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A Time-Dependent Quantum Study of $\text{Li}+\text{HF}(v=1) \rightarrow \text{LiF}(v')+H$

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Abstract: Time-dependent quantum wave packet calculations are performed for a model based (two-dimensional) $\text{Li}+\text{HF}(v=1) \rightarrow \text{LiF}(v')+\text{H}$ reaction. The reaction probabilities for a broad range of collision energies are calculated by a single solution of the time-dependent Schrödinger equation. The calculated reaction probabilities show many sharp features as a function of energy which are ascribed to scattering resonances.

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