



## PROFESSOR KIERON BURKE

Kieron Burke is a Chancellor's Professor of UC Irvine, and he is fellow/member of several scientific societies in both chemistry and physics, in the US and elsewhere. He works on developing all aspects of Density Functional Theory (DFT): formalism, extensions to new areas, new approximations, and simplifications. His work is heavily used in materials science, chemistry, matter under extreme conditions (such as planetary interiors or fusion reactors), magnetic materials, molecular electronics, and other areas. According to Google Scholar, his research papers are now cited more than 15,000 times each year.

### Semiclassical Origins Of Density Functional Approximations

**10 SEP 2019 (TUES)**  
**11.00AM–12NOON**

I will explore the relation between semiclassical methods and density functional approximations. In this lecture, I will trace how idealized mathematical treatments are connected to practical density functional calculations. This lecture will make connections between functional analysis, semiclassical approximations, and electronic structure calculations. I will end with a surprising, catastrophic failure of my own research.

### Explicit Corrections To The Gradient Expansion For The Kinetic Energy In One Dimension

**13 SEP 2019 (FRI)**  
**1.30–2.30PM**

I will report on recent work with Michael Berry in Bristol that overcomes the difficulties raised in the last lecture. We construct a mathematical framework that provides an order-by-order semiclassical expansion which reduces to the gradient expansion for slowly-varying densities, but also yields a correction when the system is finite and the spectrum is discrete. This correction is very different from any functional in current use, and greatly improves accuracy in model calculations. I will discuss the implications and future of this work. (*This lecture will be self-contained, so attendance at the first lecture is not needed to follow it.*)

### Venue

Auditorium  
Institute for Mathematical Sciences  
3 Prince George's Park  
Singapore 118402

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