due to McLaughlin *et al.* [15]. The present calculation is denoted by CCC.

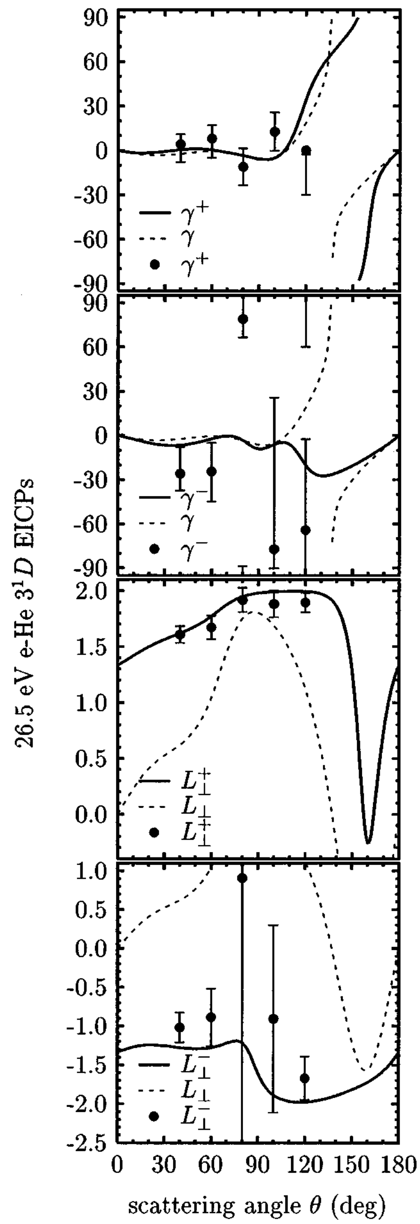

FIG. 4. The parameter set, as proposed by Andersen and Bartschat [18], for characterizing the 3^1D charge cloud after excitation by 26.5-eV electrons. The experimental values have been derived from the results presented in Ref. [15]. The theory is described in the text.

ward angles suggest that further measurements would be helpful to support one theory over the other. However, given the similar close-coupling foundation of the two theories we would argue that the CCC theory should be more accurate due to the bigger number of expansion states used. The difficulty of these experimental measurements compared with those for the 2^1P state should also be emphasized. The observed 3^1P-2^1S radiation accounts for only 2.5% of the 3^1P emission while the $3^1P/2^1P$ differential cross-section ratio is typically 1/3.

In Fig. 3 we compare the present CCC calculation for the excitation of the 3^1D state with the observed Stokes parameters measured by McLaughlin, Donnelly, and Crowe [15], and the corresponding 29-state R-matrix calculation of Ratnavelu, Fon, and Berrington [16]. Here we find agreement between the CCC theory and experiment to be satisfactory and a substantial improvement over the R-matrix calculation at the intermediate angles. Figure 3 is useful for comparison of theory with what is directly measured. The present D-state data may be expressed in terms of the parameters $(P_l, \gamma, L_\perp, \rho_{00})$ describing the shape and dynamics of the excited state [4]. However, these parameters do not provide a complete description [17] and Andersen and Bartschat [18] have very recently proposed an independent and complete

TABLE I. Measured Stokes parameters for the 3^3D state of helium excited by 26.5-eV electrons.

θ (deg)	P_1	P_2	P_3	P_4
40	0.18 ± 0.04	-0.06 ± 0.04	-0.20 ± 0.06	0.36 ± 0.05
60	0.24 ± 0.05	-0.07 ± 0.04	-0.22 ± 0.05	0.44 ± 0.05
80	0.21 ± 0.05	0.09 ± 0.04	-0.56 ± 0.05	0.41 ± 0.06
100	-0.05 ± 0.04	0.09 ± 0.04	-0.73 ± 0.07	0.42 ± 0.10
120	-0.09 ± 0.06	-0.11 ± 0.05	-0.31 ± 0.03	0.40 ± 0.07

TABLE II. The experimental coherence parameters, $\gamma,P_l,L_\perp,\rho_{00}$, for the 3^3D state of helium excited by 26.5-eV electrons.

θ (deg)	γ (deg)	P_l	$L_\perp$	ρ_{00}
40	-8.49 ± 6.25	0.35 ± 0.07	0.39 ± 0.11	0.14 ± 0.07
60	-8.53 ± 4.81	0.44 ± 0.08	0.45 ± 0.10	0.06 ± 0.07
80	10.94 ± 5.57	0.41 ± 0.08	1.12 ± 0.11	0.09 ± 0.09
100	60.91 ± 11.82	0.18 ± 0.07	1.53 ± 0.15	-0.04 ± 0.12
120	-64.67 ± 11.31	0.24 ± 0.09	0.66 ± 0.06	-0.04 ± 0.09

set $(\sigma,L_\perp^\pm,\gamma^\pm)$ of parameters for categorization of excitation of D states. These also have the advantage of providing internal checks on the consistency of the measurements, though unfortunately the error analysis for $\gamma^\pm$ is somewhat complicated. It should also be noted that two values, real and ghost [18], of both γ^+ and γ^-, are obtained from the experimental data. The real values are taken as those in agreement with the CCC results and, for clarity of presentation, only these values are shown in Figs. 4 and 6.

In Fig. 4 we give the $(L_\perp^\pm,\gamma^\pm)$ parameters. For comparison, theoretical γ and $L_\perp$ are also given. The curves are determined directly from the CCC complex scattering amplitudes. Details of the determination from the experimental $\gamma,P_l,L_\perp,\rho_{00}$ have been given by Fursa *et al.* [5]. The error bars have the usual meaning in the case of $L_\perp^\pm$. However, in the case of $\gamma^\pm$ we have used the error bars to indicate their possible range consistent with errors in the experimental data and internal consistency checks. The solid circle is then not necessarily in the middle of the error bar. A detailed discussion of the estimation of the errors in $\gamma^\pm$ is given in Ref. [5]. A number of observations can be made concerning these parameters. As would be expected from Fig. 3, there is again generally very good agreement between the CCC predictions and experiment. Theoretically $\gamma^+\approx\gamma^-\approx\gamma$, except at large angles. Other aspects of the data can be explained by consideration of the relative squares of the excitation amplitudes, in the natural frame of reference. McLaughlin *et al.* [15] show that for all measured scattering angles, a_{+2}^2 is dominant $(a_{+2}^2\geqslant 3a_{-2}^2)$ and $a_{-2}^2\approx a_0^2$. Hence $L_\perp^+$ values are close to their maximum value of $+2$ whereas $L_\perp^-$ values are closer to -2. This also accounts for the large experimental uncertainties in $L_\perp^-,\gamma^-$ compared with $L_\perp^+,\gamma^+$. An extreme example of this is the 80° data, which, within experimental error, are consistent with $a_{-2}^2=a_0^2=0$. Under these circumstances $L_\perp^-$ and γ^- are undefined.

To complete the picture at 26.5 eV we present new measurements of 3^3D excitation. The measured Stokes parameters P_1-P_4, the parameters $(\gamma,P_l,L_\perp,\rho_{00})$ and $(L_\perp^\pm,\gamma^\pm)$ are given in Tables I–III. The measured Stokes parameters have been corrected for fine-structure depolarization as discussed by Crowe *et al.* [19] before calculating the various parameters. Comparison of the measured Stokes parameters with the CCC results in Fig. 5 again shows good agreement. The $L_\perp^\pm,\gamma^\pm$ parameters are shown in Fig 6. Again $\gamma^+\approx\gamma^-\approx\gamma$ out to 100°. In this case the dominance of a_{+2}^2 over a_{-2}^2,a_0^2 is much less pronounced except at a scattering angle of 100° where, as a consequence, $L_\perp^-,\gamma^-$ are poorly defined by experiment.

V. CONCLUSIONS

We have applied the CCC theory to inelastic scattering from the ground state of helium at 26.5 eV, the lowest energy thus far. By comparison with existing 2^1P, 3^1P, and 3^1D data and the new 3^3D data we again find the same good agreement as previously observed at higher incident energies. This implies that the frozen-core model is sufficiently accurate.

It is likely that the frozen-core model works so well for helium because there are no two excited electron bound states and the energy difference between the ground and first excited states is so big. As a result for all incident energies above inelastic thresholds we can always ensure that the energy in the final channel corresponds accurately to experiment, with the resultant error in the incident projectile energy being of the order of a few percent.

Further physical insight is provided when the D-state measurements are presented in terms of the $(L_\perp^\pm,\gamma^\pm)$ parameters of Andersen and Bartschat [18]. However, problems are encountered in converting the measured Stokes parameters to

TABLE III. Experimental values of the parameters, $L_\perp^\pm,\gamma^\pm$, of Andersen and Bartschat [18] for the 3^3D of helium excited by 26.5-eV electrons. For $\gamma^\pm$ the values in brackets represent the limiting values consistent with the data.

θ (deg)	$L_\perp^+$	$L_\perp^-$	γ^+ (deg)	γ^- (deg)
40	1.69 ± 0.16	-1.54 ± 0.24	7.7 (22.5, −14.7)	−29.7(−2.2, −50.2)
60	1.88 ± 0.16	-1.81 ± 0.26	−8.5 (12.4, −13.3)	−8.5(−3.7, −34.8)
80	1.85 ± 0.15	-1.47 ± 0.55	10.9 (30.4, 5.4)	10.9 (16.5, −32.4)
100	2.06 ± 0.18	-2.47 ± 1.37	68.1 (72.7, 49.1)	−1.4(72.7, −40.9)
120	2.08 ± 0.19	-2.15 ± 0.37	−54.6(−33.8, −76.0)	−79.6(−53.4, 47.6)

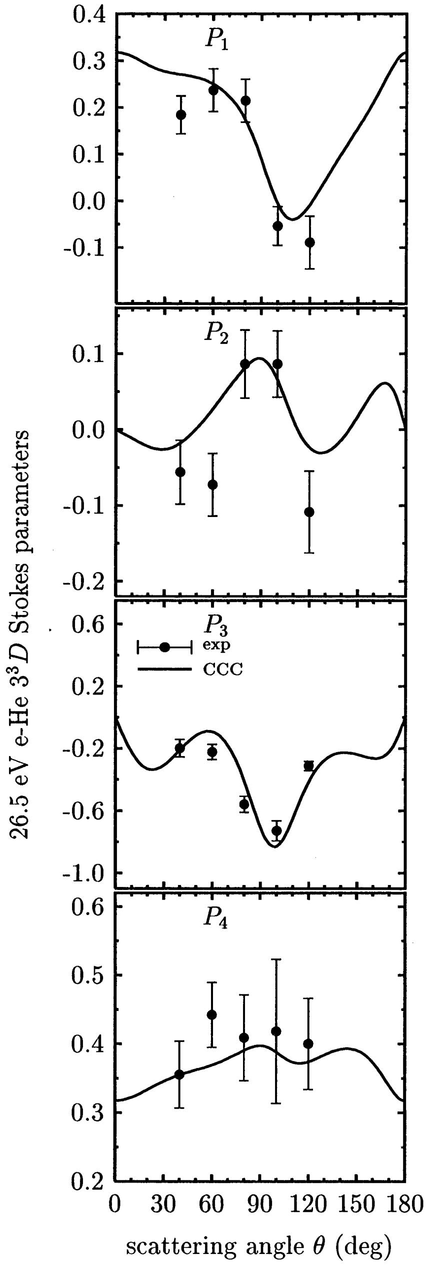

FIG. 5. Observed Stokes parameters for 3^3D excitation of the ground state of helium by 26.5-eV electrons. The present calculation and measurements are denoted by CCC and exp, respectively.

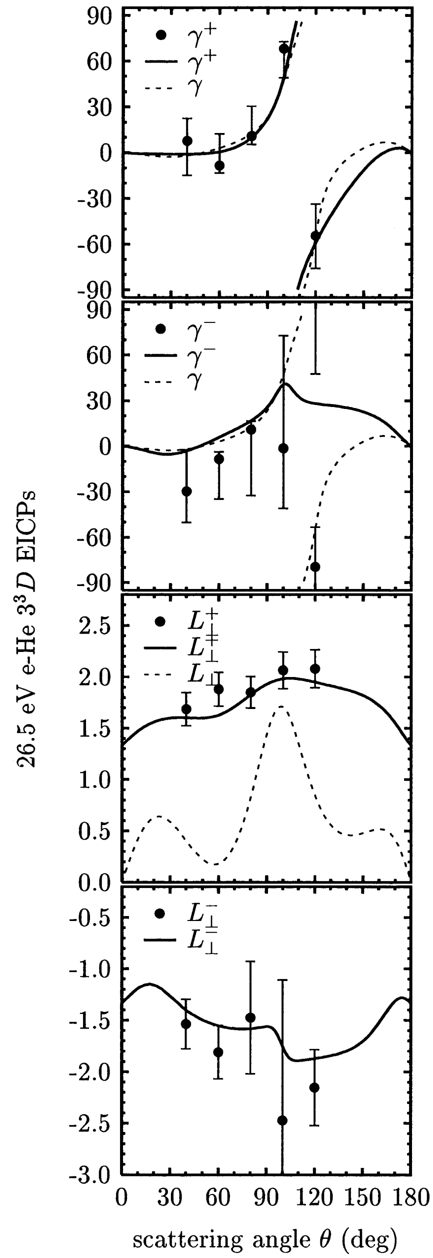

FIG. 6. The parameter set, as proposed by Andersen and Bartschat [18], for characterizing the 3^3D charge cloud after excitation by 26.5-eV electrons. Present theory and experiment are described in the text.

$L_\perp^-$, γ^- when the excitation is dominated by the $M=+2$ excitation in the natural frame. This is generally true at intermediate angles, especially for the 3^1D state. There is no problem at smaller scattering angles where the relative squares of the scattering amplitudes become similar ($a_{+2}^2=a_{-2}^2=0.375, a_0^2=0.25$) at 0°. At large scattering angles (>120°) theory predicts large variations in the $L_\perp^\pm$, $\gamma^\pm$ parameters. Experiments in this angular range would provide an even greater test of theory.

From the theoretical point of view we expect to relax the frozen-core approximation for helium, as has been done in the case of Be [11], in order to apply the CCC theory to electron-impact excitation plus ionization processes.

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