DISTINGUISHED
STAFF FELLOWS
AT ORNL

Philip Dee

Eugene P. Wigner Fellow

Where and when did you earn your PhD?

I earned my PhD in physics from the University of Tennessee, Knoxville, in Spring 2021. My advisor was Prof. Steve Johnston.

What was the subject of your dissertation?

My dissertation explored the interplay of quantum phases in materials, such as superconductivity and charge order, by simulating model Hamiltonians. These models capture general qualitative behaviors that manifest in many materials and provide helpful intuition for interpreting experiments.

What was your dissertation's major contribution to your field?

Most of my dissertation work dealt with simple quantum models containing electron–phonon interactions. In materials, these interactions are responsible for many fascinating material phases and properties. We still don't fully understand all the roles these interactions play in materials, especially when they become intertwined with other low-energy excitations. My dissertation explored how emergent phases can compete across the phase diagram. It also featured a novel way to use artificial neural networks to accelerate quantum Monte Carlo simulations. These speed-ups allowed us to simulate progressively larger systems, which is essential if you want to estimate phase transition temperatures via scaling analysis.

Who is your ORNL mentor, and which group and division are you working in?

I am working in the Computational Chemistry and Nanomaterials Sciences Group in the Computational Sciences and Engineering Division. My mentor is Thomas Maier, Advanced Computing Methods section head.

What will your fellowship research focus on?

My fellowship research will focus on developing better computational methods for simulating models of quantum materials, mainly using physics-informed machine learning approaches. I will design and use machine learning architectures to boost quantum Monte Carlo and other algorithms and extend their capabilities into challenging domains. My research will also explore incorporating domain expertise for more economical and specialized machine learning models. For instance, we can build essential symmetries and invariants into the machine learning architecture, allowing the model weights to focus on other properties.

What is your project's expected contribution to your field?

My fellowship work will contribute novel methods to efficiently simulate low-energy effective models for quantum materials research. The main project aims to evaluate where these machine learning interventions work well, where they don't, and how to improve them. I will develop a suite of methods that apply to different material models, lattice geometries, and varied interactions. This innovation will enable us to produce high-resolution spectral functions, capture the onset of phase transitions, and study transport behavior. Another project is dedicated to creating powerful computational tools for the ab initio and neutron scattering communities, both of whom are well represented here at ORNL.

What are your research interests?

My research interests lie at the intersection of condensed matter theory, computational physics, and artificial intelligence. I particularly enjoy how these fields cross-pollinate ideas and spur innovations.

What led you to science and your specific discipline?

Although my specific scientific interests varied widely, I always aspired to work in a science-related field. An experimental engineering curriculum in my high school initially drove me to study engineering at university. However, after a couple of years, I started spending all my time in the physics department and took it on as a double major. Learning about quantum mechanics and relativity had a profound effect on me intellectually. In grad school, I joined a research group specializing in computational many-body physics and learned about many exciting open questions in that field and materials research in general. Condensed matter is so broad and rich with physical insight and mystery.

What did you do before coming to ORNL?

I held postdoctoral positions at the University of Florida (UF) and the University of Tennessee. At UF, I worked on a collaboration between theorists and experimentalists focused on discovering new superconducting materials, sometimes at extreme pressures. My postdoctoral advisors there were Peter Hirschfeld and Richard Hennig. My short time as a UT postdoc concentrated on machine learning–augmented many-body simulations, much like the work I will conduct at ORNL.

Could you share an interesting fact or two about yourself?

Since my early teens, I have enjoyed writing and playing music in a band or group, especially in improvisational settings. I also enjoy hiking and ventured to the Swiss Alps last year. For experienced hikers, I highly recommend the Hardergrat ridge between Interlaken and Brienz.

What nonscience topic or activity is important to you and why?

I'm a father of two young children, and my wife and I spend most of our free time with them. I often think about the world their generation will grow up in and how best to prepare them for that world. Though the future is hard to predict, certain skills and hobbies remain timeless. Reading often, broadly, and critically is one pertinent example. We all spend a great deal of time reading and discussing what we've read.

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