My research on many-body quantum mechanics

My main interest and the topic that motivates most of the research I do is related to the mathematical study of many-body quantum systems, e.g., atoms, molecules, macroscopic charged matter, superfluids, and superconductors.

To briefly explain this consider a quantum system of N identical particles. One should in general include several species of particles e.g., protons and electrons but that would complicate the notation considerably.

Each individual particle would be described by states on a one-body Hilbert Space $\mathfrak{h}$. The collection of N particles is then described by a state on the tensor product $\mathcal{H}_N = \bigotimes^N \mathfrak{h}$. By a state I will simply mean a positive semi-definte traceclass operator Γ on $\mathcal{H}_N$ with $\mathrm{tr}\Gamma = 1$. Of particular interest are fermionic or bosonic states. Fermionic states vanish on the orthogonal complement of the antisymmetric subspace $\bigwedge^N \mathfrak{h}$ and bosonic states vanish on the orthogonal complement of the symmetric subspace $\bigvee^N \mathfrak{h}$. Here I will try to avoid the complication of considering bosons or fermions.

To define the equilibrium states of the system one would need a Hamiltonian or energy operator. Most Hamiltonians in physics may be written in terms of a one-body (in general unbounded) operator h on $\mathfrak{h}$ and a two-body (in general unbounded) operator W on $\mathfrak{h} \otimes \mathfrak{h}$, which is symmetric in interchanging the tensor product factors.

The operator on the N-body system is then given by the (in general unbounded) operator

$$H_N = \sum_{i=1}^{N} h_i + \sum_{1 \leq i < j \leq N} W_{ij}$$

where h_i means the operator h acting on tensor factor i (and as the identity on all other factors) and W_{ij} means W acting on tensor factors i and j.

The equilibrium state at temperature $T > 0$ is then (here we are setting Boltzmann's constant $k_B = 1$)

$$\Gamma = \exp(-H_N/T)/\mathrm{tr}(\exp(-H_N/T))$$

(if this is well-defined otherwise there is no equilibrium state). This Γ also minimizes the free energy

$$\mathcal{E}^{\mathrm{QM}}(\Gamma) = \mathrm{tr}[H_N\Gamma] - TS(\Gamma),$$

where $S(\Gamma) = -\mathrm{tr}(\Gamma \log(\Gamma))$ is the von Neumann entropy. For $T = 0$ in this minimization we talk about the ground state.

An example are N free particles in 3-dimensions, where $\mathfrak{h} = L^2(\mathbb{R}^3)$, $h = -\frac{1}{2}\Delta$ (the Laplacian) and $W = 0$ (using units in which the mass of the particle and Planck's constant $\hbar$ are both equal to 1). Free particles have neither ground states nor positive temperature states. This is simply because the particles will escape any region of space.

A slightly more complex system is to consider N non-interacting particles in 3-dimensions confined by a potential $V : \mathbb{R}^3 \to \mathbb{R}$. The Hilbert space is as for the free particles and we still have $W = 0$, but $h = -\frac{1}{2}\Delta - V$ is a Schrödinger operator. If V is smooth and tends to infinity at infinity then there will be both ground states and positive temperature equilibirum states. They may be analyzed using spectral theory for Schrödinger operators. A characteristic property of non-interacting systems is that the equilibrum states are characterized entirely by their one-particle reduced density matrix. This is the positive semi-definite traceclass operator (density matrix) γ on the one-body space $\mathfrak{h}$ given by satisfying

$$\mathrm{tr}_{\mathcal{H}_N}(\Gamma \sum_i b_i) = \mathrm{tr}_{\mathfrak{h}}(\gamma b)$$

for all bounded operators b on $\mathfrak{h}$.

The real challenge is to understand interacting systems where $W \neq 0$. The question that occupy me and other mathematical physicists is to establish mathematically rigorous results of physical interest. E.g., can we "state" and "prove" a statement to the effect that water freezes? Unfortunately such a question seems far beyond reach of what we are able to do today. In fact, there are only very few systems where we are able to establish the existence of phase transitions like the freezing of water.

A succesful approach to studyíng interacting systems ($W \neq 0$) is to approximate them by non-interacting systems ($W = 0$) or even better to simply restrict the class of states to be the equilibrium states of non-interacting systems. For each density matrix γ on $\mathfrak{h}$ there is a free equilibrium state Γ_γ for which γ is the one particle reduced density matrix. If we restrict an interacting systems to such states we arrive at the mean field (MF) "approximation"

$$\mathcal{E}^{\mathrm{MF}}(\gamma) = \mathcal{E}^{\mathrm{QM}}(\Gamma_\gamma).$$

I have put quotes around approximation since we often do not know how well the free energy in the mean field model approximates the true many-body free energy. We do know that the mean field free energy is always bigger as it is obtained from a restricted minimization. Good lower bounds are usually difficult to obtain and much research goes in that direction.

It is, however, also interesting to study mean field models even if we cannot establish the validity of the approximation. Mean field models are in one sense more complicated than the full many-body model as we cannot easily say what the minimizing (equilibrium) states are and whether they exist. These are often challenging mathematical questions that may require sophistaicated variational methods from non-linear functional analysis. On the other hand having established existence of minimizers it is often much easier to analyze the mean field model than the full quantum model. In many mean field models it has been possible to conclude existence of phase transitions. I am still not aware of any non-trivial model where the mean field approximation is good enough to use it to establish phase transitions in the full many-body model.

Let me finish this little overview of my research interests by highlighting a result I proved about a decade ago. This is the problem of a charged gas, one of the most fundamental physical systems. Here $\mathfrak{h} = L^2(\mathbb{R}^3 \times \{-1, 1\})$, where $\mathbb{R}^3$ is the physical space with the variable denoted by x, and $\{-1, 1\}$ corresponds to the two charge components $e = \pm 1$ (positive and negative charges). The one- and two-body operators are

$$h = -\frac{1}{2}\Delta_x, \qquad W\psi(x_1, e_1, x_2, e_2) = \frac{e_1 e_2}{|x_1 - x_2|}\psi(x_1, e_1, x_2, e_2).$$

Here W (written as a multiplication operator) represents the Coulomb potential where equal charges repel (positive potential energy) and opposite charges attract (negative potential energy). In the case $N = 2$ this problem is exactly solvable as it is simply equivalent to the hydorgen atom and we know the ground state energy explicitly. In 1967 Freeman Dyson conjectured, based on the theory for superfluidity, that for large N the ground state energy $E(N)$ satisfies an asymptotics of the form

$$\lim_{N\to\infty} \frac{E(N)}{N^{7/5}} = \inf\left\{ \frac{1}{2}\int |\nabla\Phi|^2 - J \iint |\Phi|^{5/2} \middle| \Phi \in L^2(\mathbb{R}^3),\ \|\Phi\|_2 = 1 \right\},$$

where J is an explicit constant. Using a mean field approximation essentially along the lines described above, but slightly more complicated, I established this result in 2006.