Charge transfer of He^{2+} with H in a strong magnetic field*

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By solving a time-dependent Schrödinger equation (TDSE), we studied the electron capture process in the $He^{2+}+H$ collision system under a strong magnetic field in a wide projectile energy range. The strong enhancement of the total charge transfer cross section is observed for the projectile energy below 2.0 keV/u. With the projectile energy increasing, the cross sections will reduce a little and then increase again, compared with those in the field-free case. The cross sections to the states with different magnetic quantum numbers are presented and analyzed where the influence due to Zeeman splitting is obviously found, especially in the low projectile energy region. The comparison with other models is made and the tendency of the cross section varying with the projectile energy is found closer to that from other close coupling models.

Keywords: time-dependent Schrödinger equation, strong magnetic field, charge transfer

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1. Introduction

The magnetic field may be as strong as 10^7–10^9 T in neutron stars, and 10^2–10^5 T in white dwarfs.[1,2] Such strong magnetic fields have strong influence upon the atomic structure as well as the collisional process. So far, extensive studies have been made and well understood for hydrogen[1,2] since the corresponding exact solution at an arbitrary strength of magnetic field has been found.[3] In 2013, He^- was found to be able to exist stably in a strong magnetic field.[4] Usually the magnetic field strength B is measured in terms of the parameter $\gamma = B/B_0$, where $B_0 = 2.35\times10^5$ T is the magnetic field strength in one atomic unit.

As far as we know, some studies of magnetic field effects on ion-atom collisions have been done, and the earliest study was made on symmetric resonance charge exchange of Rb^++ Rb and $H^+ + H$ collision processes in 1984[5] by the atomic orbital close-coupling (AOCC) method using a two-state basis. It was found that the magnetic field significantly reduces the charge exchange cross sections for the collision energy E_p below 200 keV/u at $B = 0.05B_0$. Later, Grosdanov and McDowell[6] studied the $He^{2+}+H$ collision process in a constant uniform magnetic field using the classical trajectory Monte Carlo (CTMC) method. They calculated the charge transfer and ionization cross sections for $\gamma \le 0.2$ with $E_p = 20$, 50, 75 keV/u and found that the ionization and capture cross sections increase by 17% with respect to that of the field-free case. After that a close coupling method was used to study the charge transfer for the same collision system with E_p between 6.25 and 400 keV/u at $\gamma \le 0.2$ by Bivona and Mcdowell.[7] They used a five-channel atomic-orbital expansion method where only He^+ $(2lm_l)$ states were included. The magnetic field was found to slightly reduce the capture cross section 8% at $E_p = 6.25$ keV/u and that it almost has no influence upon the cross section for $E_p \ge 100$ keV/u at $\gamma \le 0.2$. In all these studies, the orientation of external magnetic field was parallel to the projectile ion velocity and we call it a parallel magnetic field. Several years ago, CTMC calculation was also carried out for the system $He^{2+}+H$ by He *et al.*[8] and it was found that the parallel magnetic field would insignificantly affect the charge exchange cross sections in the energy range 25–2000 keV/u for $\gamma \le 0.2$, meanwhile it leads to an increase of excitation and ionization cross sections in the projectile energy region below 100 keV/u. However, the transverse magnetic field was found to cause a significant reduction of the total charge exchange cross section and a dramatic increase of excitation and ionization cross sections for $E_p \le 100$ keV/u.

Since so far there is no relevant experiment for the collisional process of $He^+ + H$ in the strong magnetic field, it is worth studying these problems with better methods since there are always some limitations with the above mentioned methods. Quantum effects could not be well considered in CTMC simulation and only the final states of He^+ $(2lm_l)$ were included in close coupling research of the charge transfer[7] so that the influence of other final states were ignored. It is well known that the method by solving the time-dependent Schrödinger equation (TDSE) is a powerful tool to deal with the collisional process by which many reliable results have been obtained. To the best of our knowledge, the method has not been applied to study the ion–atom collisional process with the magnetic field. The aim of the present work is to discuss the related problems with the TDSE method and compare the

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results obtained by different methods. In this paper, we shall study the charge transfer process $He^{2+} + H \rightarrow He^{+}(nl) + H^{+}$ in an external parallel strong magnetic field by the TDSE method. Here, γ is fixed at 0.2 and we will research the other magnetic field strength cases in the furture.

The rest of this paper is organized as follows. In Section 2, we give an outline of the theoretical methods, and the energy levels for He^{+} in a strong magnetic field will be given. In Section 3, the total charge transfer cross section without the external field will be presented first. Then the total and state selective cross sections under the external magnetic field are shown together with some relevant results. The comparison with other models is also made in the section and finally a summary is given in Section 4. Atomic units are used throughout unless otherwise specified explicitly.

2. Theory

The charge transfer of $He^{2+} + H$ is studied by solving the time-dependent Schrödinger equation

$$i\frac{\partial}{\partial t}\psi(\boldsymbol{r},t) = [\hat{H}_0 + V_{\rm int}(t)]\psi(\boldsymbol{r},t), \tag{1}$$

where

$$\hat{H}_0 = -\frac{1}{2}\nabla^2 - \frac{1}{r} \tag{2}$$

is the Hamiltonian of the hydrogen atom, the time-dependent interaction $V_{\rm int}(t)$ which includes the influence due to the projectile and the magnetic field is

$$V_{\rm int}(t) = \frac{-Z_{\rm p}}{|\boldsymbol{R}(t) - \boldsymbol{r}|} + \frac{1}{2}\gamma L_z + \frac{1}{8}\gamma^2 r^2 \sin^2(\theta). \tag{3}$$

In the present work, the projectile is assumed to move on a straight-line trajectory $R(t) = [b, 0, z_0 + vt]$, where b is the impact parameter, v is the velocity of the projectile He^{2+} which is along the z direction, and z_0 is the initial position of the projectile in the z direction. The magnetic field is assumed to be parallel to the z direction and L_z is the z component of the electron angular momentum. The paramagnetic term $\gamma L_z/2$ does not depend on the electron coordinates and only produces a shift in the total electron energy. $\gamma^2 r^2 \sin^2(\theta)/8$ is the diamagnetic term, which forms a parabolic potential well far away from the Coulomb centers and confines the electron motion in the direction perpendicular to the field.[8]

Here, it is necessary to give an explanation for the assumption of the straight-line trajectory for the projectile. Usually this assumption is valid when the projectile velocity $V_{\rm p}$ is high enough, for example, $V_{\rm p} = 2.0$ which corresponds to $E_{\rm p} = 100$ keV/u. However, when $V_{\rm p} \approx 0.2$ which corresponds to $E_{\rm p} \approx 1.0$ keV/u, this assumption is still valid. Two reasons are responsible for this. The first one is that when b is high enough, for example $b \geq 1.0$, the deflection of the projectile is very small which can be ignored while the deflection cannot be ignored when b is small enough, for example $b \leq 0.05$; however, when the effective range of b for it to play an important role in the calculation of the cross section is large enough, for example the range is from 0 to 9.0 shown in Fig. 1(a). Therefore, the deflection in the small range of b has little influence upon our results, which is demonstrated in Fig. 2 where the cross section obtained by us is very close to the experimental data even for $E_{\rm p} \approx 1.0$ keV/u. Another reason is that the applied magnetic field does not affect the motion of projectile since both $\boldsymbol{B}$ and $\boldsymbol{V}_{\rm p}$ are in the same direction where the Lorentz force is equal to 0.

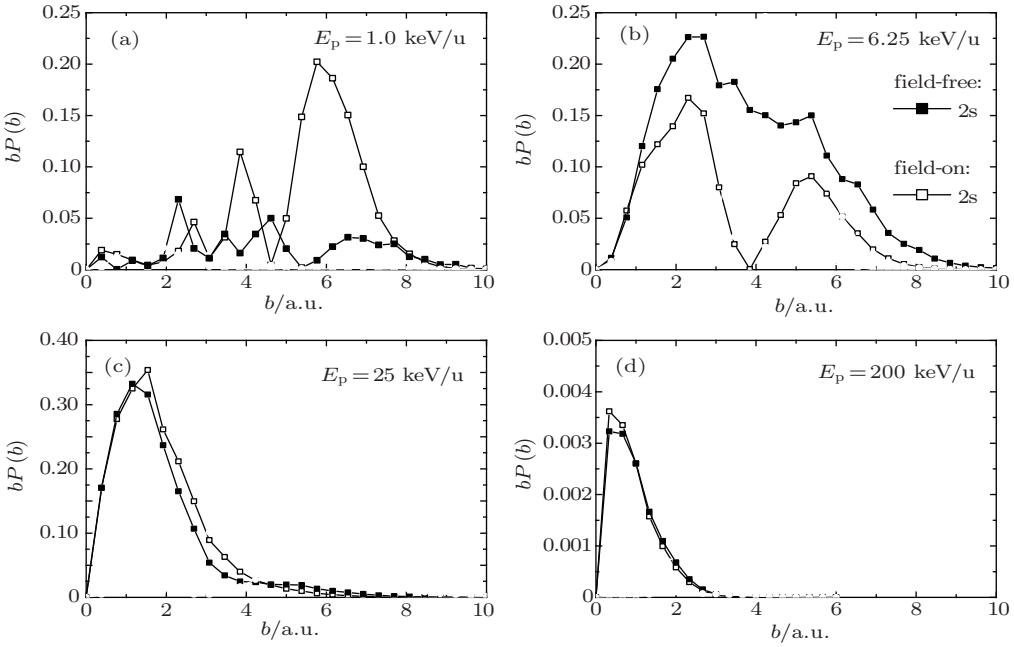


Fig. 1. The weight capture probability $bP(b)$ for 2s in magnetic field-on and field-free cases with $E_{\rm p} = 1.0$ keV/u (a), 6.25 keV/u (b), 25.0 keV/u (c), and 200.0 keV/u (d).

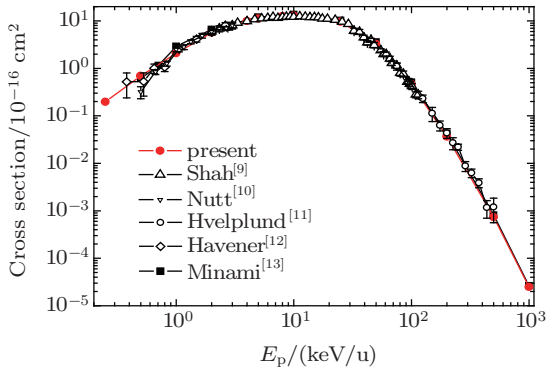


Fig. 2. (color online) Total cross sections for charge transfer in the collisions of $He^{2+}+H$. Here, Minami's result and our result are theoretical, and the others are experimental data.

Equation (1) may be solved efficiently and accurately by the well-known second-order split-operator method[14,15] given by

$$\psi(t+\Delta t) = \mathrm{e}^{-\mathrm{i}\hat{H}_0\Delta t/2}\,\mathrm{e}^{-\mathrm{i}V_{\mathrm{int}}(t+\Delta t/2)\Delta t}\,\mathrm{e}^{-\mathrm{i}\hat{H}_0\Delta t/2}\psi(t). \quad (4)$$

The computational implementation of Eq. (4) consists of the repetitive evaluation of the exponential matrices, $\exp(-\mathrm{i}\hat{H}_0\Delta t/2)$ and $\exp(-\mathrm{i}V_{\mathrm{int}}(t+\Delta t/2)\Delta t)$, times a vector of the wave function expansion coefficients, in which the evolution of the wave function is obtained. In the present work, these matrix-vector multiplications are calculated through the numerically exact and fast transform between the coordinate and spectral representations without explicitly constructing the Hamiltonian matrix. By means of the spectral representation, the total wave function $\psi(r,t)$ is expanded in terms of the eigen-functions $|nlm\rangle$ of the hydrogen Hamiltonian $\hat{H}_0$, where n, l, and m are the principle, orbital, and magnetic quantum number of the hydrogen atom, respectively. References [16]–[18] give the detailed present TDSE method, in the spectral representation. Finally, at long enough time T the charge transfer probability to a specified state nlm is defined by

$$P_{nlm}^{\mathrm{cap}}(T,b) = \left|\left\langle \psi(T)|\psi_{nlm}^{\mathrm{He}^+}\right\rangle\right|^2, \quad (5)$$

where $\psi_{nlm}^{\mathrm{He}^+}$ is the time-independent eigen-function of the projectile, the corresponding cross section can be obtained as

$$\sigma_{nlm} = 2\pi\int P_{nlm}^{\mathrm{cap}}(T,b)b\,\mathrm{d}b. \quad (6)$$

In the present TDSE method, it is important to choose adequate special grid points since the direct solution of the multidimensional TDSE is extremely computational demanding, especially when the Coulomb interaction is involved. To solve this problem, we adopt an accurate and efficient pseudo-spectral method for solving the TDSE where the radial coordinate is discredited using a grid constructed from the positive energy Coulomb wave function and it is chosen for the dense grid points near the unclear origin and sparse grid points for the large distance, which can deal with the Coulomb interaction properly. Meanwhile, the polar and azimuthal angles are discretized using the Gauss–Legendre and Fourier grids, respectively. The present algorithm is highly economical, needs no explicit construction of the Hamiltonian matrix, scales nearly linearly with the number of grid points and, moreover, it is found that the number of grid points can be orders of magnitudes less than that of evenly space grids.

For the present process in our calculation, we use $160\times320\times240$ grid points which cover the spherical region with the radius around 45.0, the initial position of projectile is $z_0=-30.0$ and the projectile is stopped at $z_{\mathrm{f}}=-35.0$. In the case of $\gamma=0.2$, the eigen-functions of the projectile for $n=2$ are very close to those without the magnetic field. For higher energy level the eigenfunctions will be highly influenced due to the strong magnetic field.

Since the strong magnetic field would influence the atomic structure, Table 1 presents the energy levels of He^+, which are the final states of charge transfer in order to know more about the relevant results of the dynamical process. The detail for the calculation can be found in Ref. [19]. In Table 1, the Landau level $(m+|m|+1)\gamma/2$ is taken away and the splitting of the level is obvious due to the strong magnetic field. Here, it is not shown for the level of $3d_{+2}$ at $\gamma=0.2$ since it is positive. It needs to be noted that it is difficult to describe the state for $n\geq3$ in a magnetic field since the expansion coefficient of the eigen-wavefunction in the base vectors is usually less than 0.5. Here, we still represent them with $|nlm\rangle$ since its contribution to the energy level is the biggest one.

Table 1. Energy levels of He^+ at $\gamma=0.0$ and 0.2.

	$\gamma=0.0$	$\gamma=0.2$
1s	–2.0	–1.997507
2s	–0.5	–0.468067
$2p_0$	–0.5	–0.485859
$2p_{-1}$	–0.5	–0.572233
$2p_{+1}$	–0.5	–0.372233
3s	–0.22	–0.098825
$3p_0$	–0.22	–0.165522
$3p_{-1}$	–0.22	–0.205031
$3p_{+1}$	–0.22	–0.005031
$3d_0$	–0.22	–0.181958
$3d_{-1}$	–0.22	–0.256481
$3d_{+1}$	–0.22	–0.056481
$3d_{-2}$	–0.22	–0.327555
$3d_{+2}$	–0.22	

3. Results and discussion

With the magnetic field, the collision dynamics and the initial state of the target particle will be changed. Firstly, we study the energy level and wave function of the hydrogen atom. The H_0 and the paramagnetic term is a diagonal matrix

in the spectral representation $|nlm\rangle$, whose matrix elements are

$$H^{(0)}_{n'l'm',nlm} = \langle n'l'm'|H_0|nlm\rangle = E_{nl}\delta_{n'n}\delta_{l'l}\delta_{m'm}, \quad (7)$$
$$H^{(1)}_{n'l'm',nlm} = \left\langle n'l'm'\left|\frac{1}{2}\gamma L_z\right|nlm\right\rangle = \frac{1}{2}\gamma m\delta_{n'n}\delta_{l'l}\delta_{m'm}.$$

In the coordinate representation $|\alpha\beta\delta\rangle$, the matrix element of the diamagnetic term is defined by

$$H^{(2)}_{\alpha'\beta'\delta',\alpha\beta\delta} = \left\langle \alpha'\beta'\delta'\left|\frac{1}{8}\gamma^2 r^2\sin^2(\theta)\right|\alpha\beta\delta\right\rangle = \frac{1}{8}\gamma^2 r_\alpha^2\sin^2(\theta_\beta)\delta_{\alpha'\alpha}\delta_{\beta'\beta}\delta_{\delta'\delta}, \quad (8)$$

so the total Hamiltonian of a hydrogen atom in a magnetic field in spectral representation is[18]

$$H^{\rm SR} = H^{(0)} + H^{(1)} + L^+H^{(2)}L. \quad (9)$$

Here, L is the transformation matrix between the two representations. Setting $m = 0$ and diagonalizing this matrix, we can first get the energy level of $H(1s_0)$ in the magnetic field. For $\gamma = 0.2$ the energy level of the ground state is $E_{1s_0} = -0.49038$, and the energy shift is less than 2%, which is very close to the result obtained by Kravchenko.[3]

By diagonalizing the matrix $H^{\rm SR}$, we can also obtain the corresponding ground state electron wave function vector in spectral representation. For the case of $\gamma = 0.2$, only very small perturbation of the ground state electron wave function is found. The base vector φ_{1s_0} contributes about 99.92% (the square of the expansion coefficient) to the ground state wave function, and the φ_{2s_0} base vector contributes about 0.046%. The other base vector's contribution is smaller than 0.01%, and their summation is about 0.034%. Although the ground state electron wave function is only very weakly perturbed by the magnetic field, this influence is still considered in our calculation.

Before discussing the magnetic field effect, we first get the total charge transfer cross sections for $He^{2+} + H$ collisions without the magnetic field with E_p from 0.25 keV/u to 200.0 keV/u. All the relevant results with TDSE and available experiment data are displayed in Fig. 2. Our result is totally in very good agreement with the experimental data obtained by Shah,[9] Nutt,[10] Hvelplund,[11] and Havener,[12] respectively. In the energy region of 75–500 keV/u, our result agrees with Hvelplund's[11] data within the experimental uncertainties. In the energy region of 2–115 keV/u, the difference between our result and Shah's[9] data is smaller than 6%, meanwhile our data is in Havener's experimental uncertainty range except for $E_p = 0.8$ keV/u. The most significant disagreement is in the energy region of 0.5–1 keV/u where Nutt's experimental data[10] are about 20%–50% smaller than ours, while our result still agrees with Havener's experimental data. Minami's theoretical data[13] are also plotted in Fig. 2, which is always larger than ours, and agree with ours within 15% except a 29% difference at $E_p = 1.0$ keV/u.

Figure 3 shows the total and state-selective charge transfer cross sections for $\gamma = 0.2$ together with the results in the field-free case, where the total cross section includes the contribution of all the final states. The effect of the parallel magnetic field on the total charge exchange cross sections is quite significant in the whole energy range. In the low energy region, the magnetic field leads to a dramatic increase in the total cross section, up to a factor of 5 at $E_p = 0.25$ keV/u. With E_p increasing the collision energy, the enhancement of total cross sections due to the magnetic field becomes smaller and smaller, and the enhancement changes to reduction at $E_p = 3$ keV/u. In the energy region of 4–50 keV/u, the total cross sections are reduced about 12%–20%. With the further increase of E_p, the total cross sections are enhanced again by the magnetic field. It is difficult to give a complete explanation about the behavior since the transfer process is much more complicated by the inclusion of the magnetic field, the relevant research by the quantum method is very scarce, and there are no experimental data to compare with. Here, we can only present part of the reasons for the observed behavior of the total cross section. We believe that there are two important reasons. One is that more avoiding crossing appears and the electrons can be transferred more easily to much more final states because of the Zeeman splitting induced by the magnetic field. The other one is the obvious decreasing of the energy levels with $m < 0$ due to the magnetic field according to Table 1, which enhances the possibility to the transfer process. Moreover, these two reasons play their roles mainly at E_p when the projectile moves very slowly so that it has enough time to interact with the target. With the increase of E_p, the capture to the states with $n > 2$ (see Fig. 4) gradually plays its role, which is ignored in Ref. [7]. Our analysis is helpful to understand the dramatic increasing of the cross sections at low E_p and a little increasing at high enough E_p. So far, it is difficult for us to explain the reduction of the total cross section for E_p around 4–50 keV/u, which was also observed in the close coupling calculation,[7] where it is ascribed to the redistribution of flux among final sublevels and the reason for this is still unclear. In addition, figure 3 suggests that for $E \leq 40$ keV/u the transfers to $n = 2$ states, especially 2p state, are the most important transferring channels, which is consistent with that in the field-free case.[13]

Another phenomenon in Fig. 3 is that the modification of transferring to 2s cross sections (σ_{2s}) is very complicated in different collision energy regions. It increases from a very small cross section to 0.2×10^{-16} cm^2 (up to two orders of

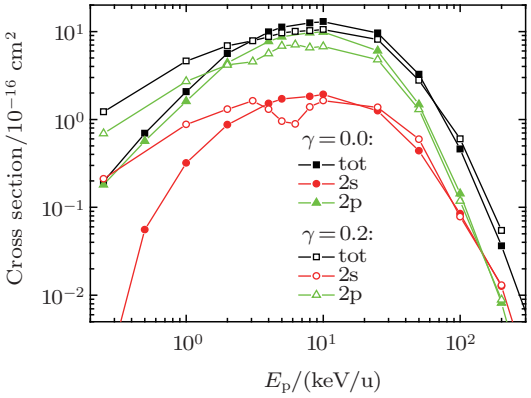


Fig. 3. (color online) Total and state-selective cross sections for charge transfer to 2l state of He^+ in $He^{2+} + H$ collisions in a parallel external magnetic field with $\gamma = 0.2$ and in the field-free case. Here, the symbol 2p means the summation of $2p_m$ with $m = -1, 0, 1$.

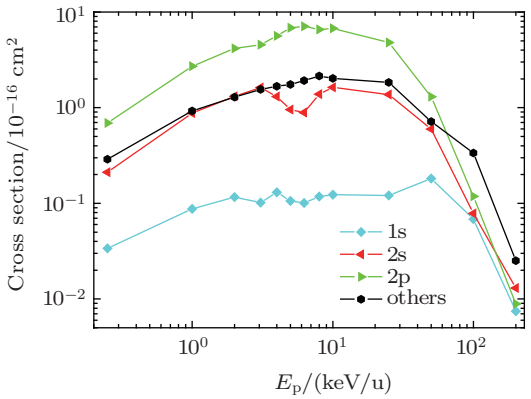


Fig. 4. (color online) State-selective cross sections for charge transfer to higher excited states (denoted with others), 1s, 2s, and 2p states of He^+ in $He^{2+} + H$ collisions with $\gamma = 0.2$.

magnitude) at $E_p = 0.25$ keV/u under the influence of a magnetic field. In the medium energy region, σ_{2s} is reduced by the magnetic field, and a minimum appears at $E_p = 6.25$ keV/u. In the energy region above 10 keV/u, the magnetic field has little influence upon the cross section. Such behavior is unknown and needs further investigation.

The cross sections to different final states are shown in Fig. 4. Here, the cross sections denoted with the symbol of others means the contribution from all the states with $n \geq 3$, which is more important than that from 1s in the whole energy range. Its contribution becomes the most important for E_p beyond 100 keV/u. The result is quite different from that in Ref. [7], where it was assumed that the contribution from the states except $n = 2$ is negligible. This means that the present calculation is more believable. Besides this, the result to 1s is always very small. We think that it is mainly due to the huge difference of the energy levels between the initial and final states. Obviously, the state-select cross section to 2p is the most important one compared with the other channels, which is consistent with the results when $B = 0$.[13] So far we have not seen an explanation for this from the others. We think one reason for this is related to the dipole transition 1s→ 2p which is optically permitted while the other transitions 1s→ *n*s are optically forbidden. Another reason is that the energy level of the 2l shell for He^+ is close to that of the initial of 1s for H^+, which makes the charge transfer to the final states of 2l on He^+ easier than to other states, especially at low E_p.

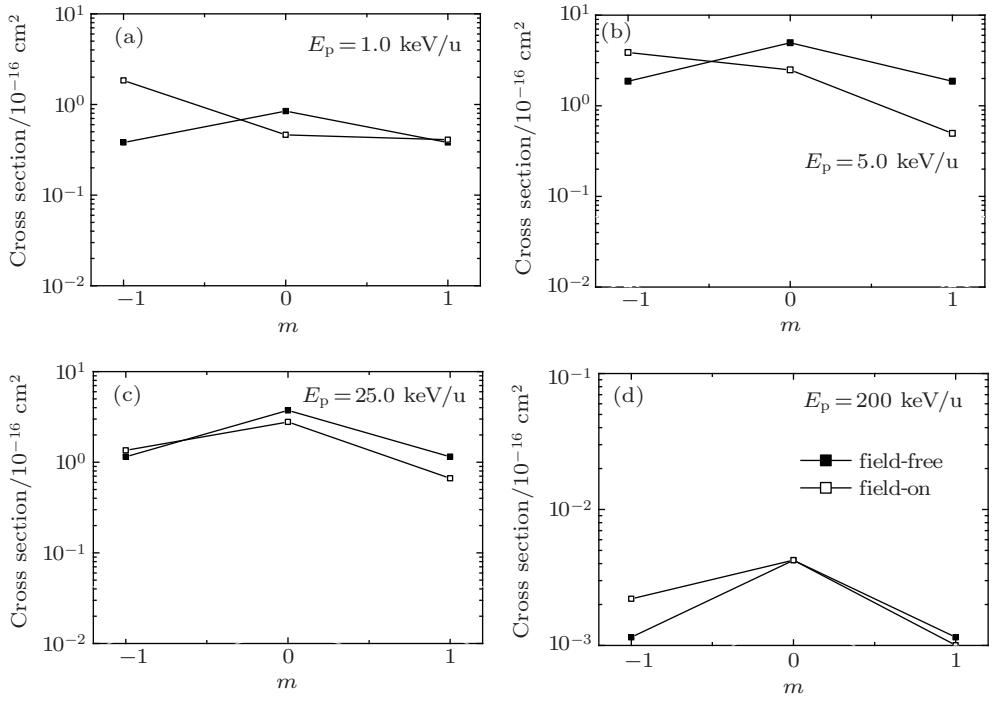


Fig. 5. State-selective cross sections for electron capture to He^+ (2p) as a function of m in magnetic field-on and field-free cases with $E_p = 1.0$ keV/u (a), 5.0 keV/u (b), 25.0 keV/u (c), 200.0 keV/u (d).

In order to know more about the behavior of σ_{2s} around $E_p = 6$ keV/u, the weight capture probability $bP(b)$ for 2s, which is deeply influenced by the magnetic field, is plotted in Fig. 1 with four different E_p. It is found that the weight capture probability for 2s at all collision energies is enhanced by the magnetic field except in the case at 6.25 keV/u. The reason for this is unclear, which needs to be further studied in the future.

Since the degeneracy of the energy levels would be removed by the Zeeman effect, the transition probabilities to the states with different magnetic quantum numbers may be quite different. In Fig. 5, we compare the most important state-selective cross sections σ_{2p} as a function of m in the cases of magnetic field on and free with $E_p = 1.0$, 5.0, 25.0, and 200.0 keV/u representing the very low, low, medium, and high energy regions. In the field-free case, it is found that the cross sections σ_{2p} are bilateral symmetrical, and the maximum is always located at $m = 0$. When the strong magnetic field is applied, it strongly influences the behavior of σ_{2p} which results in the disappearance of the bilateral symmetry at all collision energies. For $2p_{-1}$, the increase of the cross section is always dramatic, while the cross section to $2p_{+1}$ is decreased except it is almost unchanged at $E_p = 1$ keV/u. Besides this, the cross section to $2p_0$ also falls down except it is almost unchanged at $E_p = 200.0$ keV/u. This behavior is consistent with the change of the corresponding energy levels listed in Table 1. Therefore, the behavior of the change of σ_{2p} due to the strong magnetic field is determined by the competition between the increase of σ_{2p_-} and the decrease of $\sigma_{2p_{0,+}}$. Similar behaviors were also observed in Ref. [7] for $E_p = 6.25$, 12.5, and 25.0 keV/u.

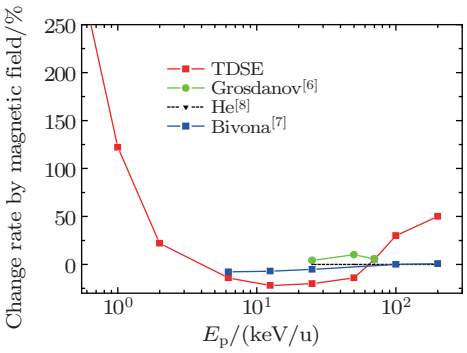


Fig. 6. (color online) The changes rates of the total transfer cross section with $\gamma = 0.2$ as a function of collision energy in different models.

Since several different models have been used to discuss the total cross section, it is necessary to compare them in order to know more about the related results. Because the data from each model may be quite different, it is convenient to compare the change rate for each total cross section influenced by the magnetic field, which is defined as $[\sigma(\gamma = 0.2)/\sigma(\gamma = 0)] - 1$. To the best of our knowledge, all the available data for the process are shown in Fig. 6. The same magnetic field strength is chosen in all the models with $\gamma = 0.2$. Except the CTMC result from He *et al*,[8] all the other results are influenced obviously by the magnetic field. In the energy region below 2 keV/u, only our result is shown with the dramatic increase of the cross section observed. In the energy region of 6–60 keV/u, our result is consistent with Bivona's[7] where the magnetic field leads to the reduction of the cross section and our result is decreased more than Bivona's. At higher energies, our calculated cross section is increased again while the others change little. We think our result is more reasonable than Bivona's since all the possible final states are considered in our calculation while only the states with $n = 2$ are included in Bivona's model. Compared with ours, the results from CTMC are not reliable since some quantum effects could not be well considered in its simulation. More work will be performed to check the difference of the results in the future.

4. Summary

In summary, we studied the electron capture process in the $He^{2+} + H$ collision system under a strong magnetic field in a wide projectile energy range based on the TDSE method. The strong enhancement of the total charge transfer cross section is observed for the projectile energy below 2.0 keV/u. With the projectile energy increasing, the cross sections will reduce a little around $E_p = 10$ keV/u and then increase again, compared with those in the field-free case. The cross sections to the states with different magnetic quantum numbers are analyzed where the influence due to Zeeman splitting is obviously found, especially in the low projectile energy region. It is found that the behavior for the change of σ_{2p} due to the strong magnetic field is determined by the competition between the increasing of σ_{2p_-} and the decreasing of $\sigma_{2p_{0,+}}$. A comparison with other calculations is made and the tendency of the cross section varying with the projectile energy is found to be closer to that from the close coupling model.

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