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MATHEMATICAL FRONTIERS
Mathematics of Quantum Physics

Rick Heller, Harvard University
Xiaosong Li, University of Washington
Mark Green, UCLA (moderator)
Abbott and James Lawrence Professor of Chemistry and Professor of Physics

Quantum Physics and Mathematics

Rick Heller, Harvard University
Wave theory

• We should not forget that quantum theory is “just” another wave theory.
• Much of classical wave physics (sound, water, earthquake,...) applies to quantum waves, but the classical waves came much earlier
Quantum Physics in many dimensions has been a wellspring of mathematics

• quantum entanglement, entropy
• decoherence,
• quantum information theory,
• quantum computing,
• quantum chaos theory and semiclassical theory
• string theory

All these aspects and many more are a wellspring of new mathematics
String theory

• String strives to be the ultimate quantum theory.

• Robbert Dijkgraaf writes: “The number of [mathematical] disciplines that it [string theory] touches is dizzying: analysis, geometry, algebra, topology, representation theory, combinatorics, probability — the list goes on and on.”
Example-Green function

• The **Dirac** delta function, with antecedents from the work of Cauchy, Poisson, Kirchhoff, Green, Helmholtz, Kelvin

• **Feynman** path integral

• Stationary phase evaluation (**Stokes, Kelvin**) of the path integral leads to the (semi)-classical limit and a window on our reality

• The **Feynman** path integral is darn close to **Huygen’s** principle and **Kirchhoff** diffraction theory
Feynman path integral

\[ S_j \equiv S(q_j, q_{j+1}, \tau) = \frac{m(q_j - q_{j+1})^2}{2\tau} - V(q_{j+1})\tau \]

\[ G(q, q', t) = \lim_{N \to \infty} \int \ldots \int \prod_j dq_j \ e^{i \sum_j S_j / \hbar} \]

\[ = \sum_{All \ Paths} e^{i S_{path} / \hbar} \]
Stationary phase on the Feynman path integral – the classical paths emerge
Quantum Chaos

• Suppose the classical path is (deterministically) chaotic. Does the stationary phase still work?

• This leads to
  – Van Vleck-Morette-Gutzwiller semiclassical propagator
  – Selberg trace formula
  – Gutzwiller trace formula
  – Deep connections between quantum chaos, random matrices, and distribution of prime numbers
Quantum Chaos

• Understanding the connections between classical chaos theory and quantum physics leads to beautiful and very deep mathematics, including number theory and the complex zeros of the Riemann zeta function,

\[
\zeta(s) = \sum_{n=1}^{\infty} \frac{1}{n^s} = \prod_{p \text{ prime}} \frac{1}{1 - p^{-s}}
\]
Scar Theory

• It came as a surprise (1984) that some quantum eigenfunctions of ergodic classical systems are not ergodic and scarred (high probability) along closed geodesics – periodic orbits. This is still under investigation.
Discover and theory of scars

• Scars were discovered graphically, by plotting eigenfunctions. This was done with a computer program implementing a new mathematical approach to finding them.

• Then, the theory of why they appear was given, using asymptotic semiclassical arguments for time domain quantum mechanics and its Fourier transform.
Many body

• Another realm, many body physics, is truly intractable; models of the real thing must be used. They are better than the exact answer anyway, because we get an intuitive grasp.

• The search for “emergent phenomena” in many body models is mathematical; pure or computational.
More Feynman quotes

• “If all mathematics disappeared today, physics would be set back exactly one week,”
• To which a mathematician replied “True – if you mean the week that God created the Universe!”
• “Shut up and calculate” (attributed to Feynman, but David Mermin claims it).
The mathematical challenges

• All but the simplest quantum systems are far too difficult to understand exactly.

• The super-challenges facing quantum physics are explaining emergent phenomena, like superconductivity, an unexpected many body effect.
MATHEMATICAL FRONTIERS
Mathematics of Quantum Physics

Harry and Catherine Jaynne Boand
Endowed Professor of Chemistry

co-Associate Chair for Graduate Education

Electron’s Dance

Xiaosong Li,
University of Washington

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What do Electrons Look Like in Molecules?

Quantum Physics

– from math to electron wave functions

\[ \hat{H} \Psi = E \Psi \]

\[ \hat{H} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \hat{V} \]
What do Electrons Look Like in Molecules?

Quantum Physics

– from atoms to molecules

\[ \psi = \sum_i c_i \phi_i \]
What do Electrons Look Like in Molecules?

Time-Dependent Quantum Physics

– from quantum physics to spectroscopy

\[ i\hbar \frac{\partial \psi(x, t)}{\partial t} = \hat{H} \psi(x, t) \]

\[ \psi(x, t) = e^{-\frac{iEt}{\hbar}} \psi(x) \]
From Quantum Physics to Spectroscopy

\[ i\hbar \frac{\partial \psi(x, t)}{\partial t} = \hat{H} \psi(x, t) \]

\[ \psi(x, t) = e^{-\frac{iEt}{\hbar}} \psi(x) \]
Electron Dynamics and Spectroscopy

\[ \mu(t) = \langle \psi(x, t) | \hat{x} | \psi(x, t) \rangle \rightarrow \mu(\omega) \]
From Time-Dependent Quantum Theory to Spectroscopy

\[ \psi(x, t) \]

\[ \hat{H} \]

\[ i\hbar \frac{\partial \psi(x, t)}{\partial t} = \hat{H} \psi(x, t) \]
Photophysics of Superposition State

\[ i\hbar \frac{\partial \psi(x, t)}{\partial t} = \hat{H} \psi(x, t) \]
Mixed Quantum-Classical Mechanics

\[ i\hbar \frac{\partial \psi(x, t)}{\partial t} = \hat{H} \psi(x, t) \]

\[ \hat{H} = \hat{H}_{QM} + \hat{V}_{eff} \]

Time = 0.012 fs
Photophysics of Chirality

2,3-(S,S)-dimethyloxirane
Resonant excitation at 11.0 eV

\[-2 \sum_{j \neq n} \frac{\omega}{\omega_j^2 - \omega^2} \text{Im} \left( \langle \psi_n | r_\beta | \psi_j \rangle \langle \psi_j | m_\alpha | \psi_n \rangle \right)\]
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