Electron-capture Process Induced by Bare Ion Impact on Biological Targets

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Abstract: Within the framework of independent electron approach, the prior form of boundary corrected continuum intermediate state (BCCIS) approximation is employed to calculate the cross sections for total single electron capture in collision of bare ions (H⁺, He²⁺ and Li³⁺) with biological molecules in the intermediate to high energy regimes. With a suitable choice of the distorting potential, the boundary condition is satisfied with a proper account of the intermediate continuum states. The cross sections have been calculated from 25 keV/amu to 10 MeV/amu. We have approximated the cross sections for molecular targets by the linear combination of atomic cross sections weighted by the effective occupation electron number. Furthermore, the multi-electronic problem is reduced to a mono-electronic one using a version of the independent electron approximation. A detailed analysis on the contributions from different molecular orbitals to total cross sections are reported. In the present investigation, we observe clearly the importance of the core contribution in the change of slope of the TCS curves. Moreover, analysis has been made on the cross section per target electron resulting in achievement of a 'universal' cross section. However, some negligible discrepancies are observed for the case of the CH₄ molecule. The present computed results in prior form of BCCIS method have been compared with the available theoretical and experimental results. We found that our computed results are in good agreement with the experimental findings.

Key words: Collision, capture, cross sections.

1. Introduction

Apart from their great importance in fundamental physics, atomic and molecular electron loss processes are of prime interest in diverse areas of science ranging from the effects of space radiation on astronauts (missions for the humour exploration of the solar system) to radiobiology, in particular for predicting the radio-induced damage at the sub-cellular scale [1]. We have gone through checking that ionization and capture cross sections of biological molecules are quite useful in medical studies, like radiobiology, medical imaging and radiotherapy [2]. Recently, it has been shown that experimental and theoretical data about the electron loss from biological systems were needed in fundamental studies of charged particle interaction in biological material (and more precisely in heavy-ion cancer therapy [3]), where water is a common modulator. Under these conditions, it appears crucial to process accurate differential and total cross sections (both ionization and capture) for light and heavy ions. Since the mid-1990s, the Cold Target Recoil Ion Momentum Spectroscopy (COLTRIMS) [4-6] technique has provided a kinematically complete insight on collision processes involving photons, ions and electrons. Different theoretical studies such as the classical trajectory Monte-Carlo (CTMC) method [7-10], the first order Coulomb Born approximation (CB1) [11-14] and continuum distorted wave-Eikonal initial state (CDW-EIS) [15-19] have been developed to study the electron loss by a fast-bare ion in biological molecule. Two main processes which contribute to the single electron loss from atomic/molecular targets are the electron capture and the electron ionization dominating at low and high impact velocities,
respectively. In this paper, studies have been made on the single-electron capture from biological molecules by fast bare ions in the energy range of 25-10,000 keV/amu using the boundary corrected continuum intermediate state approximation (BCCIS) [20-22].

The biological molecule (H₂O) has been used to study a number of recent cross section measurements for processes initiated by light particles [23, 24] and heavy particle impact [25] widely. Most of the works are featured with the electron impact ionization of molecules whereas heavy particle ion impact experiments are very rare in number. In 1968, Toburen, L. H., et al. [26] measured the total electron capture cross sections and electron loss cross sections for proton-molecule collisions over the energy ranging from 10 to 2,500 keV/amu. Two papers on the electron capture cross sections for proton [27] and α-particle [28] impact on biological molecules have been published by Rudd et al. In 1986, Bolorizadeh, M. A., and Rudd, M. E. reported differential ionization cross sections due to impact of electron [29], proton [30] and neutral hydrogen atom on H₂O [31]. Later, Gobet, F., et al. [32] reported the partial and total absolute cross sections for direct ionization and electron capture processes initiated by proton impact with water at 20-150 keV. In 2007, similar experiment [33] of ionization and capture processes appeared in the study of ion-molecule collision. The detailed cross sections of the dissociation paths along which that water undergoes electron capture and ionization by fast protons, also electron capture, ionization and projectile electron loss by fast hydrogen projectiles have been provided by them.

Theoretical calculations of single-electron capture where fast proton beams impact simple biological molecular targets (CH₄, N₂, CO and CO₂) is performed by Galassi, M. E., et al. [34] using the most successful model called CDW-EIS approximation that was first introduced by Crothers, D. S. F., and McCann, J. F. [35] to study the single ionization of hydrogen atom by bare ion impact. In this work, the influence of the molecular targets on total cross sections (TCS) has been analysed and very good agreement has been found between the theory and the corresponding existing measurements.

Later Champion and his group employed the first order Born approximation (FBA) [36] for ionization process and the CDW-EIS [37] for electron capture process to calculate the cross sections of large bio-molecules (DNA/RNA nucleobase) impacted by bare ions. Differences have been observed in TCS with existing experimental data at low impact energies (E ≤ 100 keV/amu). The ionization cross sections for protons colliding with RNA-uracil target using two theoretical models have been calculated by Champion, C., et al. [38]. These models are the 1st Born approximation with correct boundary conditions (CB1) and the CDW-EIS model. The CB1 describes the active electron as being in bound and continuum states of the target field in the entrance and exit-channel respectively, whereas in the CDW-EIS approximation, a complete representation of the active electron is introduced by considering its evolvement in simultaneous presence of the projectile and target fields in the entrance as well as exit channels. A clear theoretical overestimation of the measurements for ejection energies lower than 10 eV have been found. A similar theoretical method called distorted wave model [39] has been employed to investigate the single electron ionization as well as the single electron capture process impacted by bare ions on biological molecules like water and adenine. It is determined that tightly bound electrons are more preferable to be captured at high enough impact energies. Champion, C., and his group [40, 41] have proposed a series of quantum-mechanical models based on the first-Born approximation with correct boundary conditions (CB1) and the CDW-EIS methodology to describe the ionization and capture from water due to proton impact. Briefly, the CB1 model describes the active (ejected) electron as being in bound and continuum states of the target field in the entrance and exit
Electron-capture Process Induced by Bare Ion Impact on Biological Targets

channels, respectively, whereas the CDW-EIS description gives a more complete representation of the active electron, considering that it moves under two-centre effect (simultaneous presence of both projectile and target fields). In 2017, calculations on single ionization and capture cross sections from biological molecules; water and DNA nucleobases by H⁺, He²⁺ and C⁶⁺ impact have been reported by Quinto et al [42] within the CDW-EIS approximation and compared to the existing experimental data. In this investigation, the initial wavefunction of the active bound electron to a particular molecular orbital (MO) was described employing a complete neglect of differential overlap (CNDO) approximation originally introduced by Pople, J. A., and his group [43-45]. Even more recently, Quinto, M. A., et al. [46] calculated the electron capture cross sections from molecular targets impacted by bare ions—H⁺, He²⁺, Li³⁺ and C⁶⁺ in the framework of the quantum-mechanical CDW-EIS approximation within energy range of 50-20,000 keV/amu. A detailed analysis on the contributions coming from different molecular orbitals to TCS have been analysed. Resulting in finding the computed results in satisfactory agreement with the experimental data. Success of the BCCIS approximation [20-22, 47-49], motivated us to study the single-charge transfer cross sections from molecular targets N₂, O₂, CH₄, CO, CO₂ and H₂O interacting H⁺, He²⁺ and Li³⁺ ion beams with energies ranging from 25 to 10,000 keV/amu. The results are thoroughly compared with the existing experimental and other theoretical data.

The organization of the paper is as per following. The theoretical model is briefly described in Section 2. Our results and discussion are presented in Section 3. Finally, conclusions are given in Section 4. Atomic units have been used throughout the work.

2. Theory

Single-electron capture from molecules of biological interest by the impact of bare projectile ions (H⁺, He²⁺ and Li³⁺) may be written as Eq. (1).

\[ P^{q+} + M \rightarrow P^{(q-1)+} + M^{+} \]  

(1)

where P and M represent the projectile ion and the target molecule respectively. Let us consider an incident bare nucleus of nuclear charge Ze impacting on the molecules (M) with a velocity \( v_i \) and as a result of the collision, one or more than one electron is removed from the target. The impact energies considered here are high enough, so that vibrational and rotational time of the molecules are much larger than the characteristic time of the collision. We have been quite capable to assume that the molecules remain fixed in their initial positions during the reaction. In this work, we focus our attention on the single electron capture reaction, where only one electron is transferred from the molecular target to the projectile. This process is described within the framework of an independent electron model (IEM) approach considering the passive electrons in the target as frozen in their initial molecular orbital (MOs). This assumption bears justification in case of high impact energy values. Thus, the multi-electronic problem is reduced to a mono-electronic one involving three effective bodies, namely the projectile, the active electron and the residual target. Let \( \vec{r}_e, \vec{r}_p \) be the position vector of the electron relative to the target and projectile respectively. Furthermore, \( \vec{R} \) denotes the position vector of the passing projectile of charge \( Z_P \) and mass \( M_P \) with respect to the target centre. \( \vec{r}_i \) and \( \vec{r}_f \) are the position vector of P and T relative to the centre of mass of \( (T, e) \) and \( (P, e) \), respectively. Different initial ground states of the molecular orbitals are assumed to be described by linear combination of their atomic orbitals (LACOs) employing a complete neglect of differential overlap (CNDO) approximation for the effective occupation electron analysis of the different molecular orbitals [50]. For each MO, the TCS is seen as a LCAO weighted by the effective occupation electron number (\( \xi_0 \)). Thus, we may express TCS for electron capture [37] as Eq. (2).
where $N_j$ is the total number of atomic components of the $j$th-MO and $\sigma_{at,j}$ refers to the corresponding atomic orbital cross sections involved in the present LCAO description. However, the different ground state atomic orbitals are described using Roothan-Hartree-Fock atomic wavefunction [51]. The prior form of the transition matrix element is Eq. (3).

$$\psi_f^{BCCIS(-)} = Ne^{ik_f \cdot \bar{r}_f} \psi_i \left\{ -i \alpha_i; 1; -i \left( \bar{v}_f \bar{r}_f + v_f r_f \right) \right\} F_1 \left\{ i \alpha_2; 1; -i \left( \bar{k} \cdot \bar{r}_i + k_j r_j \right) \right\}$$

Finally, the transition amplitude can be written as Eq. (6).

$$T_f^{(-)} = N \left\{ \int d\bar{r}_f d\bar{r}_i e^{ik_f \cdot \bar{r}_i - ik_j \cdot \bar{r}_f} \phi_i^* (\bar{r}_p) \left( \frac{Z_p Z_i^{eff}}{R} - \frac{Z_p}{r_p} \right) F_1 \left\{ i \alpha_2; 1; i \left( \bar{v}_f \bar{r}_f + v_f r_f \right) \right\} \times \right\} \phi_i (\bar{r}_f)$$

Here the six-dimensional integral may be reduced to a one-dimensional integral of Leis with infinity as upper limit in compact form following an earlier investigation [45] by our group. Finally, atomic cross sections are obtained on integration over projectile scattering angular domain. These integrals are performed numerically in a 36-point and a 46-point Gauss Legendre quadrature method with an accuracy of 0.1%.

3. Results and Discussion

We have calculated the single-electron capture cross sections for collisions of $H^+$, $He^{2+}$ and $Li^{3+}$ with biological molecules (CH$_4$, N$_2$, O$_2$, H$_2$O, CO and CO$_2$) using prior form of BCCIS approximation in the energy range of 25-10,000 keV/amu. The variation of TCSs with impact energy of the projectile ion is reported in the graphical form in Figs. 1-6, respectively. In these figures, we have also shown detailed contributions coming from different molecular orbits to the TCS. In addition, we studied the dependence of TCS for single electron capture normalized by the total number of electrons of each molecule which is shown in Figs. 7 (a-c) for different bare-ion impacts ($H^+$, $He^{2+}$ and $Li^{3+}$). Exact numerical data for all cases may be obtained on request. In Figs. 1(a-c), we have displayed the calculated total single-electron capture cross sections for the collision of $H^+$, $He^{2+}$ and $Li^{3+}$ with nitrogen molecules as a function of incident projectile energy from 25 to 10,000 keV/amu. We have compared our computed results with the measurements of Toburen, L. H., et al. [26] (solid circle), Rudd, M. E., et al. [27] (open circle), Barnett, C., et al. [53] (solid square), Welsh, L. M., et al. [54] (solid triangle), Rudd, M. E., et al. [28] (solid circle for $He^{2+}$), Nikolaev, V. S., et al. [55] (solid square for $Li^{3+}$) and the theoretical results of Quinto, M. A., et al. [46] (red dotted curve) obtained by CDW-EIS approximation. The present results have overall good accordance with the experimental results [26-28, 53-55]. In Fig. 1(a) (for
Fig. 1  Total cross sections (in $10^{-16}$ cm$^2$) as a function of the incident energy $E$ (keV/amu) for three different projectiles impact (a) H$^+$, (b) He$^{2+}$ and (c) Li$^{3+}$, respectively with N$_2$ molecule (Theory: solid curve, present BCCIS results; dashed curve for N1s; dotted curve for $\sigma_{2s}$; dash-dotted for $\sigma_{2s}$; dash-dot-dotted curve for $\pi_{2p}$; short dashed curve for $\pi_{2p}$; red dotted curve, CDW-EIS [40]. Experiments: solid circle, Toburen, L. H., et al. [26]; open circle, Rudd, M. E., et al. [27]; solid square, Barnett, C., et al. [53]; solid triangle, Welsh, L. M., et al. [54]. For He$^{2+}$: solid circle, Rudd, M. E., et al. [28]. For Li$^{3+}$: solid square, Nikolaev, V. S., et al. [55]).
‘H’- N² collision’), the present BCCIS results agree well with the form of CDW-EIS results of Quinto, M. A., et al. [46] (red dotted curve) except in the energy range between 100 keV/amu and 1,000 keV/amu. In the prior version of CDW-EIS approximation [46], the target electron is distorted by the incoming projectile which was incorporated in the initial channel by an eikonal phase depending on $\vec{r}_p$. This is absent in the present BCCIS approximation. Both approximations (CDW-EIS [46] and BCCIS) are same except the Coulomb distortion between the projectile and the residual target which is present in the BCCIS model while considered in the final channel. We also note that, as the impact energy is increased, the two-quantum mechanical theoretical results merge for incident energy values larger than 1 MeV for H⁺ impact, but in case of He²⁺ and Li³⁺ impact, the present result deviates from the CDW-EIS results. It is also observed that at extremely low energy regime (below 50 keV/amu), our results overestimate the experimental results of Barnett, C., et al. [53] (solid square) only at about 30-50%. It is well known that the charge exchange is a momentum transfer reaction. So, for atomic targets, this process is preferable as the collision velocities close to the mean orbital velocities of the active electron. At high collision energy regimes charge transfer occurs from the inner orbitals, which corresponds to K-shell of the atomic components of the molecules which is shown in the Figs. 1(a-c) (dashed curve for N1s core orbital). The electron configuration of the ground state N₂ molecule is $(\sigma_g^2\sigma_u^2\pi_u^2\sigma_g^2\pi_g^2)^2$. The population and binding energy corresponding to each molecular orbital are taken from Ref. [46]. In Figs. 1, it should be noted that the π₂p (dash-dot-dotted curve) and σ₂p (short dashed curve) orbitals (binding energies -0.62 a.u. and -0.52 a.u. respectively), present N 2p character which contribute in a similar way over all the collision energy range differing only by a factor of 2 due to difference of occupation number independent of the projectile. But the σ₂s (dash-dotted curve) orbital (binding energy -0.68 a.u.), which presents a N 2s character contributes less to the TCS in the whole energy range when the charge state of the projectile increases. Furthermore, it is evident from Figs. 1(a-c) that the crossing over point of the contributions from the most bound orbital and other less bound orbitals shifts towards higher projectile energy as the projectile charge state decreases. This anomaly is observed in contrast to the CDW-EIS results [40]. It is also observed that the CDW-EIS results (red dotted curve) of Quinto et al all [46] overestimate the
Fig. 3  Total cross sections (in 10^{-16} cm²) as a function of the incident energy E (keV/amu) for three different projectiles impact (a) H⁺, (b) He²⁺ and (c) Li³⁺ respectively, with H₂O molecule (Theory: solid curve, present results (Total); dashed curve for 1A1; dotted curve for 2A1; dash-dotted curve for 1B2; dash-dot-dotted curve for 3A1; short dashed curve for 1B1; red dotted curve, CDW-EIS [40]. Experiments: filled circle, results of Toburen, L. H., et al. [26]; filled triangle, results of Gobet, F., et al. [32]; filled square, results of Barnett, C., et al. [53]. For He²⁺: filled circle, results of Rudd, M. E., et al. [28]. For Li³⁺: filled square, results of Luna, H., et al. [33]).
Electron-capture Process Induced by Bare Ion Impact on Biological Targets

Fig. 4  Total cross sections (in $10^{-16}$ cm$^2$) for single electron capture of CH$_4$ by H$^+$ and He$^{2+}$ impact as a function of incident projectile energy (Theory: solid curve, present BCCIS results; dashed curve for C1s; dotted curve for 2a1; dash-dotted curve for 1t2; red dotted curve for CDW-EIS [40]. Experiments: filled triangle, results of Toburen, L. H., et al. [26]; filled square, results of Rudd, M. E., et al. [27]; filled circle, Barnett, C., et al. [53]. For He$^{2+}$: filled square, results Rudd, M. E., et al. [28]).

Experimental results as well as present theoretical results in the whole energy regime for He$^{2+}$ (in Fig. 1(b)) and Li$^{3+}$ (in Fig. 1(c)) impact. Due to non-availability of experimental data for He$^{2+}$ and Li$^{3+}$ impact, we have only plotted the TCS as a function of projectile energy for p - O$_2$ collision (shown in Fig. 2) and compared with the experimental results of Barnett, C., et al. [53] (filled square) and Toburen, L. H., et al. [26] (filled circle). We find that the TCS results are in good agreement with the measurements [26, 53] within 30% in the energy range between 100 and 10,000 keV/amu. Oxygen molecule presents the following electronic configuration in the ground state: $(\sigma_u^4(\sigma_g^2\sigma_u^2)^2(\pi_u^2\sigma_g^2)^2)^4$. As the lower projectile energy is considered, the preference for electron capture is ordered according to ascending order of the initial orbital binding energy. Lesser the binding energy of the electron, greater is the probability of capture which is already shown for N$_2$ molecules (Figs.1 (a-c)). Henceforth the contribution...
Electron-capture Process Induced by Bare Ion Impact on Biological Targets

Fig. 5  Total cross sections (in $10^{-16}$ cm$^2$) for single electron capture of CO by H$^+$ impact as a function of incident projectile energy (Theory: solid curve, present results; dashed curve for O1s; dotted curve for C1s; dash-dotted curve for 1$\sigma$; dash-dot-dotted curve for 2$\sigma$; short-dashed curve for 1$\pi$; short dotted curve for 3$\sigma$; red dotted curve for CDW-EIS [40]. Experiments: filled triangle, results of Toburen, L. H., et al. [26]; filled square, results of Rudd, M. E., et al. [27]; filled circle, Barnett, C., et al. [53]).

Fig. 6  Total cross sections (in $10^{-16}$ cm$^2$) for single electron capture of CO$_2$ by H$^+$ impact as a function of incident projectile energy (Theory: solid curve, present results; dashed curve for O1s; dotted curve for C1s; dash-dotted curve for 3$\sigma$; dash-dot-dotted curve for 2$\sigma$; short-dashed curve for 4$\sigma$; short dotted curve for 3$\pi$; dash-dot-dotted curve for 1$\pi$; red dotted curve for CDW-EIS [40]. Experiment: filled triangle, results of Toburen, L. H., et al. [26]; filled square, results of Rudd, M. E., et al. [27]; filled circle, Barnett, C., et al. [47]).

of the outer orbital $\pi_u 2p$ (dash-dot-dotted curve) dominates the TCS. One may attribute to the fact that its occupation number is 4 whereas other outer orbitals ($\pi_g 2p$ and $\sigma_g 2p$) are occupied only by two electrons. Similar conclusions can be drawn from the Figs. 3 for H$_2$O molecule where the present quantum mechanical BCCIS cross sections are compared to the CDW-EIS [46] (red-dotted curve) as well as the available experimental data [26, 28, 32-33, 53]. BCCIS gives TCS values close to those measurement [26, 32, 53] at intermediate energy range (below 300 keV) for H$^+$ impact. Moreover, the BCCIS results
Fig. 7  Normalized (per target electron) total cross sections for electron capture as a function of incident projectile energies of (a) H⁺, (b) He²⁺ and (c) Li³⁺ respectively (Theory: present BCCIS results; solid curve, CH₄; red dashed curve, H₂O; dotted green curve, CO; blue dash-dotted curve, CO₂; cyan dash-dot-dotted curve, N₂; violet short dashed curve, O₂).
Electron-capture Process Induced by Bare Ion Impact on Biological Targets

have excellent similarity with the measurement of Luna, H., et al. [33] (filled square) for \( Li^{3+} \) impact although overestimating the results of Rudd, M. E., et al. [28] (filled circle) for \( He^{2+} \) impact. It is pleasing to note from Fig. 3(b) that the CDW-EIS and the present BCCIS give cross sections are very close to each other over the whole incident energy range. In Figs. 4(a-b), the case corresponds to the \( CH_4 \) molecule having the following electronic configuration in the ground state: \((C1s)^2(2a_1)^2(1t_2)^6\). Among three molecular orbitals, the effect of dominance of TCS comes about for less (more) bound orbitals at intermediate-low(high) impact energies which is put as evidence. A good agreement with experimental data for proton (except below 200 keV/amu) and alpha particle impact is found. Again, we see that the core contribution dominates over other less bound orbitals at higher projectile energy as the projectile charge state decreases. For example, it is 600 keV/amu for \( H^+ \) and 150 keV/amu for \( He^{2+} \) impact. In Figs. 5 and 6, we have shown the electron capture as a function of impact energy for the collision of \( CO \) and \( CO_2 \) molecules by \( H^+ \). Here \( CO \) in the ground state, having four core electrons \([O1s, C(1s)]\) and another ten electrons are distributed in four molecular orbitals \((1\sigma)^2(2\sigma)^2(1\pi)^4(3\sigma)^2\), whereas for \( CO_2 \) molecule has six core electrons and sixteen electrons distributed in six molecular orbitals when ground state is taken care. Again, we see that the core contribution does not bear importance up to the mark for TCS at intermediate energy regime. The Fig. 6 adheres that the calculations carried out with the molecular method have excellent agreement with the experimental data at intermediate and high energy values. It is well-known that for electron capture from atomic targets, total cross section is dominated when the projectile momentum approaches the electron orbital momenta. Therefore, the reaction is likely to occur in ascending order from outer orbitals to inner ones as the collision energy increases. For the present molecular case, we observe the same behaviour. The core capture predominates the TCS at enough high impact velocities. Figs. 7(a-c) show that the normalized (per target electron) total cross sections for electron capture as a function of projectile energy for different bare ion impact (\( H^+, He^{2+} \) and \( Li^{3+} \)). A ‘universal’ cross section is obtained. This behaviour was already reported by Champion and co-workers for the case of both ionization and electron capture processes in collision of proton impact with DNA nucleobases and water vapour [56]. We found close agreement for all the target molecules except \( CH_4 \). For \( H^+ \) impact, the normalized TCS for all the molecules are in close proximity in the wide range of projectile energy, whereas for \( He^{2+} \) and \( Li^{3+} \) impact, we see nature of that the total cross sections are evidently depending upon the nature of molecules as the collision energy decreases (shown in Figs. 7(b-c)).

4. Conclusions

This paper presents calculated cross sections based on the three-body BCCIS approximation for \( H^+, He^{2+} \) and \( Li^{3+} \) in the energy range of 25-10,000 keV/amu impacting on biological molecules (\( N_2, O_2, H_2O, CH_4, CO \) and \( CO_2 \)). The obtained cross sections are found to be in very good agreement with the available experimental data. We took charge transfer as the target ionization on averaging over the final state momentum distribution and it is expected that the inclusion of target continuum states is essential in such studies. In this work, we have taken into account the many-electron collision problem having used the independent-particle model (IPM) for pure electron capture where only one electron is considered as active. Moreover, the orbitals of the bio-molecular targets investigated here are described by linear combinations of atomic states corresponding to the atomic components of each of them. Moreover, the total cross sections have been computed within the CNDO approximation. The contribution of no molecular orbital to the TCS has been discarded. In general, in the low-intermediate energy range, the
dominance of contribution to the TCS is ordered from less bound to more bound orbitals. This feature reverses as the collision energy increases. Therefore, the reaction is prioritized in ascending order from less bound orbitals (outer orbitals) to the tightly bound orbitals (inner orbitals) as the collision energy increases. However, more theoretical works are required to be carried out and experimental investigations for electron capture in other large biological molecules are necessary to test the validity of the present theoretical investigation.

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