Resonance Phenomena in Electron Capture Processes by Multiply Charged Ions

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At low collision energies, interesting phenomena such as shape resonance and orbiting appear in electron capture processes [1-3]. Shape resonance causes peaks in cross sections at particular collision energies because quasi-molecules are formed during collisions. Furthermore, orbiting causes a monotonic increase in cross sections with decreasing velocity. Mechanism of orbiting is usually explained by classical scattering trajectories such as projectile ions rotating around target atoms [4].

Shimakura and Kimura (1991) have reported that shape resonance and orbiting occur in electron capture by N^{5+} ions from H atoms [2]. However, the dynamical mechanism of shape resonance was not evident because a time-independent close-coupling method was used in their calculation. In this work, we show the examples of the shape resonance for some systems and then provide a dynamical picture of shape resonance for the case of (N^{5+} + H) system by using a multi-channel wave packet method that can solve the time-dependent close-coupling equations in order to elucidate the mechanisms of shape resonance. The method based on the split-operator technique is efficiently implemented with the aid of fast Fourier transform [5].

Figure 1 shows the cross sections of the N^{5+} + H collision calculated by using a time-independent close-coupling method. In this calculation, only three Σ states are considered, *i.e.*, 1Σ, 2Σ, and 3Σ states corresponding to the $N^{4+}(4s) + H^+$, $N^{4+}(4p) + H^+$, and N^{5+} + H (1s) states at the separated atom limit, respectively. The solid and broken lines in figure 1 represent the partial cross sections of the $N^{4+}(4s) + H^+$ and $N^{4+}(4p) + H^+$ states, respectively. Several peaks appear below E = 0.02 eV/amu. Squared scattering matrices around collision energies at which peaks appear show that each peak is dominated by the partial wave with a particular angular momentum K. This indicates that in the effective potentials with such angular momenta quasi-bound states are formed and the effective potential produces a well with a centrifugal barrier. Thus, shape resonance occurs when the collision energy coincides with that of the rovibrational state of the quasi-molecule. The peaks can be assigned to vibrational v and rotational K states. The rovaibrational states (v, K) used for the assignment in Fig.1 are quasi-bound states of the adiabatic 3Σ effective potential and the states (v, K)* are those of the diabatic potential smoothly connecting the adiabatic 2Σ and 3Σ effective

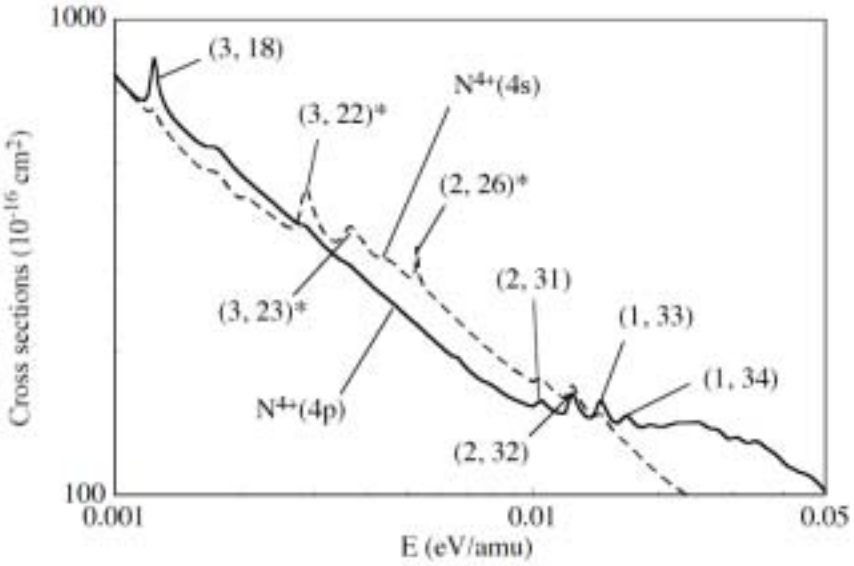

Fig. 1. Electron-capture cross-sections in the (N^{5+} + H) collision system. The partial cross sections of the N^{4+}(4s) + H^+ and N^{4+}(4p) + H^+ states are denoted by solid and broken lines, respectively. The peaks are assigned to resonance rovibrational states (v, K) and (v, K)*. The definitions of these states are given in the text.

potentials. These rovibrational states and energies were obtained by using the Rydberg-Klein-Rees method [6-9].

To demonstrate the time-dependent picture of shape resonance for the resonance state, we calculate the wave packet dynamics. In the calculation of the dynamics, all the three potentials and non-adiabatic couplings between them are taken into account. The calculated results show many useful concepts about the shape resonance. After some times elapse, part of the wave packet is trapped into the quasi-bound potential of the 3Σ state; the other part is scattered by the centrifugal barrier. As obvious from the increase in the 2Σ component, the wave packet trapped into the quasi-bound potential transfers to the N^{4+}(4p) + H^+ channel rather than returns to the initial channel by tunneling again. We also examine a case where the collision energy is off from that of the rovibrational state. In this case, the wave packet does not tunnel through the centrifugal barrier when the collision energy does not match with the resonance energy.

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