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Triplet-triplet excitation in helium

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Differential cross sections for the electron impact excitation from the metastable $2\,^3S$ state to the $3\,^3S$ state of helium, at impact energies 50 to 500 eV, are calculated in the two-potential model and the modified Born approximation using Coulomb waves with a screened nuclear charge. The exchange effect is included in the framework of the Ochkur-Rudge approximation. The results are compared with recent theoretical calculations. It is shown that the present approach provides a significant improvement over the plane-wave Born approximation at large scattering angles.

I. INTRODUCTION

In the past, considerable work has been done both theoretically and experimentally in the study of the elastic and inelastic collision processes between electrons and atoms which are initially in the ground state. Relatively little work has been done to investigate collision processes involving target atoms and ions which are found initially in an excited state.[1] The knowledge of collision processes involving excited atomic systems is of great importance in problems in astrophysics and plasma physics. Further, the study of the above process is of direct relevance to the development of lasers and in the understanding of gaseous discharges and other related phenomena where the excitation from the excited states represents one of the major channels for the absorption of the electron energy.

In this paper we shall be interested in the study of inelastic scattering of electrons from metastable helium atoms. This study is considered useful since metastable helium atoms play important roles in Penning ionization processes and in other gaseous phenomena by virtue of their long radiative lifetimes.

The excitation of metastable helium provides a test of various approximations. Since loosely bound electrons are involved, not much is known concerning the validity of the Born approximation for these transitions. In the low-energy region, Marriott[2] has used the two-state close-coupling approximation to calculate the significant partial cross sections for elastic and inelastic scattering of electrons by helium in the singlet and triplet metastable states.

In the intermediate and high-energy region, Flannery and McCann[3] calculated the $2\,^{1,3}S \rightarrow n\,^{1,3}L$ ($n=2,3$; $L=S,P,D$) collisional excitation cross sections of helium by electron impact in the multichannel eikonal approximation. Chen and Khayrallah,[4] and Khayrallah *et al.*[5] have calculated the elastic and inelastic scattering of electrons by the metastable helium atom using the Glauber approximation. Kim and Inokuti[6] studied $2^{1,3}S \rightarrow n\,^{1,3}L$ ($n=2,3,4$ for $L=P$, and $n=3$ for $L=S,D$) transitions of helium by charged-particle impact in the Born approximation. Flannery *et al.*[7] have calculated the total excitation cross sections for transitions to $2\,^{1,3}P$, $3\,^{1,3}S$, $3\,^{1,3}P$, $3\,^{1,3}D$, and $4\,^{1,3}P$ from the $2\,^{1,3}S$ state of helium for up to 500-eV electron-impact energies in the Born, and Vainshtein-Presnyakov-Sobel'man (VPS) approximations. Ochkur and Bratsev[8] computed the excitation cross sections of a series of triplet and singlet helium levels from the metastable $2\,^3S$ state by electron impact in a first approximation to the perturbation theory. Ton *et al.*[9] determined the cross sections for the $2\,^3S \rightarrow n\,^3L$ ($n=2-5$, $L=S-F$) excitation and for the single ionization in e^-+He ($2\,^{1,3}S$) collisions in the Born approximation.

The main drawback of the Born approximation is that it fails to explain the large-angle inelastic scattering. This is because the contribution from the nuclear scattering to the plane-wave Born cross sections vanishes due to orthogonality of the wave functions of the bound states involved. One can improve upon the plane-wave Born approximation by retaining the nuclear interaction term as is done in the Glauber approximation,[10] using a Coulomb wave for the free electrons as in the Geltman-Hidalgo approach,[11] or by using a distorted wave[12] which amounts to a Coulomb-Born approximation with variable nuclear screening.

In some recent work[13,14] an approach similar to that of Geltman and Hidalgo[11] has been used to study the electron-atom inelastic scattering. In this approach, the two-potential model and the modified Born approximation, using Coulomb waves with a screened nuclear charge instead of the plane wave, have been used with considerable success to study the inelastic scattering of electrons from the ground states of atomic hydrogen and helium. It was found that the above approach led to a significant improvement for the differential cross section (DCS) over the plane-wave Born approximation, particularly at large scattering angles.

In the present paper, we extend our study[14] to the excitation of the $3\,^3S$ state of helium from its metastable $2\,^3S$ state by electron impact. Exchange effect is also included in the framework of the Ochkur-Rudge approximation.[15] The results for DCS are found to be in satisfactory agreement with the Glauber calculation of Khayrallah *et al.*,[5] but differ considerably from the Born calculations at large angles. No experimental data on DCS exist at present for the above transition.

II. THEORY

The T-matrix element for the excitation of a helium atom from an initial state i to a final state f in the two-potential modified Born (TPMB) approximation, is given by[14]

$$T_{i\to f}^{\mathrm{TPMB}} = \langle \chi_f^{(-)} | W_2 | \chi_i^{(+)} \rangle , \qquad (1)$$

where superscripts $(\pm)$ refer to the outgoing and incoming wave boundary conditions, respectively. χ is the total wave function defined as

$$\chi(\vec{r}_1, \vec{r}_2; \vec{r}_3) = \Psi(\vec{r}_1, \vec{r}_2) F(\vec{r}_3) , \qquad (2)$$

where $\vec{r}_1$ and $\vec{r}_2$ are the position coordinates of the atomic electrons, and $\vec{r}_3$ of the incident electron. $\Psi(\vec{r}_1, \vec{r}_2)$ is the wave function of the helium atom and $F(\vec{r}_3)$ is a Coulomb wave function of nuclear charge δ:

$$W_2 = -\frac{(Z-\delta)}{r_3} + \frac{1}{r_{13}} + \frac{1}{r_{23}} ,$$

where Z is the nuclear charge and δ is a screening parameter.

Ignoring exchange, one sees that for the case of direct inelastic scattering, the nuclear term in Eq. (1) does not contribute due to the orthogonality of the initial and final-state atomic wave functions, thereby making W_2 effectively equal to $1/r_{13} + 1/r_{23}$. Hence the result of Eq. (1) for inelastic scattering becomes identical to the Coulomb-Born results with a screened charge $Z - \delta$.

To include exchange effects in Eq. (1), one needs to consider the spin functions explicitly. In the present study, we are considering the case of triplet-triplet transitions and, therefore, we take the combination of an electron ($S = \frac{1}{2}$) with the triplet two-electron function ($S = 1$). The three-electron spin function corresponds to a total spin of $S = \frac{1}{2}$ and $\frac{3}{2}$. Therefore, the total antisymmetric spatial spin-state function for an incident electron plus an initial triplet target state will belong either to a doublet (D) or a quartet (Q) spin state. We thus write for $\chi_i^{(+)}$, the total antisymmetrized wave function

$$\chi_i^{(+)} = \mathcal{A} \Psi_2(\vec{r}_1, \vec{r}_2) F_2(\vec{r}_3) S_{Q,D}(1, 2; 3) , \qquad (3)$$

where $\mathcal{A}$ is the antisymmetrization operator. $S_{Q,D}(1, 2; 3)$ are the three-electron normalized spin functions given by[16,7]

$$S_Q(1,2;3) = \alpha_1\alpha_2\alpha_3 \times (1/\sqrt{3})(\alpha_1\alpha_2\beta_3 + \alpha_1\beta_2\alpha_3 + \beta_1\alpha_2\alpha_3) \qquad (4a)$$

for the quartet spin state with total magnetic components $M_s = \frac{3}{2}$ and $\frac{1}{2}$, respectively, and

$$S_D(1,2;3) = (1/\sqrt{6})[2\alpha_1\alpha_2\beta_3 - \alpha_3(\alpha_1\beta_2 + \alpha_2\beta_1)] \qquad (4b)$$

represents the doublet state with the total magnetic component $M_s = \frac{1}{2}$. The function $\chi_f^{(-)}$ is given by

$$\chi_f^{(-)} = \mathcal{A} \Psi_3(\vec{r}_1, \vec{r}_2) F_3(\vec{r}_3) S_{Q,D}(1, 2; 3) . \qquad (5)$$

$\Psi_2(\vec{r}_1, \vec{r}_2)$ and $\Psi_3(\vec{r}_1, \vec{r}_2)$ are the spatial parts of the atomic antisymmetric wave functions for the initial and final state, respectively. $F_2(\vec{r}_3)$ and $F_3(\vec{r}_3)$ are the scattered electron wave functions[14] which, in the present approach, are represented by the Coulomb wave function of charge δ.

The differential cross section for a collision in which the helium atom is excited from an initial state ($2\,^3S$) to a final state ($3\,^3S$) is given by

$$\left(\frac{d\sigma}{d\Omega}\right)^{\mathrm{TPMB}} = \frac{K_f}{4\pi^2 K_i} \left[\tfrac{1}{3} |T(D)|^2 + \tfrac{2}{3} |T(Q)|^2\right] . \qquad (6)$$

$\vec{K}_f$ and $\vec{K}_i$ are the momenta of the scattered and the incident electron, respectively. The T matrices for the doublet and quartet states are obtained as

$$T(D) = \Gamma(1 - ia_i)\Gamma(1 - ia_f) \times e^{\pi(a_i + a_f)/2} (I_D + I_E) , \qquad (7)$$

and

$$T(Q) = \Gamma(1 - ia_i)\Gamma(1 - ia_f) \times e^{\pi(a_i + a_f)/2} (I_D - 2I_E) , \qquad (8)$$

where

$$I_D = \int d\vec{r}_3\, e^{i\vec{q}\cdot\vec{r}_3} {}_1F_1(ia_i; 1; iK_i r_3 - i\vec{K}_i\cdot\vec{r}_3) {}_1F_1(ia_f; 1; iK_f r_3 + i\vec{K}_f\cdot\vec{r}_3) \langle \Psi_3(\vec{r}_1, \vec{r}_2) | W_2 | \Psi_2(\vec{r}_1, \vec{r}_2) \rangle \qquad (9)$$

and

$$I_E = \int d\vec{r}_1 d\vec{r}_2 d\vec{r}_3\, e^{i(\vec{K}_i\cdot\vec{r}_1 - \vec{K}_f\cdot\vec{r}_3)} {}_1F_1(ia_i; 1; iK_i r_1 - i\vec{K}_i\cdot\vec{r}_1) {}_1F_1(ia_f; 1; iK_f r_3 + i\vec{K}_f\cdot\vec{r}_3) \Psi_3(r_1, r_2) W_2 \Psi_2(r_3, r_2) . \qquad (10)$$

I_D and I_E can be expressed as

$$I_D = -N_2N_3\Bigg[\frac{A_{21}A_{31}}{\lambda_1^3}\left(2[G(q,\lambda_1)] - \lambda_1\frac{\partial}{\partial\lambda_1}[G(q,\lambda_1)]\right) + \frac{A_{21}A_{32}}{\lambda_2^4}\left(6[G(q,\lambda_2)] - 4\lambda_2\frac{\partial}{\partial\lambda_2}[G(q,\lambda_2)] + \lambda_2^2\frac{\partial^2}{\partial\lambda_2^2}[G(q,\lambda_2)]\right)$$
$$+\frac{A_{21}A_{33}}{\lambda_3^5}\left(24[G(q,\lambda_3)] - 18\lambda_3\frac{\partial}{\partial\lambda_3}[G(q,\lambda_3)] + 6\lambda_3^2\frac{\partial^2}{\partial\lambda_3^2}[G(q,\lambda_3)] - \lambda_3^3\frac{\partial^3}{\partial\lambda_3^3}[G(q,\lambda_3)]\right)$$
$$+\frac{A_{22}A_{31}}{\lambda_4^4}\left(6[G(q,\lambda_4)] - 4\lambda_4\frac{\partial}{\partial\lambda_4}[G(q,\lambda_4)] + \lambda_4^2\frac{\partial^2}{\partial\lambda_4^2}[G(q,\lambda_4)]\right)$$
$$+\frac{A_{22}A_{32}}{\lambda_5^5}\left(24[G(q,\lambda_5)] - 18\lambda_5\frac{\partial}{\partial\lambda_5}[G(q,\lambda_5)] + 6\lambda_5^2\frac{\partial^2}{\partial\lambda_5^2}[G(q,\lambda_5)] - \lambda_5^3\frac{\partial^3}{\partial\lambda_5^3}[(q,\lambda_5)]\right)$$
$$+\frac{A_{22}A_{33}}{\lambda_6^6}\left(120[G(q,\lambda_6)] - 96\lambda_6\frac{\partial}{\partial\lambda_6}[G(q,\lambda_6)] + 36\lambda_6^2\frac{\partial^2}{\partial\lambda_6^2}[G(q,\lambda_6)] - 8\lambda_6^3\frac{\partial^3}{\partial\lambda_6^3}[G(q,\lambda_6)] + \lambda_6^4\frac{\partial^4}{\partial\lambda_6^4}[G(q,\lambda_6)]\right)\Bigg], \tag{11}$$

and

$$I_E = \frac{N_2N_3}{2[K_f - i(2I_p)^{1/2}]^2}\left(-A_{21}A_{31}\frac{\partial}{\partial\lambda_1}[G(q,\lambda_1)] + A_{21}A_{32}\frac{\partial^2}{\partial\lambda_2^2}[G(q,\lambda_2)] - A_{21}A_{33}\frac{\partial^3}{\partial\lambda_3^3}[G(q,\lambda_3)]\right.$$
$$\left. + A_{22}A_{31}\frac{\partial^2}{\partial\lambda_4^2}[G(q,\lambda_4)] - A_{22}A_{32}\frac{\partial^3}{\partial\lambda_5^3}[G(q,\lambda_5)] + A_{22}A_{33}\frac{\partial^4}{\partial\lambda_6^4}[G(q,\lambda_6)]\right), \tag{12}$$

with

$$G(q,\lambda) = \int d\vec{r}_3\frac{e^{-\lambda r_3}}{r_3}e^{i\vec{q}\cdot\vec{r}_3}{}_1F_1(ia_i;1;iK_ir_3 - i\vec{K}_i\cdot\vec{r}_3)\,{}_1F_1(ia_f;1;iK_fr_3 + i\vec{K}_f\cdot\vec{r}_3). \tag{13a}$$

Carrying out this integration[17] one obtains

$$G(q,\lambda) = \frac{4\pi e^{-\pi a_i}}{(q^2+\lambda^2)}\left(\frac{(q^2+\lambda^2)^{ia_i}(K_i+K_f+i\lambda)^{-i(a_i+a_f)}}{(K_i-K_f+i\lambda)^{i(a_i-a_f)}}\right){}_2F_1\left(1-ia_i; ia_f; 1; \frac{4K_iK_f\sin^2\theta/2}{(q^2+\lambda^2)}\right), \tag{13b}$$

where $a_i = \delta/K_i$ and $a_f = \delta/K_f$. λ's are defined in Eq. (16). I_p is the ionization potential of the target atom in the initial state. $\vec{q}$ $(=\vec{K}_i - \vec{K}_f)$ is the momentum transfer vector.

In arriving at the above expression for I_E, we have followed the Ochkur-Rudge approximation.[15] Furthermore, following Byron and Joachain,[18] we have retained only that part of the potential which represents the interaction between the incident and ejected electrons, since it gives the dominant contribution for the range of energies studied in this paper.

In evaluating I_D and I_E, we use the Hartree-Fock wavefunctions. They are the variationally determined orthonormal sets given by[19]

$$\Psi_2(\vec{r}_1,\vec{r}_2) = (N_2/\pi)[\phi_{1s}(r_1)\phi_{2s}(r_2) - \phi_{1s}(r_2)\phi_{2s}(r_1)], \tag{14a}$$

$$\Psi_3(\vec{r}_1,\vec{r}_2) = (N_3/\pi)[\phi_{1s}(r_1)\phi_{3s}(r_2) - \phi_{1s}(r_2)\phi_{3s}(r_1)], \tag{14b}$$

where the ϕ's are linear combinations of Slater orbitals defined by

$$\phi_{ns} = \sum_{i=1}^{n} A_{ni}r^{i-1}e^{-\alpha_{ni}r}, \tag{15}$$

$$\lambda_1 = \alpha_{21}+\alpha_{31};\quad \lambda_2 = \alpha_{21}+\alpha_{32};$$
$$\lambda_3 = \alpha_{21}+\alpha_{33},$$
$$\lambda_4 = \alpha_{22}+\alpha_{31};\quad \lambda_5 = \alpha_{22}+\alpha_{32};$$
$$\lambda_6 = \alpha_{22}+\alpha_{33}. \tag{16}$$

The parameters A_{ni}, N_2, N_3, and α_{ni} for $2\,^3S$ and $3\,^3S$ states are the same as given by Khayrallah *et al.*[5] which are based on the earlier work of Morse *et al.*[19] and Marriott,[2] respectively.

III. RESULTS AND DISCUSSION

We have used Eq. (6) to obtain the differential cross sections for the excitation of helium to the $3\,^3S$ state from the metastable $2\,^3S$ state. As in our earlier work,[14] we have taken δ to be a free parameter. In the figures, we have presented our results for the two values of δ equal to 1.4 and 2.0.

Figures 1–4 show the results of our calculation of the differential cross sections for the $2\,^3S \to 3\,^3S$ excitation of helium by electron impact at the energies of 50, 100, 200, and 500 eV. In these figures, we have compared our results with the Born calculation and the other sophisticated theoretical results.

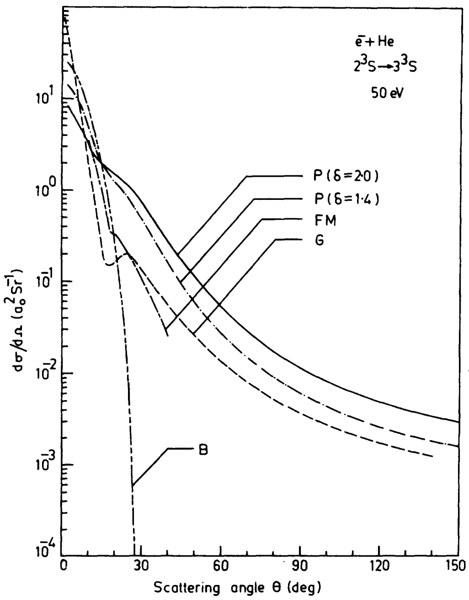

FIG. 1. Differential cross section for the excitation of helium from $2\,^3S$ to the $3\,^3S$ state at an energy of 50 eV •—— •—— •——,; present calculation (curve P) corresponding to $\delta = 1.4$, ——; present calculation (curve P) corresponding to $\delta = 2.0$, ——————; present calculation in the Born approximation (curve B); ------, calculations of Khayrallah *et al.* (curve G, Ref. 5); —— ——— ——, calculation of Flannery and McCann (curve FM, Ref. 3).

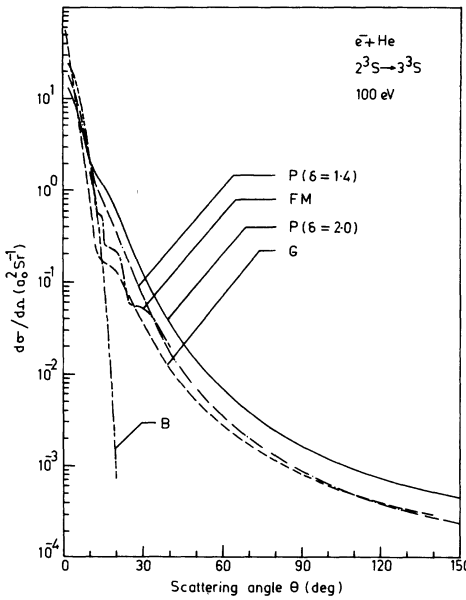

FIG. 2. Differential cross section for the excitation of helium from $2\,^3S$ to the $3\,^3S$ state at an energy of 100 eV. Description is same as in Fig. 1.

Figure 1 shows our results (curves P) at 50-eV energy. The other theoretical results shown are (i) the calculation of Flannery and McCann[3] (FM) (taken from the figure of Khayrallah *et al.*[5]) based on the ten-channel eikonal treatment (ii) the calculation of Khayrallah *et al.*[5] (G) based on the Glauber approximation, and (iii) the calculation based on the Born approximation (B). It is evident from this figure that the Glauber calculation (G) as well as both the present calculations (P), give a much higher cross section in the large-angle region as compared to the Born-approximation calculation (B), which shows a very rapid fall towards large angles. In the lower-angle region, we do not get the prominent dip as obtained in the Glauber calculation.[5] However, we get a slight shoulder in the cross section at about the same position where the dip is obtained in the Glauber results. A similar shoulder is noticed in the calculation of Flannery and McCann[3] (FM).

Figure 2 shows our results (curves P) at 100-eV energy. From the figure we notice that our results (P) (corresponding to $\delta = 1.4$), agree well with the FM calculation between 10 to 40°. Beyond this angular range, our results show a good agreement with the (G) calculation. A large difference is again noticed between all the other theoretical calculations and the Born results (B) at large scattering angles.

Figure 3 shows our results (curves P) at 200-eV energy. Here we compare our results with the (G) and (B) calculations. At this energy, our results (corresponding to $\delta = 1.4$) show a reasonably good

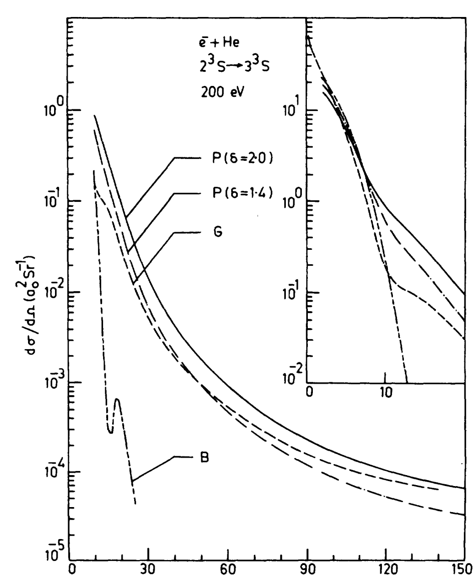

FIG. 3. Differential cross section for the excitation of helium from $2\,^3S$ to the $3\,^3S$ state at an energy of 200 eV. Description is same as in Fig. 1.

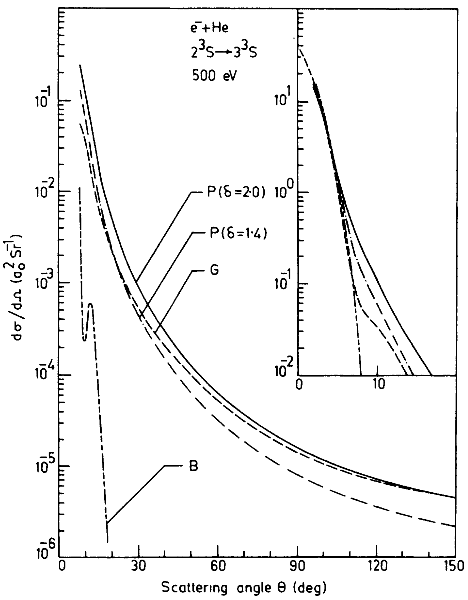

FIG. 4. Differential cross section for the excitation of helium from $2\,^3S$ to the $3\,^3S$ state at an energy of 500 eV. Description is same as in Fig. 1.

agreement with the (G) calculation up to 80° while beyond this angular range, our results (corresponding to $\delta = 2.0$) begin to agree better with the Glauber results.

Figure 4 shows our results (P) at 500-eV energy. At this energy, the general features of our results (P) and the Glauber calculation (G) are similar to those of Fig. 3. It is noted that as the energy increases, our results (P) (corresponding to $\delta = 2.0$) show a better agreement with the Glauber calculation (G) at larger scattering angles. The Born approximation calculation (B) greatly underestimates the cross sections at all the energies in the backward direction.

Since the Glauber and distorted-wave approximations use, in effect, a variable nuclear charge, they converge to our results with $\delta = 2$ at large angles and to our results with smaller δ ($\delta = 1.4$) at intermediate angles. For high energies and small angles, all the results tend to the plane-wave Born approximation results.

In comparison to the direct scattering amplitude, the contribution of exchange is quite small in the range of energies studied here. Further, this exchange contribution becomes still smaller as the energy increases from 50 to 500 eV. Our calculations for exchange amplitude, which are based on the Ochkur-Rudge approximation,[15] are expected to be reasonable. Truhlar *et al.*[20] have pointed out that the Born-Oppenheimer approximation gives an erroneously large contribution to the exchange scattering amplitudes at low and intermediate energies.

It is concluded that by using the present approach, which is very simple in nature and requires much less computer time compared to the Glauber and the ten-channel eikonal calculations. one can obtain a reasonable estimate of the cross sections for the excitation of helium to the $3\,^3S$ state from the initial $2\,^3S$ metastable state.

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