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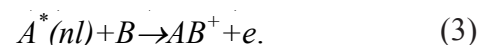
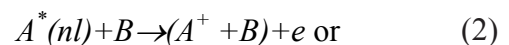
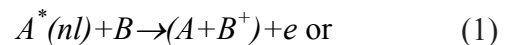
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PENNING AND STOCHASTIC COLLISIONAL IONIZATION OF ATOMS IN AN EXTERNAL MAGNETIC FIELD: MODEL POTENTIAL SCHEME

The key physical aspects of the Penning and stochastic collisional ionization of atoms in an external magnetic field are considered and new model potential approach has been implemented in order to take into account an effect of magnetic field on multi-electron atom energy parameters and to compute the wave functions basis for next using in the collisional block. The corresponding Schrödinger equation for atom in a magnetic field and the Focker-Plank stochastic equation are solved within the standard differences-grid method.

1. Above a great number of different elementary atomic and molecular processes to be studied in collisions physics, physics and chemistry of plasma, gases and other mediums one should note such complicated phenomena as an ionization of excited atoms by means of the photon and electron impact, atom-atom or ion-atom collisions, including these processes at presence of the external field. As a rule in any case an adequate treating these processes requires an accurate account of different exchange-correlation and even relativistic corrections [1-25]. Indeed to fulfill an accurate account of the inter electron correlation effects in the atomic collisions is very difficult as these effects and other ones are not adequately described within many simplified models. Situation changes dramatically under consideration of the different atomic collisional processes under availability of the external electromagnetic fields. Even more simple case of the external static electric or magnetic field is remained hitherto quantitatively undeceived. Several theoretical attempts were taken to make formulation of the consistent quantum theory for the atomic collisional processes in presence of the external magnetic field. [11-20].

Usually there are considered the key interatomic collisional processes, which are of a great interest for many applications, namely [1-4]:



As usually, in these formula A^* denotes the atom in an excited state, B^+ is the ionized atom. The first process (1) occurs and runs very effectively in a case when the excitation energy of the A atom is more than the ionization potential of the atom B. Here one can introduce the Penning process, which is corresponding to the situation when the atom A is in the metastable state. The process (3) is corresponding to the associative ionization. It takes a place when the dissociation energy of molecular ion AB^+ is more than the ionization potential of the excited atom [1,2].

The most widespread theoretical schemes for description of the cited processes (look, for example, [1-5,17-22]) are based on the computing the capture cross-section of collisional particles

by field of the wan der Waals interaction potential. Above other consistent methods one should mention a few versions of the rectilinear classical trajectories model too [1-3,20]. Besides, standard problems of adequate treating complex inter electron correlations, there are other difficulties in a correct description of collisional processes studied.

Remember that the above cited models do not account for any difference between the Penning process and resonant collisional processes. Though the Penning and stochastic collisional ionization of atomic systems remains a subject of intensive theoretical and experimental interest, however, at present time an available level of modelling these processes is still not satisfactory. The most important tasks include more accurate modelling of an external electromagnetic field on the corresponding Penning and stochastic collisional ionization processes. As for the last years a great interest has been renewed after discovery of the quantum chaos phenomenon in atomic systems in the static magnetic field [1-13,22], it is of a importance studying stochastic collisional ionization processes.

In series of papers [17, 22-24] the different aspects of new theoretical methods to the treating elementary atomic processes (1)-(3) in a presence of external electric and magnetic field were considered . In this paper we formulate a consistent, computationally effective model potential approach of accounting the external magnetic field effect in many-electron atomic system and further using in collisional problem.

2. Further we formulate the simple physical model of elementary collisional process with additional stochastic block. Let us remind the main moments of the elementary model for collisional process, in particular (1). A definition of complete cross section for the collisional process can be written as [24]:

$$\sigma = \int_0^{\infty} 2\pi\rho d\rho \{1 - \exp[- \int_{-\infty}^{+\infty} G(R)dt]\} \quad (4)$$

where $G(R)$ is a probability of the Auger effect $G(R) = 2p|V_{12}|^2 g_2$ (indexes 1 and 2 are relating to states: A^*+B and $A+B^++e$; g is a density of the final states; V is operator of interaction between atoms).

In a case when ionization process is realized in the repulsive potential of interaction between atoms in the initial channel, the cross-section is :

$$\sigma = (4\pi f_w / v) \int_{R_m}^{\infty} R^2 G(R) \sqrt{1 - U(R)/E} dR \quad (5)$$

Here v is the relative velocity of collision, R_m is the minimally possible distance of rapprochement (the turning point); f_w is the probability that the process is permitted on full electron spin of system of the collisional atoms.

The important step is to account for a possibility of decay in the second and higher orders of perturbation theory on $V(R)$. Such approach may be used as for the Penning ionization description as for ionization through the wan-der-Waalse capture [3,5, 17,24].

Let us remind that in the perturbation theory second and higher orders it is introduced the ma-

trix element: $\langle 1|V(R)G_{E_{\infty}}V(R)...V(R)|2\rangle$ consist of the simple matrix element $\langle 1|V(R)|2\rangle$ in expression for probability of collisional decay. Here $[1] \equiv [A^*+B]$ is the initial state, $[2] \equiv [A+B^++e]$ is the final state; $G_{E_{\infty}}$ is the Green function (see below); E_{∞} is an energy of quasi-molecule A^*B under $R \rightarrow \infty$.

Further one can use for operator $V(R)$ the standard expansion on non-reducible tensor operators:

$$V(R) = \sum_{l_1, l_2=1}^{\infty} V_{l_1 l_2}(n) / R^{l_1 + l_2 + 1} \quad (6)$$

$$V_{l_1 l_2}(n) = (-1)^{l_2} \sqrt{\frac{(2l_1 + 2l_2)!}{(2l_1)!(2l_2)!}} C_{l_1 + l_2}(n) \{Q_{l_1}^A \otimes Q_{l_2}^B\} \quad (7)$$

$$n = \frac{R}{R}$$

where \widehat{Q}_m is an operator of the 2^l-pole moment of atom and $C_{l_m}(n)$ is the modified spherical function. If we suppose that atom A^* is in the state with the whole moment J_i and projection on the quantization axe M_i ; in the final state the corresponding quantum numbers are $J_f M_f$; The final expression for the full probability of the electron ejection is similar to expressions in different approximation is, for example, presented in ref. [17-24].

Above the theoretical consideration concerns the standard collisional process without accounting any stochastical (or chaotic) elements. In ref. [22,23] it has been considered the perspective for realization the stochastic collisional process for a case when the atom A in process (1) is highly excited (Rydberg state). This physical situation can be adequately treated within generalized theory of chaotic drift for the Coulomb electron in the external microwave field (see refs. [4-6,19-23]).

The function of distribution $f(n,t)$ of the Rydberg electron on space of effective quantum numbers n should be introduced. The equation of motion of the Rydberg electron has the well known form:

$$\frac{\partial f(n,t)}{\partial t} = \frac{\partial}{\partial n} [\Theta(n-N_{min})D(R)n^3 - \Theta(n-N_{max})G(n,R)f(n,t)] \quad (8)$$

Here $\Theta(n-N_{min})$ is the Heviside function. It served here as additive multiplier in the coefficient of diffusion: Dn^3 and provides freezing of the stochastic processes in region of the low lying states in accordance with the known Cirikov criterion: $N_{min} < n < N_{max}$. For the Rydberg states ($n > N_{max}$) a direct channel of ionization is opened and the electron ejection takes a place. It is important to note that process will be realized with more probability under availability of the external magnetic field. So the task is further resulted in implementation of an adequate theoretical model of an external magnetic field accounting or in more details the model for computing the corresponding electron wave functions of the Zeemane problem.

3. The next step is implementation of the model potential approach to multi-electron atom in a magnetic field into collisional problem. Let us remind that despite a long history since the discovery of the Zeemane effect and sufficiently great number papers on atomic systems in an external magnetic field, hitherto a majority of results are as a little acceptable for many applications as related only the hydrogen atom (look, for instance, [4-6,11-13]). The problem of the treating many-electron atom in a magnetic field remains very complicated especially in a case of the strong field. Below we implement a simple scheme to

treating multi-electron atom in a static magnetic field. The purpose is to present the basis scheme for definition of the electron wave functions for further using in the collisional task.

The Hamiltonian of the many-electron atom in magnetic field is different from the operator of the hydrogen atom by the presence of the operator of electron-electron Coulomb interaction, which, of course, exacerbates the problem of separation of variables in the Schrödinger equation.

Because of the invariance of \hat{H} in relation to rotations around the axe Oz (it is parallel to field B and crossing a nucleus of an atom), naturally z-component of the orbital moment $L_z = \hbar M$ is the conserving variable. In the cylindrical coordinates with axe Oz||B with account of the trivial dependence of the wave function upon the rotation angle φ around the axe z ($\Psi \sim e^{M\varphi}$), one could write the corresponding equation in the form (in atomic units: $e=\hbar=m=1$):

$$\left\{ \frac{\partial^2}{\partial \rho^2} + \frac{1}{\rho} \frac{\partial}{\partial \rho} + \frac{\partial^2}{\partial z^2} - \frac{M^2}{\rho^2} - 4\gamma^2 \rho^2 + \frac{4}{r} + V_c(r) + \left(\frac{E}{R_y} - \gamma M \right) \right\} \Psi(\rho, z) = 0 \quad (9)$$

where $V_c(r)$ is the self-consistent model potential (analog of the Hartree-Fock potential). It can be, for example, chosen in the Green et al like form (look details in Ref. [5,16], which indeed well approximates the Hartree potential:

$$V = -\frac{(N_c - 1)\Omega(r)}{r} \quad (10)$$

where the screening function is

$$\Omega(r) = 1/[\exp(r/d_1 - 1) + d_2]$$

and $d_{1,2}$ are the known parameters of the model potential.

Naturally the equation (9) has not an analytical solution as the Coulomb interaction term with $r = (\rho^2 + z^2)^{1/2}$, prevents to the variables separation. As usually the equation (9) can be in some approximation rewritten as follows:

$$Hy(r,z) = Ey(r,z) \quad (11)$$

$$\begin{aligned}
H &= -1/2(\partial^2 / \partial \rho^2 + 1/\rho \partial / \partial \rho + \\
&+ \partial^2 / \partial z^2 - m^2 / \rho^2) \\
V(\rho, z) &= -(\rho^2 + z^2)^{-1/2} + (N_c - 1) \times \\
\Omega(\rho^2 + z^2)^{-1/2} + 1/8\gamma^2 \rho^2 + \gamma m / 2,
\end{aligned} \quad (12)$$

Where, as usually, $g = B/B_o$ ($B_o = 2,3505 \times 10^9$).

The potential $1/8\gamma^2 \rho^2$ limits a motion in the direction, which is perpendicular to the B direction. In the region $\gamma \gg 1$ the electron motion along (or perpendicular) magnetic field is defined by the Coulomb interaction (by a size of the cyclotronic orbit $\lambda = (\hbar c / \mathcal{M})^{1/2}$). The simplified circumstance is that the potential of the longitudinal Coulomb interaction can be received by way of the averaging the total Coulomb potential $e^2(\rho^2 + z^2)^{-1/2}$ on the little radius of the transverse motion.

The one-particle energy for given values of magnetic field B is defined as:

$$\varepsilon_{B\mu} = (m_\mu + |m_\mu| + 2s_{z\mu} + 1)\gamma / 2 - \varepsilon_\mu \quad (13)$$

where ε_m - one-particle energy (the field is absent), $S_z m$ is the spin projection on the axe z .

After the analytical integration on the angles, two-dimensional (r, z) Schrodinger equation (12) is solved by the finite difference method. One-electron function is represented in the form:

$$\Psi_\mu(\rho, \phi, z) = (2\pi)^{-1/2} e^{-im_\mu \phi} \psi_\mu(z, \rho) \quad (14)$$

where m is the number of electrons numbers, each of which is described by a certain value of the magnetic quantum number m_m . Note that unlike the hydrogen-like system for a multi-electron atom is an essential consideration of the effects of electron correlations and exchange. The numerical solution of the written equations can be performed on the basis of the differences-grid standard method. Really, according, for example, to [5], under the differences solving, an infinite region was replaced by rectangular area: $0 < r < L_\rho$, $0 < z < L_z$ by sufficient large size, in which there

is constructed a uniform grid with steps h_ρ , h_z . On the outer boundary there are set conditions: $(\partial \Psi / \partial n)_r = 0$. In the absence of a field, the wave function decreases at infinity like $\exp[-(-2E)^{1/2} r]$. In the presence of E must be replaced with the ionization energy of the stationary state in the lowest Landau level: $(-E)$. A rough estimate for L :

$L = 15(-2E)^{-1/2}$. Derivatives of r are approximated $(2m + 1)$ -point symmetric difference schemes obtained by differentiating the interpolation formula of Lagrange. For the second derivative z used symmetric three-point difference scheme. The eigenvalues of the Hamiltonian are calculated based on the method of inverse iterations. The corresponding system of inhomogeneous equations solved by Thomas (look details, for example, in Ref. [5]). Naturally, the concrete realization of such a algorithms and its further implementation into collisional problem block requires significant computational work and will be considered in the next paper. Here let underline that using the simple model potential model simplifies all theory. Though, it is obvious that in a case of the stochastic collisional process, in particular, with Rydberg collided atoms, the model became more complicated to take into account the possible essential changing stochastic mechanism due to an effect of the external field.

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Abstract.

The key physical aspects of the Penning and stochastic collisional ionization of atoms in an external magnetic field are considered and new model potential approach has been implemented in order to take into account an effect of magnetic field on multi-electron atom energy parameters and to compute the wave functions basis for next using in the collisional block. The corresponding Schrödinger equation for atom in a magnetic field and the Focker-Plank stochastic equation are solved within the standard differences-grid method.

Key words: Penning and stochastic collisional ionization, magnetic field, model potential approach

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ПЕННИНГОВСКАЯ И СТОХАСТИЧЕСКАЯ СТОЛКНОВИТЕЛЬНАЯ ИОНИЗАЦИЯ АТОМОВ ВО ВНЕШНЕМ МАГНИТНОМ ПОЛЕ: СХЕМА НА ОСНОВЕ МОДЕЛЬНОГО ПОТЕНЦИАЛА

Резюме.

Рассмотрены ключевые физические аспекты пеннинговской и стохастической столкновительной ионизации атомов во внешнем магнитном поле и сформулирован новый подход к решению задачи учета влияния внешнего магнитного поля на энергетические параметры многоэлектронных атомов и вычисления базиса волновых функций для последующего использования в столкновительном блоке. Соответствующее уравнение Шредингера для атома в магнитном поле и стохастическое уравнение Фоккера-Планка решаются в рамках стандартном конечно-разностного метода сеток.

Ключевые слова: пеннинговская, стохастическая столкновительная ионизация, магнитное поле, подход на основе модельного потенциала

Г. О. Кузнецова

ПЕННІНГІВСЬКА ТА СТОХАСТИЧНА ЗА РАХУНОК ЗІТКНЕНЬ ІОНІЗАЦІЯ АТОМІВ У ЗОВНІШНЬОМУ МАГНІТНОМУ ПОЛІ: СХЕМА НА ОСНОВІ МОДЕЛЬНОГО ПОТЕНЦІАЛА

Резюме.

Розглянуті ключові фізичні аспекти пеннінговской і стохастичною зіткнень іонізації атомів у зовнішньому магнітному полі і сформульований новий підхід до вирішення завдання врахування впливу зовнішнього магнітного поля на енергетичні параметри багатоелектронних атомів і обчислення базису хвильових функцій для подальшого використання в блоці зіткнення. Відповідне рівняння Шредінгера для атома в магнітному полі і стохастичне рівняння Фоккера-Планку вирішуються в рамках стандартного скінченно-різницевого методу сіток.

Ключові слова: пеннінгівська, стохастична за рахунок зіткнень іонізація, магнітне поле, підхід на основі модельного потенціалу