Charge transfer in positronium-proton collisions: Comparison of classical and quantum-mechanical theories

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Abstract

Charge transfer in positronium-proton collisions is calculated using the quantum-mechanical convergent close-coupling method and classical trajectory Monte-Carlo method. Previous calculations revealed that at low incident energy the cross section in both theories scales as $n_{\rm Ps}^2/E_{\rm Ps}$, where $n_{\rm Ps}$ and $E_{\rm Ps}$ are the principal quantum number and the center-of-mass energy of the incident positronium atom, respectively. However, the quantum cross section is systematically lower than classical one in absolute magnitude. To investigate the origin of this quantum suppression effect, we compare the charge transfer probabilities as functions of the impact parameter. We show that the quantum suppression in the cross section is mainly due to the low-impact parameter behavior of the probabilities governed by the quantum uncertainty principle.

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I. INTRODUCTION

Quantum-classical correspondence has been a fascinating and challenging topic since the early days of the quantum theory. It is particularly peculiar with regard to systems interacting by the Coulomb force. Although it is usually suggested that quasiclassical and semiclassical methods work better for highly excited states, the Bohr quantization rules give the exact spectrum for the hydrogenlike atom including its ground state. The Bohr-Heisenberg correspondence principle allows us to obtain exact formulas for spontaneous emission of the hydrogen atom [1], although their rigorous derivation requires not only quantum mechanics, but also quantum field theory. With regard to collisions of two charged particles, it is well known that the Rutherford formula for elastic scattering cross section is exactly the same in classical and quantum mechanics. When other processes, for example inelastic collisions and bremsstrahlung are considered, the classical domain corresponds to a large Coulomb parameter $e^2/\hbar v$ [2], that is, it corresponds to *low* velocities v, rather than to high velocities which would be expected from treatment of scattering by a short-range potential.

The dipole interaction decaying as $1/r^2$ with the distance is another interesting example. In both classical and quantum mechanics the integrated elastic cross section is divergent, and the differential cross section is inversely proportional to the collision energy [2, 3]. Although the spherically symmetric $1/r^2$ potential does not exist in nature, the $1/r^2$ dependence is relevant to scattering of a charged particle by a polar molecule and by a hydrogenlike atom. In the latter case the effective $1/r^2$ interaction appears due to the degeneracy of excited states belonging to manifolds with the fixed principal quantum number n [4, 5].

Of a special interest is the charge transfer in collisions of positronium (Ps) atoms with protons/antiprotons leading to formation of hydrogen/antihydrogen atoms

$$\mathrm{Ps}^* + p \to \mathrm{H}^* + e^+ \tag{1}$$

$$\mathrm{Ps}^* + \bar{p} \to \bar{\mathrm{H}}^* + e^- \tag{2}$$

where the asterisk labels excited states. The second process is of crucial importance for the physics of the antihydrogen creation [6–10]. Quantum calculations [11–14] of this process become extremely challenging with the growth of the principal quantum number n, and researchers have to turn to more feasible classical methods like Classical Trajectories Monte

Carlo (CTMC) calculations. Then the question arises: how much CTMC results can be trusted? It was suggested by Krasnicky et al [15, 16] that classical trajectory Monte Carlo (CTMC) calculations describe this process quite well, and indeed comparisons of CTMC and convergent close-coupling (CCC) results exhibit a remarkable agreement both in energy dependence of the cross sections and their absolute values if the Ps is initially in excited states. However, a substantial disagreement between classical and quantum results was found in l-mixing collision process [17], that is the process of changing of the Ps angular momentum due to collisions with protons. More recently we pointed out [18] that quantum results in the charge transfer process are lower than classical due to the special quantum-mechanical low-energy behavior of the partial cross sections. Specifically, it was shown that for a given collision energy the maximum angular momentum contributing to the charge transfer cross section depends linearly on n. As a result, at low energies the cross section for a fixed energy scales as n^2 rather than n^4 which would be expected from simple classical arguments. However, as Krasnicky *et al* [16] correctly pointed out, the classical cross section as a function of n and velocity v scales as

$$\sigma(n, v) = n^4 \sigma(1, nv).$$

(This classical scaling law was derived in 1966 by Abrines and Percival [19]). Therefore only in case when σ is independent of velocity, it scales as n^4. However, if it depends on velocity as $1/v^2$, we obtain n^2 law for a fixed v. Another important characteristic of collisions is the maximum value of the impact parameter contributing to the charge transfer, or the cut-off impact parameter. It was shown that the cut-off impact parameter in classical calculations is proportional to n/v [16], in accordance with the quantum-mechanical result [18].

Nevertheless, a thorough inspection of the results of Krasnicky et al [16] show a systematic disagreement between classical and quantum-mechanical values, the quantum-mechanical cross sections are almost always lower, sometimes by 50-60%, sometimes by a lower amount. It looks like quantum suppression does exist, but its nature is more subtle than suggested before. The physics analysis of the discrepancies between classical and quantum results is crucial for estimation of reliability of any future CTMC calculations of the charge transfer process. The present paper aims to investigate the origin of these discrepancies. We will be discussing cross section for the process (1), but the results apply, of course, to the process (2) as well due to the charge conjugation symmetry. Atomic units are used throughout the

paper unless stated otherwise.

II. DEPENDENCE ON THE IMPACT PARAMETER

The classical cross section for the charge transfer process is computed via the integral of the product of transition probability $P(b)$ and the impact parameter b, i.e., $2\pi bP(b)$ over a range of impact parameters. Since in collision problems quantum and classical mechanics usually disagree in a certain range of impact parameters, we want to investigate how $P(b)$ for the charge transfer process depends on the impact parameter b. While in CTMC method calculation of this quantity is straightforward, in quantum calculations we operate with the relative angular momentum rather than with the impact parameter. Moreover, in contrast to the impact parameter, it is a discrete quantity and it is not conserved during collisions. To get a rough idea about the quantum analog of the $P(b)$ function, we introduce the "quantum" impact parameter as

$$b = (L + \frac{1}{2})/k,$$

where k is the initial Ps momentum in a.u., and calculate $P(b)$ at discrete values of b corresponding to the relative angular momentum $L = 0, 1, 2, ...$ Alternatively, we can vary b continuously and calculate probabilities $P(L)$ corresponding to $L = \{bk - 1/2\}$, where $\{x\}$ is the integer closest to x. Quantum-mechanical probability is given by

$$P(b) = \frac{\sigma^L k^2}{\pi(2L+1)} = \frac{\sigma^L k}{2\pi b},$$

where σ^L is a partial cross section.

For detailed comparisons we have performed two types of calculations, one for $n_{\rm Ps} \to n_{\rm H}$ rates averaged over the initial angular momentum states of Ps and summed over final angular momentum states of H. This probability in quantum calculations is given by

$$P(k,b) = \frac{k}{2\pi n_{\rm Ps}^2 b} \sum_{l_{\rm Ps} l_{\rm H}} (2l_{\rm Ps}+1)\sigma^L_{l_{\rm H} l_{\rm Ps}}(k,b). \tag{3}$$

In the other set of calculations we choose a specific initial angular momentum $l_{\rm Ps}$ but sum over final $l_{\rm H}$. In both calculations we average over the orientation of the initial orbit and sum over all orientations of the final orbit. In quantum calculations this corresponds to averaging over initial magnetic quantum number and summing over final magnetic quantum number.

The description of CCC calculations are extensively described in refs. [11, 12]. For specific applications of the CCC theory to the problem of interest see [13, 14, 20]. In CTMC calculations we follow a methodology similar to that described in ref. [16] and use the microcanonical distribution [19, 21] for initial states. In brief, for a given principal quantum number, $n_{\rm Ps}$ of Ps atom, the following quantities for the relative motion of the electron and positron (elliptical orbits) can be obtained:

$$E_{\rm Ps} = -\frac{1}{4n_{\rm Ps}^2}, a = 2n_{\rm Ps}^2, e^2 = 1 - l_{\rm Ps}^2/n_{\rm Ps}^2, \tag{4}$$

where $E_{\rm Ps}$ is the binding energy of the Ps atom, a is the semi-major axis, e is the eccentricity of the ellipse and $l_{\rm Ps}$ is the magnitude of the orbital angular momentum. With these parameters, the equations for the elliptical orbit on the zx plane (z directed along the perihelion axis of the orbit) can be written as,

$$\begin{gathered} x = a\sqrt{1-e^2}\sin\xi,\ \ z = a(\cos\xi - e), \\ \dot{x} = \frac{l_{\rm Ps}\cos\xi}{n_{\rm Ps}^2(1-e\cos\xi)},\ \ \dot{z} = -\frac{\sin\xi}{n_{\rm Ps}(1-e\cos\xi)}, \end{gathered} \tag{5}$$

where ξ is the eccentric anomaly which is related to the mean anomaly ζ according to

$$\zeta = \xi - e\sin\xi \tag{6}$$

In the microcanonical distribution (fixed $n_{\rm Ps}$), we randomly select $e^2 \in [0,1]$ from a uniform distribution and identify the classical orbital angular momentum values $l_c = n_{\rm Ps}\sqrt{1-e^2}$ according to the criterion $l_{\rm Ps} < l_c \leq l_{\rm Ps}+1$. Note that classically $l_c \in (0, n_{\rm Ps})$ whereas in quantum mechanics $l_{\rm Ps} = 0, ..., n_{\rm Ps}-1$. Another random selection is done for the mean anomaly $\zeta \in [0, 2\pi]$ and Eq. (6) is then numerically solved for $\psi \in [0, 2\pi]$ in order to obtain the equations of motion (Eq. (5)). Next, we do successive Euler rotations about the fixed axes $z-y-z$ with angles $\phi \in [0,2\pi], \theta \in [0,\pi]$ and $\psi \in [0,2\pi]$, respectively. These angles are also obtained randomly with uniform distribution in their allowed ranges. Once the rotated coordinates and velocities are brought to the lab frame, they are used as initial conditions for the classical trajectories in CTMC calculations. In propagating the classical trajectories, we implement the regularization technique of the three-body problem as explained in [22]. For each impact parameter, about 5×10^4 trajectories are sampled from the initial microcanonical distribution. Each trajectory is then propagated until the positron reaches an asymptotic distance after a close encounter with the proton. At the

end of the integration, the energies of the relative motion of the $p-e$ and $e-e^+$ pairs are computed in order to determine the formation of $p-e$ bound system. The transition probability, P(b) is then computed as the ratio between the number of trajectories leading to a $p-e$ bound pair and the total number of trajectories propagated. Sample results for integrated cross sections agree very well with the results published in [16].

III. RESULTS AND DISCUSSION

Figure 1 shows the total and partial cross sections for hydrogen formation as a function of the incident positronium center-of-mass energy. Here we have presented the partial and summed cross sections for the Ps($n_{\rm Ps}=3$) $\rightarrow$ H($n_{\rm H}=4$) transitions. The summed cross sections obey the $n_{\rm Ps}^2/E_{\rm Ps}$ scaling investigated in detail in Ref. [18]. The quantum cross section always appears to be lower than the classical cross section for very low Ps incident energy. Similar behavior is observed also in the Ps($n_{\rm Ps}=4$) $\rightarrow$ H($n_{\rm H}=5$) transition as shown in Fig. 2. To understand the difference between the quantum and classical results, we explore the probabilities for the above two transitions as functions of the impact parameter. In Figs. 3 and 4 we present our results of calculations of the first type (average over initial Ps angular momentum states) for the $n_{\rm Ps}=3\rightarrow n_{\rm H}=4$ and $n_{\rm Ps}=4\rightarrow n_{\rm H}=5$ probabilities at two different energies. Irregularities in the CTMC probabilities are due to statistical uncertainties in the random selection of the parameters of the orbits, and irregularities in the quantum results are due to the discrete representation for the impact parameter $b=(L+\frac{1}{2})/k$. The alternative approach based on the equation $L=\{bk-1/2\}$ leads to sudden jumps in the probability dependence on b, and the corresponding results are not shown here. The general features of the partial and summed probabilities shown in Figs. 3 and 4 can be summarized as follows. At low impact parameters the classical probabilities always appear to be higher than the quantum results. At large impact parameters, the quantum probabilities in some cases show higher values compared to the classical results. Within an intermediate range of impact parameters, some agreement between the classical and quantum probabilities can be observed (see, for example, Fig. 3e).

The quantum suppression of the probability at lower impact parameters can be interpreted in terms of the uncertainty principle. Indeed, classical calculations at $b<2n_{Ps}^2$ involve hard head-on collisions between the electron and the proton which lead to formation

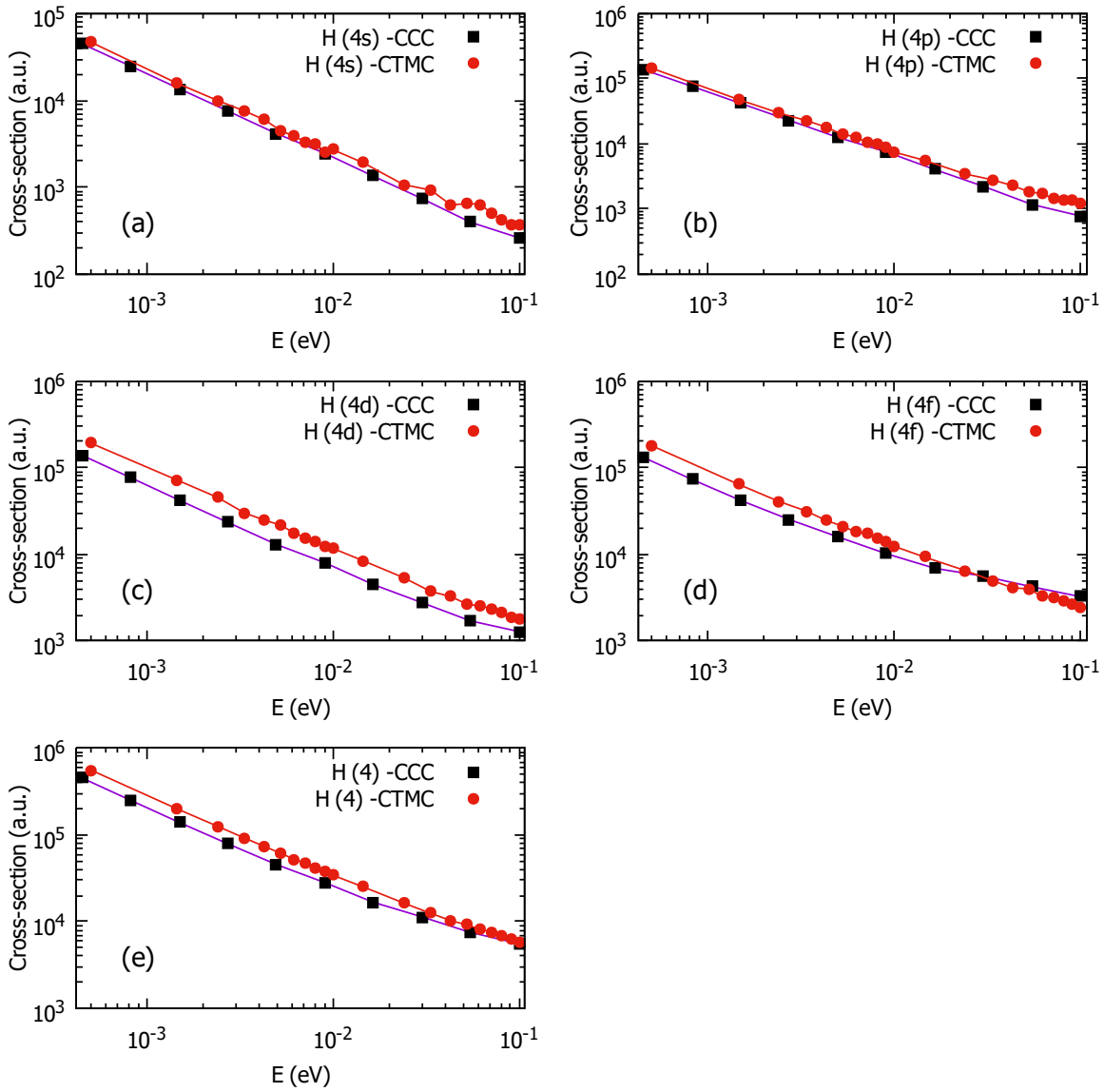

FIG. 1: Cross sections for hydrogen formation as a function of Ps center-of-mass energy. From panels (a)-(d), quantum and classical cross sections for $\mathrm{Ps}(n_{\mathrm{Ps}} = 3) \rightarrow \mathrm{H}(n_{\mathrm{H}} = 4, l_H = 0, 1, 2, 3)$ are presented. Panel (e) shows the summed cross section over the final angular momentum states. All cross sections are averaged over the initial angular momentum states.

of H with a large probability. Even when $b > 2n_{Ps}^2$, the Ps electron can have several close encounters with the proton before it lands on a bound orbit forming hydrogen. In contrast, in quantum calculations the uncertainty in the electron position prevents electron from approaching the proton. In some cases we observe quantum enhancement of the probabilities at large impact parameters which can be explained due to the quantum tunneling effects in

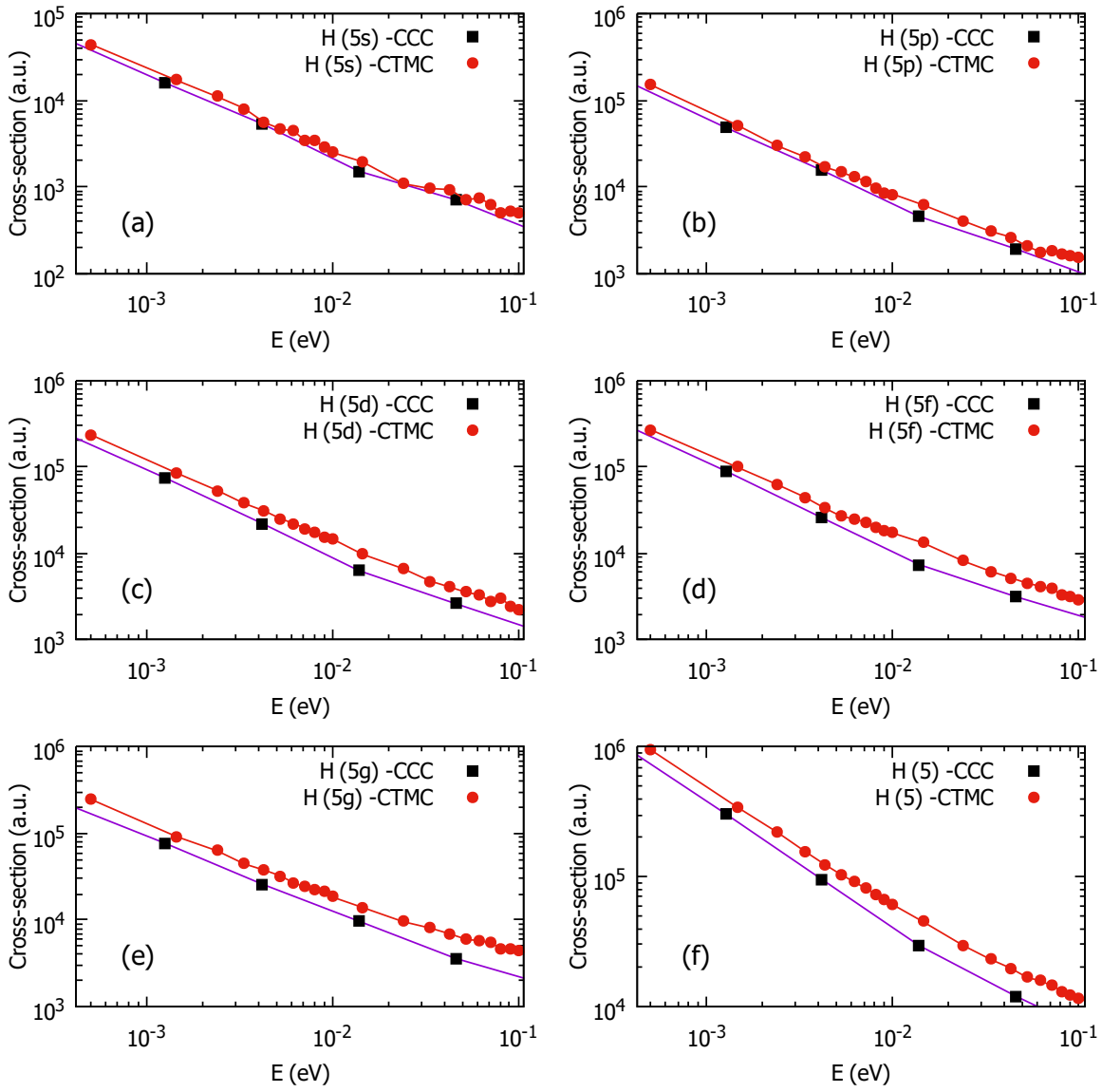

FIG. 2: Same as in Fig. 1, but for the Ps($n_{\rm Ps} = 4$) $\rightarrow$ H($n_{\rm H} = 5, l_H = 0, 1, 2, 3, 4$) transitions.

$1/r^2$ potential.

This argument is valid for any initial Ps angular momentum. To demonstrate this, in Fig. 5, we present calculations performed for specific initial angular momentum of Ps, $l_{\rm Ps} = 0, 1, 2, 3$ (calculations of type 2). The same trend is observed in these cases.

IV. CONCLUSIONS

With the help of CTMC simulations, we have computed the cross sections and probabilities for (anti)hydrogen formation in specific final states $n_{\rm H} = 4, 5$. Comparison between the

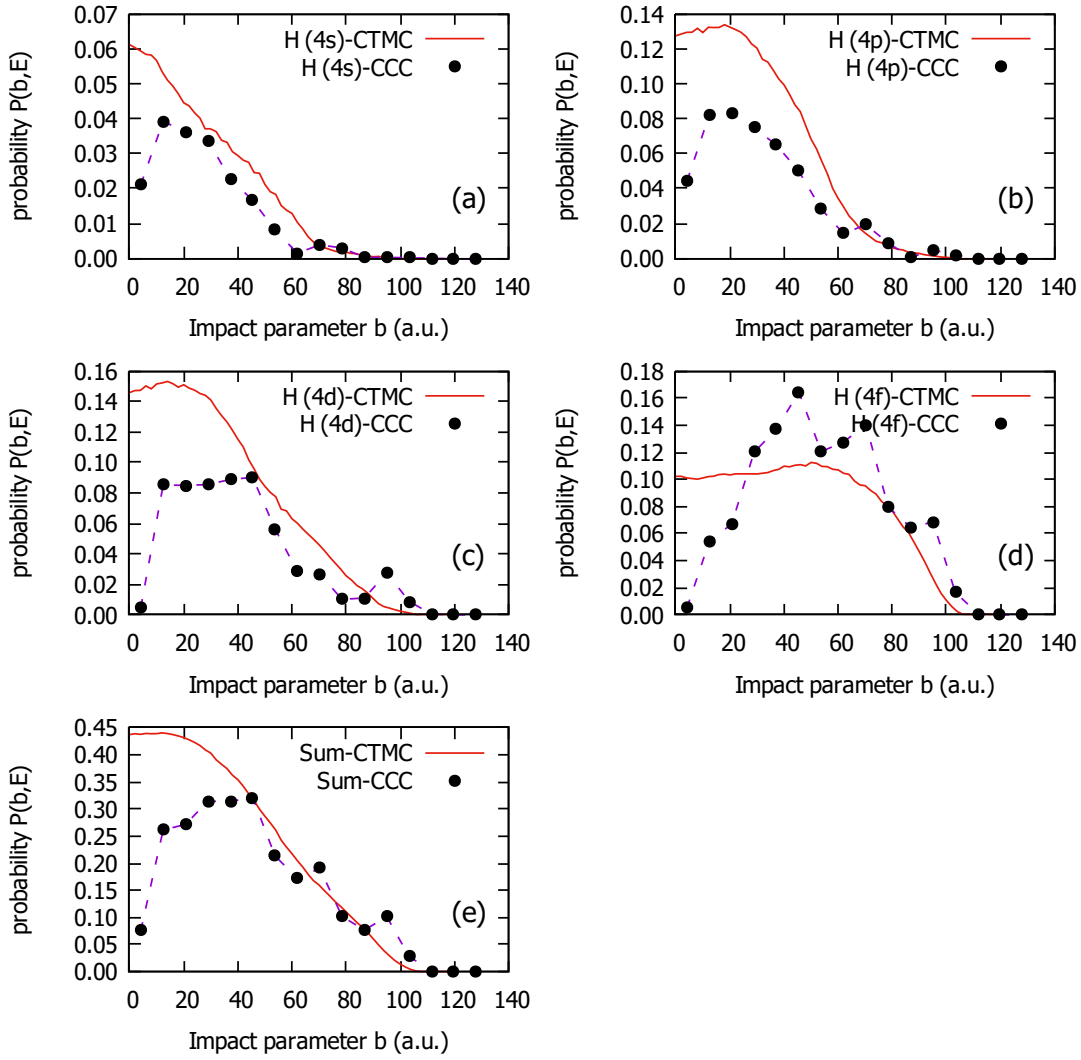

FIG. 3: Probabilities for the $n_{\rm Ps} = 3 \rightarrow n_{\rm H} = 4$ transition as a function of the impact parameter b at collision energy 0.099603 eV. Panels (a)-(d). Quantum (solid circles) and classical (red line) probabilities when the final hydrogen state is at $l_{\rm H} = 0, .., 3$. These probabilities are averaged over the initial angular momentum states of Ps. Panel (e). Probability summed over the final angular momentum of states of H.

CCC and CTMC cross sections reproduced the similar observation that were reported in [16]. In the present work, we analyzed the behavior of CTMC and quantum probabilities as functions of the impact parameters. The quantum suppression in the cross sections can be explained by the low-impact-parameter behavior of transition probabilities: in this region the quantum uncertainty principle prevents localization of electron near the proton site and suppresses the transition probability. Although at high impact parameters the quantum

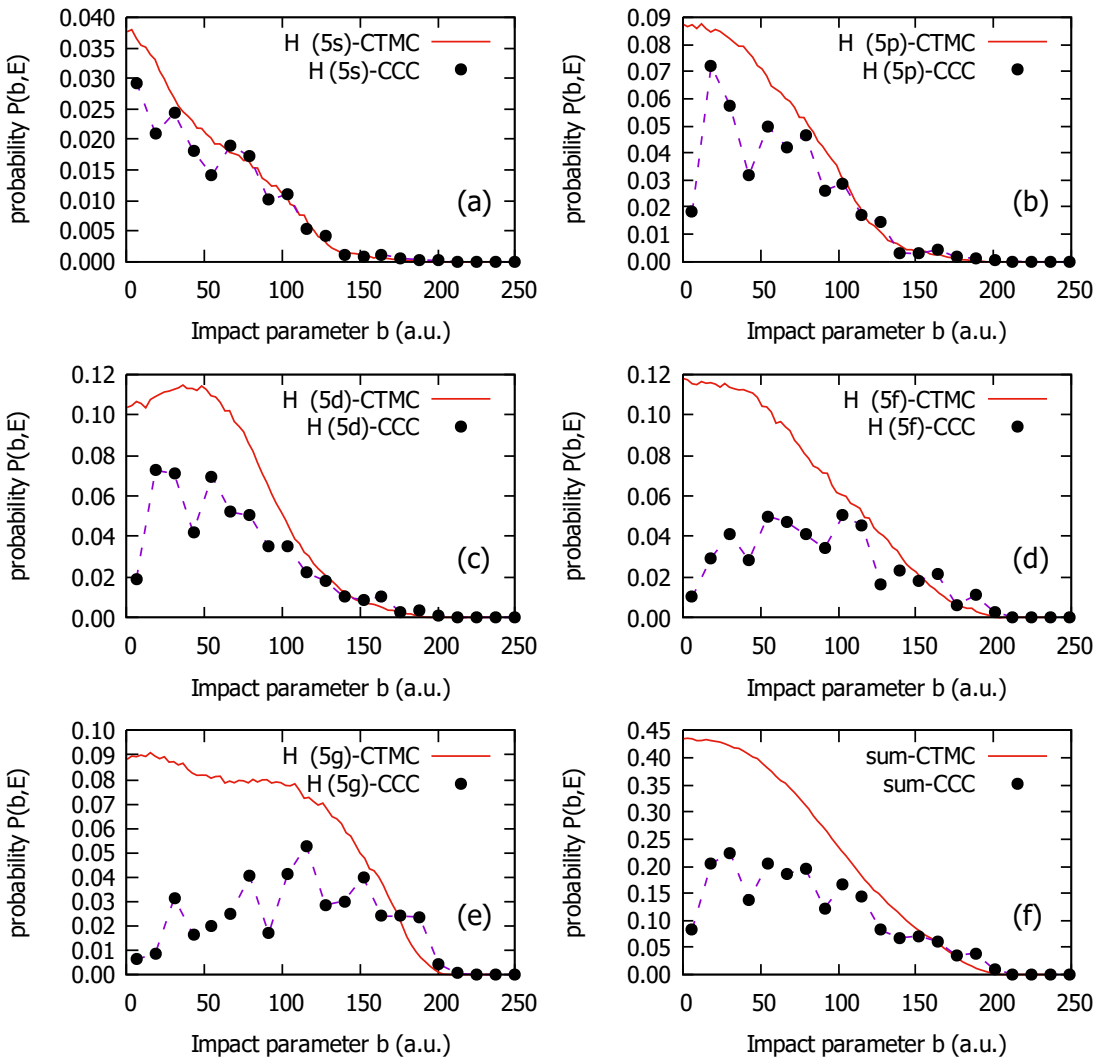

FIG. 4: The same as in Fig. 3, but now the probabilities are calculated for the $n_{\rm Ps} = 4 \to n_{\rm H} = 5$ transition at collision energy 0.046101 eV. The latter corresponds to the collision energy where the quantum cross section is lower than the CTMC results shown in Fig. 1.

transition probability is somewhat higher than classical due to the tunneling effect, the quantum integrated cross section is still lower than the classical one.

We conclude that $1/r^2$ potential presents the case where the difference between classical and quantum results is very subtle: although the energy dependence of both cross sections at low energies is similar, a certain discrepancy in magnitude is still observed. Another discrepancy might appear due to resonance scattering which is quantum-mechanical phenomenon observed below thresholds for excitation of Ps or hydrogen [23]. It is also apparent from the present analysis that a more substantial discrepancy would appear in angle-differential cross

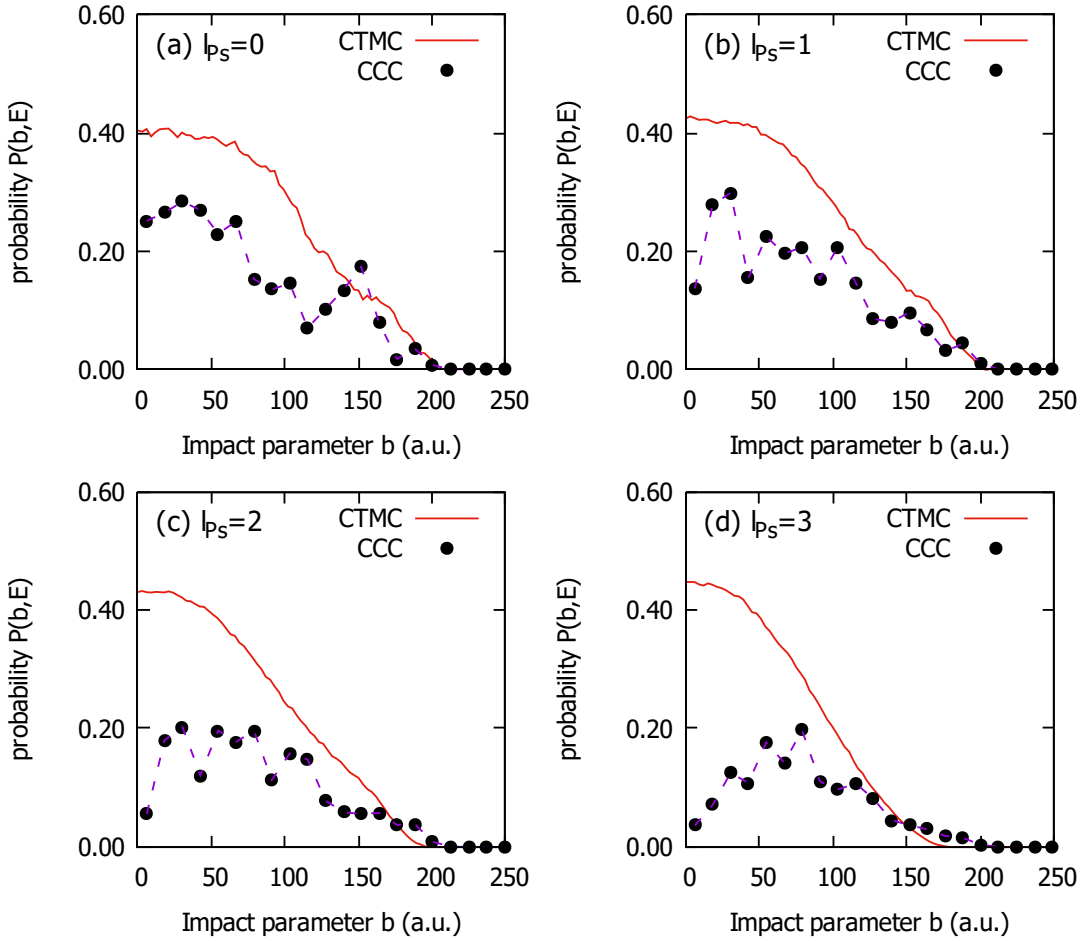

FIG. 5: Panels (a)-(d). Quantum (solid circles) and classical (red line) probabilities as functions of the impact parameter b for the $n_{\rm Ps} = 4(l_{\rm Ps} = 0, 1, 2, 3) \rightarrow n_{\rm H} = 5$ transitions. Ps collision energy at 0.046101 eV. Probabilities are summed over the final angular momentum states.

section. In particular the Gailitis-Damburg oscillations [4, 5], a pure quantum-mechanical phenomenon, although smeared out completely in the total charge transfer cross sections [23], might appear in an angle-differential cross section.

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