

$$\rho_{\alpha\alpha}^{rs}(t=0) = w_{\alpha} |r\rangle \langle s|, \quad (2)$$

where  $|r\rangle$  refers to a Gaussian or Coulomb wave packet describing the internuclear motion on a radial grid [18]. We have tested two different initial wave packets with the same Gaussian envelope but two different boosts,  $\mathcal{B}(k_0 r)$ , namely a plane wave ( $e^{-ik_0 r}$ ) and an incoming Coulomb wave,  $H_{L=0}^{-}(k_0 r)$ :

$$\psi(r, r_0, \sigma_0, k_0) = \mathcal{N}^{-1} \exp\left[-\frac{(r-r_0)^2}{2\sigma_0^2}\right] \mathcal{B}(k_0 r), \quad (3)$$

where  $\mathcal{N}$  is a normalisation constant,  $r_0$  is the initial, central position of the wave packet,  $r$  is a radial grid position,  $\sigma_0$  is the spatial dispersion, and  $k_0$  is the average wave number, which depends on the average incident energy  $E_0$ ,  $r_0$  and  $\sigma_0$  and is found by solving  $E_0 = \langle \psi | \hat{H} | \psi \rangle$ ,  $\hat{H}$  being the Hamiltonian of the collision. Eq. (3) with a plane-wave boost is a Gaussian wave packet, while this is a Coulomb wave packet when a Coulomb-wave boost is used.

In Eq. (2), the density matrix is diagonal in the energy eigenstate basis, denoted by  $|\alpha\rangle$ . The initial population of the energy eigenstates is given as,

$$w_{\alpha} = \frac{(2I_{\alpha} + 1) \exp\left\{-\frac{e_{\alpha}}{\mathcal{T}}\right\}}{\sum_{\alpha'=1}^N (2I_{\alpha'} + 1) \exp\left\{-\frac{e_{\alpha'}}{\mathcal{T}}\right\}}, \quad (4)$$

where  $I_{\alpha}$  is the spin value. Since the present calculations only include excited states of the  $^{188}\text{Os}$  ground-state rotational band, the spin degeneracy factors in Eq. (4) will be irrelevant. Excited states are thermally populated before the target and projectile interact with each other and thermodynamic equilibrium is assumed at the start of the reaction [19, 20]. As known from coupled channels calculations, coupling of the radial motion to energy eigenstates can cause changes in fusion probability. Population of excited states in either the target or projectile nucleus due to surface vibrations or rotational excited states lead to an overall increase in fusion probability due to coherent coupled channels effects [21]. For the dynamical calculations, we use the same equation of motion for the density matrix of the reduced system as the one used in Ref. [18], Eq. (5). This method uses the Lindblad master equation, allowing coupling between the radial and energy eigenstate bases, and uses Lindblad operators to introduce novel effects into the calculation. An energy projection technique is used to calculate the fusion probability for specific collision energies [18].

In the following calculations, we use a  $^{188}\text{Os}$  target nucleus due to its low-lying  $2^+$  rotational excited state at 155 keV [22] and a  $^{16}\text{O}$  projectile nucleus due to its

high 6.13 MeV first excited state. Hence we only consider the ground state of  $^{16}\text{O}$  and the ground and first excited state of  $^{188}\text{Os}$ . The parameters used in these calculations are the same as in Ref. [18], except from the potential parameters which are unique to the projectile and target pair. The Woods-Saxon nuclear interaction potential parameters used in this work are:  $V_0 = 60.64$  MeV,  $R_0 = 1.2$  fm,  $a_0 = 0.63$  fm, and these parameters provide the same height of the uncoupled Coulomb barrier ( $V_B = 71.7$  MeV) as the microscopic São Paulo potential [23]. The deformation parameter of the 155 keV excited state is  $\beta_2 = 0.184$  [24].

*Atomic effects.* NPI effects are included in the calculations by introducing new matrix elements into Eq. (5) of Ref. [18],

$$\Gamma_{12}^{rr} = \gamma_{12} \quad (5)$$

$$\Gamma_{21}^{rr} = \gamma_{21}, \quad (6)$$

where  $\gamma_{12}$  and  $\gamma_{21}$  are the respective excitation and de-excitation rates between the ground state and first excited state of  $^{188}\text{Os}$ . These affect the excited state population, dependent on the temperature and density of the plasma. The relevant rates for this work are shown in Table I, and were calculated using the ISOMEX code [25], which is based on the relativistic average atom model and assumes local thermal equilibrium. The considered excitation processes due to NPIs are: resonant photon absorption, inelastic electron scattering, NEEC and NEET. The de-excitation processes include spontaneous photon emission, induced photon emission, internal conversion, bound internal conversion (BIC), and super-elastic electron scattering. Since the excited state of  $^{188}\text{Os}$  is much higher than the binding energy of the K-shell atomic orbitals, NEET and BIC do not contribute to the plasma induced nuclear transition rates.

It was found that the effects of NPIs were negligible ( $< 10^{-6}$  % increase in fusion probability) for a  $^{16}\text{O}$  projectile and  $^{188}\text{Os}$  target, at all temperatures and densities considered. Considering that the timescale of the fusion reactions is of the order of  $10^{-22}$  s, the effective excitation rates are too low to have an impact on the population of the excited state [26] and therefore the overall effect on fusion is weak.

Nuclear fusion reactions are commonly initiated from the ground state of the collision partners. Should scenarios exist where fusion reactions are initiated from long-lived intrinsic high angular momentum excited states, the NPIs would be more effective [27]. Additionally, a recent experiment [28] showed that missing excited electronic configurations could be a reason for discrepancy between theory and experiment for NEEC reactions.

*Results and discussion.* We construct the coupled channels fusion probability of a zero temperature, environment-less fusion reaction for an inert  $^{16}\text{O}$  projectile and  $^{188}\text{Os}$  target with two states (ground and first excited state), given in Fig. 1. Multiple wave packets with different initial mean energies ( $E_0$ ) were used to