Resonances in Quantum Chemistry: Complex Absorbing Potential Method for Systems

M. Melgaard

The Complex Absorbing Potential (CAP) method is widely used to compute resonances in Quantum Chemistry, both for scalar valued and matrix valued Hamiltonians. In the semiclassical limit $\hbar \to 0$ we consider resonances near the real axis and we establish the CAP method rigorously in an abstract matrix valued setting. The proof is based on pseudodifferential operator theory and microlocal analysis.

The talk is based on a joint work with J. Kungsman.