

# DIFFERENTIAL GEOMETRY/PDE SEMINAR

FRIDAY, OCTOBER 28, 2005

THO 231

2:30-3:20

A Review of Rigorous Results on Molecular Propagation

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(VIRGINIA TECH)

We review several mathematical results concerning the time-dependent Born–Oppenheimer Approximation. It is the main source of information about molecular propagation. It leads to an asymptotic expansion in powers of  $\epsilon$  for solutions to the molecular Schrödinger equation. Here  $\epsilon^4$  is the electron mass divided by the mean nuclear mass. By applying an optimal truncation technique to this expansion, we obtain an approximation whose errors are bounded by  $C_1 \exp(-C_2/\epsilon^2)$ . Born–Oppenheimer approximations break down in situations called electron energy level crossings and at avoided crossings of electron energy levels with small gaps. We describe these phenomena and their effects on the propagation of molecular wave packets.

For more information about this seminar, visit the DG/PDE Seminar Web page (from the Math Department home page, [www.math.washington.edu](http://www.math.washington.edu), follow the link **Seminars, Colloquia, and Conferences**).

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