Transition from heating to cooling of channeled ion beams

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Experiments showing a transverse heating or cooling of channeled ion beams are explained in terms of electron capture and loss processes between the projectile ions and the target. Such processes violate reversibility as the projectile captures electrons from occupied bound states and loses them to unoccupied weakly bound or continuum states. The transition probabilities for the transfer of electrons are calculated in the impact parameter Born approximation. Their dependence on the distance from the crystal strings is determined by scale factors which depend in turn on the relative velocity and the binding energies of the transferred electrons in the projectile and in the crystal, respectively. The appearance of transverse heating and cooling depends on the relative size of the scale factors for capture and loss. The transition from heating to cooling as function of velocity is described in good agreement with the experiments.

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I. INTRODUCTION

Ion beams can be cooled effectively by interaction with laser beams which must be colinear for a large overlap region. Likewise, cooling by comoving electron beams predominantly takes place in the longitudinal direction, where the electron temperature (i.e., the momentum spread) is much smaller than in the transverse direction due to the acceleration from the electron gun. For transverse cooling, other methods must be developed. Experiments on the angular distribution of initially isotropic heavy ions show a redistribution of flux after passage through Si crystals. In some cases, an enhancement along the channeling directions has been observed (transverse cooling); in other cases, a reduction (transverse heating) [1–5]. This seems to contradict the principle of detailed balance for the scattering of channeling ions which rests on the time reversibility of trajectories [6,7]. The observations have been explained in terms of a mechanism in which the cooling or heating of the transverse motion of the channeling ions is due to the transfer of electrons between the projectile and the crystal atoms. As the transverse potential $V_\perp$ between the ion and the atomic rows of the crystal is repulsive and decreases with distance, the ion loses transverse energy if capture tends to take place at smaller distances r_c from the atomic row than loss r_l, and vice versa. Typical parameters were deduced from total cross sections for capture and loss [8]. The proposed mechanism is shown in a schematic manner in Fig. 1 which has been adapted from Ref. [1]. Later experiments showed that there is no heating of channeled ions at low velocities if the projectile is lighter than the crystal atoms [2]. However, for heavy ions, a transition from heating to cooling has been observed if the relative velocity is increased [3–5]. This cannot easily be explained in terms of effective impact parameters for capture and loss. Instead, the experiments have been simulated by classical trajectory Monte Carlo calculations of the projectile with two strings of N atoms each carrying n electrons [4,5,9]. Such a simulation aims at a self-consistent description of the inelastic processes accompanying the passage of the channeling projectile through the target. Electrons are exchanged between the target atoms and the projectile, whose fluctuating charge state in turn influences the interaction with the target. In the experiments under consideration, a local charge equilibrium has been reached. In the simulations, reversibility is broken as the probabilities for electron capture and loss have a different dependence on the impact parameter. While the experimentally observed transition velocities were fitted to the charge of the projectile, no reference to an underlying model has been made. Moreover, a recent study of transport cross sections [10] indicates that classical mechanics is only marginally applicable for the ion charge states and projectile velocities occuring in these experiments.

For the special case of hydrogenic orbits there exist closed quantum mechanical expressions for the impact parameter dependence of the transfer amplitudes [11]. These involve scale factors which depend in turn on the binding energies of the transferred electron in the projectile and in the target, respectively, and on the relative velocity. In such a model system, the transition from heating to cooling can be

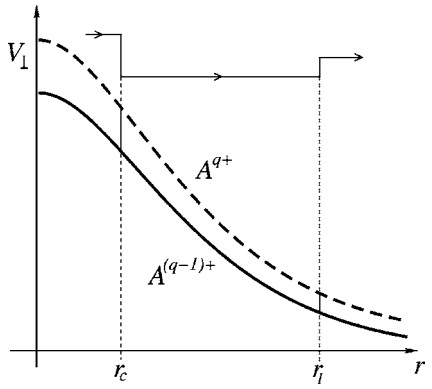

FIG. 1. Transverse potential for a channeling projectile, which loses transverse energy by capturing an electron at r_c and gains transverse energy by losing an electron at r_l (Ref. [1]).

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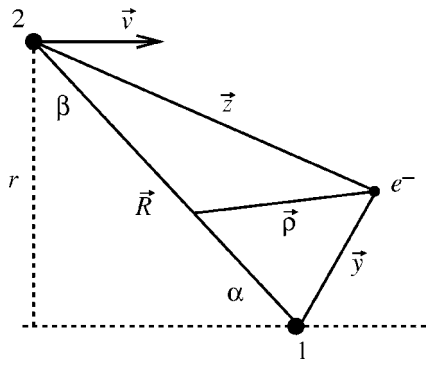

FIG. 2. Coordinate system for the transfer of an electron between Target 1 and Projectile 2.

demonstrated in a transparent manner [12]. An inspection of the transfer amplitudes shows that there are leading terms from the transitions between *s* states. The contributions from all other terms cancel in averaged quantities, such as the cross section for the transfer between major shells. Adopting the *shape* of these leading terms for the general case, the impact parameter-dependent transfer amplitudes are parametrized by binding energies taken from many-body calculations for arbitrary atoms and ions [13,14]. This allows a derivation of a closed formula for the transition velocity in terms of the binding energies of the transferred electrons in the target and the projectile, respectively.

II. SCHEMATIC MODEL: TRANSFER BETWEEN HYDROGENIC STATES

The channeling projectiles move on nearly straight trajectories between the crystal strings and they are confined by the transverse potential to regions outside the atomic core. The amplitudes of the individual transitions can be calculated in the impact parameter Born approximation [11]. Atomic units (a.u.) will be employed, i.e., impact parameters r are measured in units of the Bohr radius $r_0=\hbar^2/(e'^2m)$, the projectile velocity v in units of $v_0=e'^2/\hbar\approx c/137$, energies in units of $e'^4m/\hbar^2$, and times in units of $\hbar^3/(e'^4m)$, where $e'^2=e^2/(4\pi\varepsilon_0)$ with the elementary charge e, the electron mass m, and the permittivity of the vacuum ε_0. Assuming hydrogenic wave functions, the transfer amplitude A can be evaluated in closed form. The matrix element for the transfer from a single-particle state $\varphi^{(1)}$ in the target atom to a state $\varphi^{(2)}$ in the projectile with (effective) charge number Z_2 is

$$V_{12}(\vec{R})=\int \varphi^{(2)*}(\vec{z})\frac{(-Z_2)}{z}\varphi^{(1)}(\vec{y})e^{-i\vec{v}\cdot\vec{\rho}}d^3\rho \tag{1}$$

in the post form [11]. Here $\vec{R}$ is the distance vector between the projectile and target nuclei, $\vec{\rho}$ is the vector from the cm to the electron while $\vec{z}=-\beta\vec{R}+\vec{\rho}$ and $\vec{y}=\alpha\vec{R}+\vec{\rho}$ are the electron coordinates in the projectile and the target, respectively, see Fig. 2.

Because of the relative motion with velocity $\vec{v}$, the transition amplitude

$$A_{12}=\int_{-\infty}^{\infty} V_{12}(\vec{R})e^{-i(E_1-E_2)t}e^{(i/2)v^2(\beta^2-\alpha^2)t}dt \tag{2}$$

involves not only the difference of the binding energies E_1-E_2 but also translation factors. It is advantageous to express the wave functions in Fourier space

$$F(\vec{k})=\int d^3y\varphi^{(1)}(\vec{y})e^{i\vec{k}\cdot\vec{y}},$$

$$G(\vec{k})=Z_2\int d^3z\varphi^{(2)}(\vec{z})z^{-1}e^{i\vec{k}\cdot\vec{z}}, \tag{3}$$

and to introduce cylindrical coordinates along $\vec{n}=\vec{v}/v$, i.e., $k_\parallel=\vec{k}\cdot\vec{n}$ and $\vec{k}_\perp=\vec{k}-k_\parallel\vec{n}$. Because of $\vec{R}=\vec{r}+\vec{v}t$, the time integral in Eq. (2) yields a δ-function and the transition amplitude which is axially symmetric, can be expressed as

$$A_{12}(r)=-\frac{1}{4\pi^2v}\int d^2k_\perp e^{-i\vec{k}_\perp\cdot\vec{r}}\cdot G^*\left(\vec{k}_\perp,\frac{1}{2}v-\frac{E_1-E_2}{v}\right)F\left(\vec{k}_\perp,-\frac{1}{2}v-\frac{E_1-E_2}{v}\right). \tag{4}$$

The cross sections for a transfer

$$\sigma_{12}=\int d^2r|A_{12}(r)|^2=\frac{1}{(2\pi)^4v^2}\int d^2k_\perp\cdot\left|G\left(\vec{k}_\perp,\frac{1}{2}v-\frac{E_1-E_2}{v}\right)\right|^2\left|F\left(\vec{k}_\perp,-\frac{1}{2}v-\frac{E_1-E_2}{v}\right)\right|^2 \tag{5}$$

between hydrogenic subshells $n_1, l_1\leftrightarrow n_2, l_2$ have been evaluated in closed form using parabolic coordinates [15]. Much simpler expressions result if one also sums with respect to the angular momenta l_1 and l_2 [16]. Using the Fourier transforms of hydrogenic wave functions [17] in Eq. (5), the result for the transition between states with principal quantum numbers n_1 and n_2 is

$$\sigma_{n_1,n_2}=\frac{1}{n_1^2}\frac{2^{11}\pi(Z_1Z_2)^2(E_1E_2)^{3/2}}{5v^2x^{10}}. \tag{6}$$

This shows explicitly the symmetry between capture and loss, or equivalently, between the post and prior formulations of the transfer processes, as the extra factor n_1^{-2} results from the averaging with respect to the initial states. Here, x is a scale factor which depends on the relative velocity v and the binding energies E_1 and E_2 in the target and the projectile, respectively

$$x^2=\frac{v^2}{4}+E_2+E_1+\frac{1}{v^2}(E_2-E_1)^2. \tag{7}$$

As discussed above, the heating or cooling of channeling ion beams is related to the dependence of the transfer amplitude A on the impact parameter r. For hydrogenic wave functions, the $\vec{k}_\perp$ integrations in Eq. (4) can be done in closed form, explicit examples are presented in the Appendix. The general form of the transfer amplitudes is the linear combination

$$A(r) = \sum_{m\geqslant 0} \sum_{p\geqslant 2} c_{p,m}(rx)^{p+m} K_p(rx), \tag{8}$$

where the $K_p(z)$ are modified Bessel functions of order p. All contributions $(rx)^p K_p(rx)$ behave in a similar manner as functions of rx: An inverted parabola for $rx \lesssim 1$ and an exponential tail for $rx \gtrsim 1$. This determines then also the shape of the transition amplitude on a scale set by the parameter x (7). Insertion of the explicit expressions (8) into Eq. (5) and performing the integration with respect to the impact parameter return the expression (6) for the averaged total transfer cross section. This suggests that the transitions are dominated by the exterior tails of the wave functions rather than by the details of the interior node structure. Moreover, explicit calculations demonstrate that this leading term is also sufficient to describe the *shape* of the transfer amplitude (8) [12]. This encourages one to generalize Eq. (7) for the scale factors by employing binding energies taken from many-body calculations for arbitrary atoms and ions [13,14].

III. EFFECTIVE MODEL: RESULTS AND DISCUSSION

The transition amplitude A depends through the scale factor x on the projectile velocity v and the binding energies of the electron in the target and the projectile. As A is a decreasing function of its argument, a larger scale factor favors transitions at smaller impact parameters. Thus, if the scale for capture x_c is larger than that for loss x_l, capture tends to take place at smaller distances from the crystal strings than loss, $r_c < r_l$, which leads to transverse cooling, and vice versa for heating. Assuming that the unoccupied target states which are populated through electron loss from the projectile have a negligible binding energy the scale factors (7) are

$$x_l^2 = \frac{v^2}{4} + E_2 + \frac{E_2^2}{v^2}, \tag{9}$$

$$x_c^2 = \frac{v^2}{4} + E_2 + E_1 + \frac{1}{v^2}(E_2 - E_1)^2, \tag{10}$$

for loss and capture, respectively. Here, E_2 is the binding energy of the transferred electron in the projectile and E_1 is the binding energy of the occupied state in the target. For highly charged heavy projectiles, the binding energies E_2 in the projectile are larger than the target binding energies E_1. Graphs of x_l (solid curve) and x_c (dashed curve) as functions of v are shown in Fig. 3 for $E_2 = 10$ and $E_1 = 4.3$.

The two graphs intersect at the critical velocity v_t for the transition between heating and cooling

$$v_t = (2E_2 - E_1)^{1/2}. \tag{11}$$

At low velocities $v < v_t$, the scale factor for capture is smaller than that for loss, leading to heating, and vice versa cooling is obtained for $v > v_t$. For $E_2 < E_1/2$, there is no such transition in accordance with the experimental observation [2] of the absence of heating for light projectiles, i.e., small binding energies E_2.

For an explicit evaluation of the transition velocity, the excitation energy of the projectile ion must be taken into account. The average energy $\overline{E_2}$ of the states populated in the projectile is estimated with the help of the cross section (6):

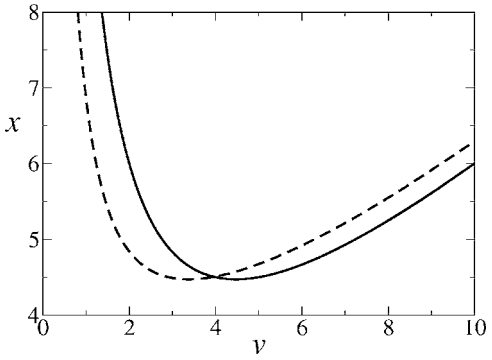

FIG. 3. Scale factors x_l for loss (solid curve) and x_c for capture (dashed curve) as function of the velocity v for a binding energy $E_2 = 10$ in the projectile and $E_1 = 4.3$ in the target.

$$\overline{E_2} = \frac{\int_0^{E_2^{(0)}} E_2 \sigma dE_2}{\int_0^{E_2^{(0)}} \sigma dE_2} \approx \frac{5}{7} E_2^{(0)}, \tag{12}$$

where $E_2^{(0)}$ is the ground state ionization energy of the projectile. Inserting this average energy $\overline{E_2}$ into Eq. (6) the transition velocity is

$$v_t = \left(\frac{10}{7} E_2^{(0)} - E_1\right)^{1/2}. \tag{13}$$

For a comparison with experiments on channeling of heavy highly charged ions in Si [4,5], we assume in accordance with the earlier treatment [1] that the projectile captures electrons mainly from the Si L shell with a binding energy $E_1 = 4.3$. This and the other binding energies are obtained from the tables of Fricke *et al.* [13] for ions and atoms up to an atomic number $Z \leqslant 54$ and for Pb [14]. The ground state ionization energies $E_2^{(0)}$ were taken for various charge states q around the estimate $v_{t,\mathrm{exp}} Z^{1/3}$ [8], where $v_{t,\mathrm{exp}}$ are the transition velocities as observed in the experiments. Such charge states are also obtained from the tables of Shima *et al.* [18].

In Table I, the theoretical values v_t for the transition velocity are compared with the measurements. The present model gives a good account of the transition from heating to cooling both as the absolute values of the transition velocities and their dependence on the projectile are concerned. In the experiments, the excitation energy and the charge state fluctuate in the course of the numerous transfer processes during the passage of the projectile through the crystal. This masks any shell effects, e.g., for Ne-like Ni. The dependence of the transition velocity on the energy E_1 of target states from which electrons are captured is weak for $E_2^{(0)} \gg E_1$ as in the present application. Moreover, larger energies E_1 are improbable because of Eq. (6). Because of shielding, the actual binding energies in the projectile depend on their charge number in a complicated manner. So, this model provides no physical basis for a simple power law as in Refs. [4,5].

TABLE I. Experimental [4,5] and theoretical transition velocities (9) for projectiles with atomic number Z and various charge states q around $v_{t,\mathrm{exp}}Z^{1/3}$.

Projectile	Z	$v_{t,\mathrm{exp}}$ [4,5]	q	$E_2^{(0)}$ [13,14]	v_t (8)
Ti	22	5.4	14	31.7	6.2
			15	34.5	6.7
			16	38.2	7.1
Ni	28	6.0	17	20.9	5.1
			18	22.2	5.2
			19	56.8	8.7
Br	35	6.7	22	33.7	6.6
			23	35.3	6.8
			24	39.4	7.2
Y	39	7.0	23	39.2	7.2
			24	41.0	7.4
			25	41.4	7.4
Ag	47	7.7	27	51.0	8.2
			28	53.7	8.5
			29	56.5	8.8
J	53	8.1	29	60.0	9.0
			30	63.4	9.3
			31	66.8	9.5
Pb	82	9.9	42	73.8	10.3
			43	76.8	10.7
			44	79.6	11.1

Obviously the model presented here cannot exactly account for transfer processes between definite states. Rather, it aims at an average description for which the redistribution of strength due to collective effects is not so important. The occurence of transversal heating and cooling for channeling ions is traced back to the matrix elements for the transfer of electrons between the projectile ions and the crystal atoms. The dependence of these amplitudes on the impact parameter depends sensitively on the velocity of the projectile and the binding energies of the transferred electrons in the projectile and the target. Reversibility is violated as the projectile captures electrons from occupied strongly bound target states and loses them to weakly bound or unbound states. The excitation of the projectile above its ground state is estimated with the help of total cross sections. The model predicts no heating for light projectiles and a transition from heating to cooling with increasing velocity of heavy projectiles. The transition velocities obtained in this model which contains no adjustable parameters are in good agreement with the experiments. The quantum mechanical estimate of the impact parameter-dependent transition amplitudes confirms on a microscopic basis the validity of the charge exchange model [1].

It seems desirable to exploit the features of the individual transfer processes in simulations of the complete passage of the channeling projectiles through the target crystal in order to obtain a more transparent understanding for the absolute values of observables like the mean charge state and the deviations of the energy loss from their random values.

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APPENDIX

For an explicit evaluation of the transfer amplitude (4), the Fourier transforms

$$F_{nlm}(\vec{k}) = f_{nl}(k)Y_{lm}(\hat{\vec{k}}) \tag{A1}$$

can be expressed in terms of Gegenbauer polynominals in the hydrogenic case [17]. With the help of the Schrödinger equation, one obtains

$$G_{nlm}(\vec{k}) = \left(\frac{1}{2}k^2 + E_2\right)F_{nlm}(\vec{k}). \tag{A2}$$

Explicit expressions in cylindrical coordinates for the transition between s-states from $n_1=3$ to $n_2=2$ are, for example

$$F_{300}\left(\vec{k}_\perp, -\frac{1}{2}v - \frac{E_1 - E_2}{v}\right) = 2^{15/4}3^{-1}\pi^{1/2}Z_1E_1^{3/4} \cdot \left[\frac{3}{(k_\perp^2 + x^2)^2} - 32E_1\left(\frac{1}{(k_\perp^2 + x^2)^3} - \frac{2E_1}{(k_\perp^2 + x^2)^4}\right)\right] \tag{A3}$$

and

$$G_{200} = 2^{11/4}\pi^{1/2}Z_2E_2^{3/4}\frac{k_\perp^2 + x^2 - 4E_2}{(k_\perp^2 + x^2)^2} \tag{A4}$$

with x given in Eq. (7).

The transition amplitude (4) has the form (8) with the leading term

$$A_{300,200}(r) = -\frac{2^{5/2}}{v}Z_1Z_2(E_1E_2)^{3/4}\frac{r^2}{x^2}K_2(rx) + \ldots \tag{A5}$$

The contribution from this term to the cross section

$$\sigma = \frac{2\pi}{3^2}\int drr|A(r)|^2 = \frac{1}{9}\frac{2^{11}\pi(Z_1Z_2)^2(E_1E_2)^{3/2}}{5v^2x^{10}} \tag{A6}$$

already exhausts the total cross section (6) from the major shell $n_1=3$ to $n_2=2$, i.e., all other contributions to that cross section cancel.

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