THE WHOLE IS MORE THAN THE SUM OF ITS PARTS - OR IS IT?
Surprises in many-particle theory and nanoscience.

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(The mathematical equations appearing here are included for completeness, and most do not appear in the slides presented orally. The reader can follow the general argument without examining the equations in detail.)

INTRODUCTION

The world we live in is certainly a very complicated place, in many different senses. On a global scale we have delicate negotiations over war and terrorism, climate change and the world economic order. On a more private scale we have the seemingly inexplicable behaviour of the opposite sex. In fact anything involving human behaviour depends on the workings of perhaps the most complex structure in the universe, the human brain. But there are many other instances of complexity that do not directly involve biology. For example, we know that the hydrodynamic flow of our atmosphere, the determiner of our weather and climate, is chaotic - intrinsically complex and unpredictable over long time scales. This is true despite the fact that the underlying phenomena are accurately described by relatively simple mathematics. Nevertheless numerical weather prediction over a few days is now a highly successful venture, responsible for the great improvement in forecasting in recent years. Solution of the hydrodynamic equations also reveals emergent properties such as cold fronts, which of course do correspond to reality, but whose existence one would not easily guess by looking at the equations.

Complication is everywhere. As a theoretical physicist, I know that even a tiny crystal of common salt contains billions upon billions of charged atoms (ions) undergoing elaborate, coordinated motions (phonons) even though the crystal appears to be just lying there doing nothing. Understanding these structures and motions allows us to predict the physical properties: salt crystals are cubic in shape, hard and brittle, and melt at a very high temperature. An even more detailed description, involving the quantum mechanical motions of the electrons within and between the atoms (or ions), is needed to get a full understanding of the chemical and electrical properties. These include (e.g.) salty taste and the ability to be an insulator when in crystalline form, but a conductor when in solution.

These days we wish to be able to predict such properties “from scratch”, in order to create new “designer substances” for particular technological needs. Only recently, in the last forty years or so, has this started to become possible, and the development of the necessary methods is by no
means finished. A recent Nobel Prize, awarded to John Pople and Walter Kohn in 1998, recognised the importance of our ability to predict chemical, physical and even some biological properties to a useful accuracy from first principles, via many-electron quantum mechanics.

The present Lecture is partly about just this venture: the explanation, design and prediction of chemical and material properties from basic theoretical physics. Where this is possible, it has the attractive feature that a very few simple basic concepts, rules and mathematical equations are sufficient to explain and predict complicated phenomena and properties. Thus many aspects of the complex world can be reduced to simple considerations after all.

The practical spinoffs from this kind of theoretical physics are very widespread, including for example several aspects of magnetic resonance imaging, a very important modern medical diagnostic tool. Another application that I will discuss later on is the absorption of hydrogen into carbon-based graphitic materials, of importance in creating a greenhouse-safe world energy economy. On the other hand, the mathematical solution of the equations to sufficient accuracy is often extremely challenging, and it is generally agreed that the prediction of holistic properties from simple basic equations is not in general an exactly soluble mathematical problem.

To many, the ambitions described above amount to reductionism, and might be seen in a negative light within some philosophical frameworks. Personally, I take a pragmatic view on this. My own work involves cases where the current paradigms do not work to sufficient accuracy, and where there is a very good chance to do something useful about this, with spinoffs in solid state physics, chemistry and clean energy technology.

**HOW TO BE A “GOOD” REDUCTIONIST**

(i) *Pick an appropriate level of detail and don’t be too ambitious.*

E.g. (a) in explaining global social networks, it’s probably not a good idea to start by thinking about electrons moving inside the participants’ bodies.

E.g. (b) Consider trying to describe chemical reactions that involve rearrangement of the motions of electrons in the outer parts of atoms. It’s not necessary or useful to consider the very complex phenomena constantly occurring within the nucleus deep inside the atom – these processes are scarcely changed by the chemical reactions. (Nuclear Magnetic Resonance is an exception). They are important in radioactivity, however
In these and many other cases, the appropriate levels are pretty well agreed at this point in time. For example, in describing the self-assembly of nanostructures – large assemblies of particles each in the size range between on billionth and one millionth of a metre – most workers do treat molecular units as “sealed” and work with models of the forces between these units. One of the “surprises” referred to in the title of this talk is that soft nanostructures are not in fact adequately treated in this fashion, and I am currently working on a new way of treating this problem. This new approach will have the effect of defining new levels of detail that can be kept separate after all.

(ii) Be very clear what are your starting assumptions and end goals. A true reductionist theory aims to obtain predictions logically and doesn’t allow unproven additional hypotheses or ad-hoc adjustable parameters to be introduced. Reductionism is not of much use if the underlying, reduced problems cannot be expressed in simple mathematics and the results obtained by consistent logic and mathematics.

(iii) Pick a good (i.e. important and unsolved) problem to work on, one that justifies the enormous theoretical and computational effort that is often required to carry through the reductionist approach.

Having set out the general framework of my endeavours, I will now explain in more detail what I mean by the title “the whole is more than the sum of its parts”. In particular, I will now explain what are “the parts”. I will do this in three steps, and then I will discuss what is the “whole”.

“THE PARTS” I - DESCRIBING THE MOTION OF ONE CLASSICAL PARTICLE DUE TO A GIVEN FORCE

This is by now a solved problem. The classical description was largely worked out by Isaac Newton in the 1600s. Newton had the insight, astonishing in his time, that the natural state of a particle free from outside influences (forces) was not to be stationary, but rather to move with constant velocity \( v \) (both in magnitude – known as speed – and direction). This condition is commonplace for particles in the depths of space, but we rarely see this type of motion on Earth: objects slow down and stop because there are almost always large forces (friction, air resistance, gravity, etc.) The rolling motion of a well-lubricated railway car (at nearly constant speed on a level track) approximates the zero-force conditions envisaged by Newton, at least in the horizontal direction. He named the external influences that modify the natural uniform motion forces, and specified their size by the rate at which they change the velocity. In one dimension, this gave Newton’s’ second Law in the form of the differential equations
\[ \frac{dx}{dt} = v, \quad \frac{dv}{dt} = \frac{F}{m} \]  \hspace{1cm} \text{(Equation 1)}

These equations describe how a force \( F \) influences the spatial position \( x \) of a particle of mass \( m \), by changing its velocity \( v \) over a time \( t \). He applied his equations successfully to describe the motions of the planets, which feel the gravitational force due to the Sun, but do not experience frictional forces because they move in the vacuum of space. In his initial work he ignored the gravitational forces acting \textit{between} the planets, and thus needed to solve only one-body problems, treating one planet at a time. The special inverse-square nature of the gravitational force allowed him to obtain his solutions in closed algebraic form, suitable for numbers to be “plugged in” to obtain numerical predictions for the position of planets at any time.

When the force does not have such a simple dependence on position, we may not be able to obtain a closed algebraic solution, but we can resort to numerical solution of Newton’s equations. For the motion of one particle in three dimensions, this is trivial on a modern computer, requiring one merely to follow the values of a particle’s three position coordinates \((x,y,z)\) over time according to three equations like Equation (1).

\textbf{“THE PARTS” II: THE FUNDAMENTAL PARTICLES AND FORCES OF PHYSICS}

Where do forces come from? There are four fundamental types of force that are currently believed to explain all of Nature (although persistent rumours keep cropping up of a possible fifth force). Other commonly-discussed forces (as in covalent chemical bonds, for example, or the contact force between one’s finger and a pen) are emergent properties that follow from the fundamental ones, together with the laws of particle motion. In order of relative strength, the four well-accepted fundamental forces are

(i) the “strong” nuclear force that acts between neutrons, protons and their constituents (quarks)
(ii) the electromagnetic force that affects electrically charged particles such as electrons and protons
(iii) the “weak” nuclear force that affects nuclear particles and is responsible for radioactive beta decay
(iv) the force of gravity that affects all massive particles (and even massless ones, in general relativity).
One of the basic aims of physics is to explain as much of Nature as possible, by starting from an understanding the above forces, and combining these with equations (classical or quantum mechanical as appropriate) describing the motion of the particles under the forces.

My main aim today is to throw some light on advances in chemistry, solid state physics and materials/nanoscience. For these purposes the above list of forces can be drastically curtailed. Forces (i) and (iii) are active mainly inside atomic nuclei, and are not normally needed in the condensed matter and materials science cases that I will be considering, except where radioactivity is involved. I will therefore not include these forces. Similarly gravity, though ubiquitous, is weak at the nanoscale and is rarely the determiner of the kind of nanostructures that I will be talking about. Thus I will discard it also. This leaves the electromagnetic force.

The simplest part of the electromagnetic force is the Coulomb force $F$ between electrically charged objects with charges $Q_1$ and $Q_2$, separated by a distance $R$:

$$F = \frac{KQ_1Q_2}{R^2} \quad \text{(Equation 2)}$$

This is known as an inverse square law. For example, suppose that I move two ions, each with a positive electric charge, so that they are now twice as far apart as when I started. Then formula above tells us that the repulsive force between them is reduced by a factor of 4, compared with its original strength. The same applies, but with an attractive force, if the two objects have a positive charge ($Q_1 > 0$) and a negative charge ($Q_2 < 0$) respectively. An example of this attractive Coulomb force is the force that keeps negatively-charged electrons revolving around the positively charged nucleus of an atom, instead of cruising off into space. On the other hand, the repulsive force between the two similarly-charged electrons in a helium atom tends to keep them on opposite sides of the atom, during their joint motions. This behaviour of moving particles is known as "correlated" motion, something that will be of crucial importance later in this talk.

"THE PARTS" III: QUANTAL DESCRIPTION OF SINGLE-PARTICLE MOTION

A quantum mechanical (wave mechanical) description is required for small particles such as electrons moving in atoms, molecules or in a solid, the situations of interest in my own work. (The classical or Newtonian description described in previous paragraphs is an approximation to the quantum description: its accuracy increases as the mass of the particle increases.) The need for this description was highlighted, for example, in the Davisson-Germer experiment the early 1900s when it was found that electrons scattered off a crystal exhibited wavelike behaviour. (They formed
a diffraction pattern, previously familiar from water waves and light waves, but unknown at that time for objects like electrons, that were believed to be particles). It was found that the wavelength \( \lambda \) was inversely proportional to the speed. This is encapsulated by the De Broglie relationship,

\[
\lambda = \frac{h}{mv}
\]

(Equation 3)

where \( m \) is the particle’s mass and \( h \) is Planck’s constant.

The Schrodinger equation describes motion of one particle in a force field \( F(x) = -\frac{dV}{dx} \) that is specified by the corresponding potential energy \( V(x) \). It takes the Newtonian prediction for the momentum \( mv \), and then uses de Broglie’s relationship to specify the local wavelength of the waves. This, along with a similar consideration linking energy and time, gives the famous Schrodinger equation for one particle, specifying the time evolution of the system

\[
i \frac{h}{2\pi} \frac{d\Psi}{dt} = -\frac{h^2}{8m\pi^2} \frac{d^2\Psi}{dx^2} + V(x,t)\Psi
\]

(Equation 4)

Here \( V(x,t) \) is the potential energy function, directly determined once we know what force is acting on the particle. \( \Psi(x,t) \) is the wavefunction, which guides the motion of the particle, and whose square gives the probability density for finding the particle at position \( x \) at time \( t \).

Equation (4) applies for motion in one space dimension. In three dimensions (4) becomes

\[
i \frac{h}{2\pi} \frac{d\Psi}{dt} = -\frac{h^2}{8m\pi^2} \left( \frac{d^2\Psi}{dx^2} + \frac{d^2\Psi}{dy^2} + \frac{d^2\Psi}{dz^2} \right) + V(x,y,z)\Psi
\]

(Equation 5)

The mathematical situation is more complicated in quantum mechanics than in classical physics because one effectively allows for all paths that a particle could follow. Thus instead of a single velocity \( v(t) \) and position \( x(t) \), the condition of a particle at a particular time “t” is described in quantum mechanics by the wavefunction \( \Psi(x,t) \). This is basically an infinite set of numbers \( \Psi \), one for each point \( x \) in space and each time \( t \). In very simple situations, exact algebraic solution can often be found for \( \Psi \), as for example in the hydrogen atom. In more complicated situations, by sampling the wavefunction at a grid of discrete points, we can obtain a numerical solution of the Schrodinger equation to obtain \( \Psi \). For a typical atomic quantum mechanics problem in three space dimensions, a grid of 100 points in each space direction might be sufficient, giving \( 100 \times 100 \times 100 = 1 \) million points. Solving this version of the one-particle Schrodinger equation numerically is these days fairly routine. One typically uses more efficient ways to sample \( \Psi \) than the \( 100 \times 100 \times 100 \) grid just described.
Some of the specifically quantum-mechanical phenomena described by the Schrödinger equation are:

**Tunnelling:** Particles can move from one low-energy location to another by “tunnelling” through high-energy regions that they would be forbidden to traverse within the classical, Newtonian description. The phenomenon of electrons tunnelling between atoms gives rise, for example, to the covalent chemical bond that holds many molecules together.

**Diffraction:** This is a wavelike phenomenon which sometimes causes fewer particles to reach a given point in space, when more paths to that point are opened up (waves can cancel as well as adding). This is vital in understanding the motion of electrons in crystalline solids.

**Zero-point motion:** In classical physics, the lowest-energy (zero-temperature) state of any system is one of zero motion – a stationary particle. This is untrue in quantum mechanics: whenever a force confines a particle to a finite region of space (as in an atom), the wavefunction has to vary in space and this leads, via De Broglie’s relationship, to a nonzero momentum and a finite zero-point kinetic energy. This is one way of understanding, for example, why the electron in a hydrogen atom does not simply go to the nucleus and stay there, as the attractive Coulomb force would favour. This phenomenon is also necessary to understand the weak van der Waals forces that hold many nanostructures together.

In the context of the title of this talk “The whole is more than the sum of its parts” we now know the “parts”, for the problems of current interest. They are (a) the electrical Coulomb force, and (b) the Newton or Schrödinger equations for the motion of each particle under the influence of a given force. Now we need to consider a description of “the whole”.

**MANY-PARTICLE PHYSICS - “THE WHOLE”**

Luckily it is found that the Coulomb force is additive: the force $F$ on particle A due to two other charged particles B and C is just the sum of the forces due to B and C,

$$F = F_B + F_C$$  \hspace{1cm} (Equation 6)

*The classical many-body problem.* Unfortunately this simple additivity does not apply to solutions of the equations of motion, and this is why many-particle physics is hard – the whole, in this mathematical sense, is certainly more than the sum of its parts. We could imagine that all particles
but one are fixed, and then solve for the motion of the one remaining particle, as described above. The force on this last particle would be just the sum of the forces due to the others.

Unfortunately, however, the other particles do NOT stay in fixed positions while our chosen particle moves. Thus we have to keep track of all the moving particles simultaneously. In the classical case this is not too hard: to describe N particles we need 3N coupled differential equations for the position coordinates of the N particles. The direct numerical solution of these equations is known as “molecular dynamics” and can these days be carried through successfully for many thousands of interacting particles. These particles could, for example, be molecules in a classical fluid, and this approach is being carried out by my colleague Dr. Debra Bernhard to understand the behaviour of fluids in very small (nanosized) pores, where the conventional hydrodynamic equations are not adequate.

General form of the quantum many-body problem. In the quantum mechanical case appropriate to electron motions in molecules and solids, things are much harder. The simultaneous motions of the electrons are described by a many-electron wavefunction that depends on all the particle coordinates simultaneously:

\[ \psi_N(x_1,x_2,x_3,\ldots,x_N,t). \]  
\[ \text{(Equation 7)} \]

It satisfies the many-body Schrödinger equation

\[ i\hbar \frac{d\psi_N}{dt} = -\hbar^2 (2m)^{-1} \left( \frac{d^2}{dx_1^2} + \frac{d^2}{dx_2^2} + \frac{d^2}{dx_3^2} + \ldots + \frac{d^2}{dx_N^2} \right) \psi_N + V(x_1,x_2,x_3,\ldots,x_N) \psi_N. \]
\[ \text{(Equation 8)} \]

Friendly and unfriendly particles.

One further fact needs to be accounted for. It is found that Nature does not distinguish between different particles of the same species - e.g. “all electrons are the same”. This means that the magnitude \(|\psi_N|\) of the many-particle wavefunction must remain unchanged when we swap the labels of two particles. Two ways for this to be satisfied are

(i) The wavefunction \(\psi_N\) can change sign when we swap two particle labels. This means that we cannot build a wavefunction \(\psi_2(x_1,x_2) = \phi(x_1) \phi(x_2)\) with two particles undergoing the same motion described by the one-particle wavefunction \(\phi\). For interchanging \(x_1\) and \(x_2\) does not change this wavefunction, so \(\psi_2(x_1,x_2)\) would have to equal minus itself, and so could only be zero. Thus there are no states with two particles undergoing the same motion (i.e. occupying the same orbital). This is the famous Pauli principle, and types of particle that obey this type of exchange symmetry are in
general termed “fermions”, after Nobel prizewinner E. Fermi. Electrons, protons and neutrons are all fermions. The fact that electrons are fermions, and hence obey the Pauli Principle, is essential in our understanding of atoms. Fermion many-body wavefunctions $\psi_N$ vanish whenever two particles have the same coordinates, which means that these wavefunctions are essentially oscillatory quantities.

(ii) The wavefunction $\psi_N$ can stay the same when we swap two labels. Particles with this feature are in general termed Bosons, after Indian physicist S. Bose. Elementary bosons include Pimeson but these nuclear particles are not very stable and are not of interest here. More commonly-encountered bosons are formed from tightly-bound combinations of an even number of fermions – e.g. the common isotope of helium contains 2 electrons, two protons and two neutrons. (When two atoms are swapped holus bolus, the many-body wavefunction is multiplied by six fermion factors of (-1) and so is unchanged since $(-1)^6 = 1$.)

**Summary:** Fermions (e.g. electrons) are “unfriendly” particles – they cannot move in unison. Bosons, by contrast, are “friendly” – they are more likely to move in unison than otherwise.

**Difficulty of solving the quantum many-body problem.** The quantum many-body problem is very daunting from a computational point of view. Just to store the many-body wavefunction $\psi_N$ for, say, a system of 200 interacting electrons, is impossible. With $\psi_N$ sampled at 100 grid points in each of the three space directions for each particle, the number of computer storage locations required is

$$(1,000,000)^{200} = 10^{1200} = 1 \text{ followed by 1200 zeros.}$$

This is hugely more than the combined storage of all the world’s computers.

Thus a direct solution of the Schrodinger equation requires clever statistical sampling of a small minority of the tabulation points (the “Diffusion Quantum Monte Carlo Approach”, “DMC”). For electrons, with their intrinsically “wriggly” fermionic many-body wavefunction, this has proved possible for at most a hundred or so electrons, in very favourable cases. When a well-converged wavefunction $\psi_N$ from these solutions is used to predict measurements, however, the agreement has always been impressive, so that we are very confident of the correctness of the many-body Schrodinger equation.

**Jellium.** One system that has been solved this way is the so-called “jellium”, “homogeneous electron gas” or “uniform electron gas”. This is a fictitious system somewhat akin to a metal, but where the lattice of discrete positive ions that are present in a real metal has been replaced by a
uniform “jellium background” consisting of a smear of positive charge. The density (charge per unit volume) of the background is the same throughout all space. The electrons move freely through this background, and achieve an average number density \( n \) electrons per unit volume, so as to neutralise the positive background, giving an overall charge-neutral system. While this jellium is of minor interest as a crude model of simple metals such as sodium, it has a much greater importance. The groundstate energy per electron \( \varepsilon(n) \), tabulated for various number densities \( n \), is the essential input into the “Local Density Approximation”, a practical approximation method for obtaining groundstate electronic energies of real physical systems. This will be outlined a few Sections further on.

**THE SIMPLEST NON-TRIVIAL MANY-BODY APPROXIMATIONS – MEAN FIELD, PERTURBATION AND VARIATIONAL TREATMENTS**

Very few many-electron systems of interest are small and simple enough to be analysed via the Diffusion Quantum Monte Carlo methods just described, and therefore approximations or inspired guesswork are required in order to make progress. Three common approximation methods are described below.

*Mean field theory.* Here we focus on one particle at a time. The remaining moving pointlike particles are replaced by a smeared-out effective cloud whose density function \( n(x) \) does not vary with time. \( n(x) \) is determined self-consistently. The force acting on our one chosen particle is calculated using the known microscopic force law (Coulomb’s Law in our case) using the smeared distribution, instead of the point particles, as source. The particles both create and respond to the mean field. This approach is especially suitable for seeing emergent *cooperative* effects, in which very many particles participate in motions that are quite unlike the motions of individual particles (e.g. density waves or “plasmons”). The wave motion is manifested in the density function \( n(x) \), and is not the same thing as the wavelike structure of the underlying quantum mechanical wavefunction. Cooperative effects are one case where the whole is “more” (or different) from the sum of the parts taken independently.

*Perturbation theory.* In this method one treats the effect of forces between the particles as a small correction to the motion without forces. More sophisticated versions start, not with zero forces, but with a smeared mean-field version of the forces, and then the difference between the true and the smeared forces is treated as a small correction. By treating the forces as small one can perform a highly systematic mathematical analysis, sorting the effects of the force by their “order of smallness” (first order perturbation, second order perturbation.). This procedure will only give exact answers
when taken to infinite order of perturbation. This is perhaps the most systematic way to approach the many-body problem, but it does not directly or easily yield the emergent properties (the “more-than the sum-of-its-parts” phenomena such as cooperative wave motion).

Variational theory. Here one focusses on some aspect of the motion and builds a “guessed” many-body wavefunction $\psi_N$ "by hand", in order to incorporate this aspect. For example, if the forces present are repulsive one can build a wavefunction that becomes small when any two particles get close to one another. By adjusting the degree of this smallness until the energy is minimised, one picks the “best” wavefunction in this class. This is quite a powerful way to proceed, but it requires excellent physical insight into the physics of the particular systems being studied. Many Mean Field Theories can be obtained formally by this approach, building a many-body wavefunction that is a product or determinant of one-body wavefunctions. The well-known Hartree and Hartree-Fock descriptions of atoms and molecules fall into this category.

In the next section I discuss how these and other approaches have explained some surprising emergent properties of large collections of particles.

**SOME PAST SURPRISES – UNEXPECTED EMERGENT PROPERTIES OF MANY-PARTICLE SYSTEMS**

*Example 1: Newton’s balls – lecture demonstration*

The apparatus known as “Newton’s Balls” is a collection of 5 steel balls suspended on strings so that they can move freely in the horizontal direction until they collide. The ball at one end (ball #1) is pulled aside leaving balls #2-5 sitting stationary in a clump. Ball #1 crashes into the nearest ball (#2) which is part of the cluster of 4 sitting stationary.

A reasonable person would probably guess that the impact of #1 would cause the cluster (#2 - #5) to start moving away together. What actually happens is that #5 flies away from the rest, leaving #1 - #4 sitting stationary.

This behaviour can be understood if one removes all but #1 and #2. When #1 is now pulled aside and allowed to collide with #2, after the impact #2 flies off leaving #1 stationary. In fact #1 and #2 simply swap velocities. This in turn is readily understood in terms of Newton’s laws of motion, which can be rewritten to express the conservation of momentum and of energy.
The original behaviour of the five balls can now be understood as a sequence of two-ball collisions in which all of the momentum of #1 is successively transferred to #2, then to #3, then to #4, and finally to #5 which has no further neighbour and so moves away unimpeded.

So in this case the surprising emergent behaviour of the collection of 5 balls can in fact be understood by breaking the problem down into smaller “pieces”, and applying known simple laws to the pieces. A classic reductionist success!

Example 2: Sausages and kinks: the quest for plasma confinement to supply clean energy

It has been known for a long time that nuclear fusion—the process that makes the Sun burn—could provide much “cleaner” energy than the traditional nuclear fission reactors that now supply (e.g.) some 80% of France’s electric power needs. (In fusion, small atomic nuclei join together, releasing energy. In fission, a large nucleus breaks apart, also releasing energy.) In order to allow the atomic nuclei to approach closely enough to fuse and thereby release useful energy, it is necessary to heat the gas to a very high temperature. Then the nuclei are moving fast enough to overcome their mutual coulomb repulsion and hence to collide closely. At the required high temperatures, gases become plasmas in which outer electrons leave the atoms. Then the negatively charged electrons and positively charged ions move independently. One of the interesting properties of a plasma is its high electrical conductivity, due to independent streaming of the positive and negative particles under an electric field.

It is not easy to keep a gas confined when heated to the necessary temperature for ignition of the nuclear fusion reaction. The high electrical conductivity of a hot plasma was the basis of an ingenious scheme known as a “pinch machine” proposed in the 1940s. If the gas can be heated enough to ionise it (an easily achievable goal) then the idea was to pass an electric current through it. It was then expected that the pinch effect would occur: the current passing through the plasma would create a surrounding magnetic field which would then compress (pinch) the plasma, thus both heating the plasma and helping to confine it against thermal expansion.

When the experiment was tried, what actually happened was that after pinching initially as expected, the column of plasma underwent violent wriggling motions (the “sausage” and “kink” instabilities) and ultimately broke up, interrupting the current. These motions are an emergent property of a charged fluid, but are easily understood from a mean-field point of view. The moving charges both create the magnetic field and are influenced by it. The sausage instability occurs if one part of the pinch becomes a little narrower than neighbouring sections. Its more concentrated current creates a stronger field, which then pinches the plasma more tightly. This in turn makes the narrow section of the pinch become even narrower, squeezing plasma out into neighbouring
sections. These expand, weakening the field and hence expanding further. This “sausage” instability eventually cuts the column of current at the narrow sections. In the related “kink” instability, the plasma column is disrupted by sideways motions.

The sausage and kink instabilities are just the first examples discovered from among a host of ways in which the particles in plasmas “conspire” to escape rapidly from their confining magnetic fields. Only in the last few years, 60 years after the initial suggestions for confinement, have plasma physicists begun to tame these unwanted emergent properties sufficiently to approach the necessary conditions for fusion energy production.

**Example 3: Superconductors**

Metals conduct electricity because some of their electrons are relatively free to move under the influence of an applied voltage or electric field. If the electrons were completely free, Newton’s laws imply that they would accelerate constantly under the applied electric field, resulting in an electric current that increased over time as long as the voltage was maintained. The current would also not decay after the voltage was removed. Normal metals contain defects in their crystal structure, however, and these limit this process, so that the current rapidly settles down to a steady value proportional to the applied voltage (Ohm’s law). This *resistance* due to the defects also halts the current again when the voltage is removed.

In 1908, however, Kammerlingh Onnes and co-workers discovered that mercury loses all electrical resistance when cooled below about 4° Kelvin (≈ -269° C). For example, an electric current initiated on a closed mercury loop is found to be flowing undiminished a year later. Many other substances were found to have the same behaviour when cooled sufficiently. This superconducting phenomenon, involving electric current without resistance and hence without power consumption, is today used to create very large electromagnets used in Magnetic Resonance Imaging (MRI). MRI is a medical diagnostic tool that can view soft tissues, unlike X-rays.

A full reductionist theory of this superconductivity phenomenon took fifty years to come, and won a Nobel prize in 1972 for John Bardeen, Leon Cooper and Robert Schrieffer. There are several aspects to this understanding. Surprisingly, despite their mutual Coulomb repulsion, the electrons in superconductors experience a net effective attraction by polarising the crystal lattice of ions. Accordingly, they form two-electron bound states somewhat like large atoms. These “Cooper pairs” heavily overlap one another, but a mean field theory allowed them to be treated one at a time. The pairs in this ensemble behave more like bosons than fermions. Accordingly they move in unison, and one can imagine that all pairs will need to change their motion together if a defect is to slow the current down. This is too hard to achieve, so defects are ineffective in causing electrical resistance.
The fact that the charge carriers (Cooper pairs) have two electronic charges has been well verified experimentally.

In the 1980s a new class of “high temperature superconductors” was discovered. They are technologically important because they superconduct at higher temperatures than conventional superconductors, permitting use of inexpensive liquid nitrogen for cooling, rather than the scarce and expensive liquid helium required for conventional superconductors. In order to achieve the highest possible operating temperature, a comprehensive reductionist theory is required, to relate the superconducting properties right back to the chemical composition. Unfortunately, 16 years after the experimental discovery of these “high-Tc” superconductors, such a predictive theory is not yet to hand. The mechanism of high-Tc superconductors seems to be fundamentally different from that of the conventional superconductors. This highlights the difficulty of the quantum mechanical many-body problem.

*Example 4: Electrons falling apart?? The fractional quantum Hall effect.*

Electrons can be trapped in a very thin (two-dimensional) layer at the interface between two types of semiconductor in a solid-state device. When this device is cooled to sub-Kelvin temperatures, the electrical conductivity shows a series of sharp oscillations as a function of magnetic field (the fractional Quantum Hall effect). Amazingly, the charge transport characteristics (shot noise) suggest that the particles carrying the electric current have one-third of the electron charge. There is no doubt that the electrons are carrying the current, and there is equally no doubt, under current understanding, that the electron with charge e is a truly indivisible elementary particle. It seems that the apparent charge $\frac{e}{3}$ is a many-body effect. The motions of the electrons are strongly correlated with each other, forming a kind of quantum soup in which each electron is bound to three magnetic flux quanta. The fuzzy nature of quantum wavefunctions allows $\frac{1}{3}$ of an electron to move across a boundary along with one flux quantum, simulating charge $\frac{e}{3}$. Robert Laughlin shared a Nobel prize in 1998 for his theory of this phenomenon. With remarkable physical insight, he guessed a suitable many-electron wavefunction for these systems, leading to the “$\frac{e}{3}$” phenomenon in a natural way.

**NOBEL PRIZE FOR QUANTUM CHEMISTRY: COMPLETING THE REDUCTIONIST PROGRAM FOR SMALL MOLECULES**

Chemistry was once a largely empirical science, in which accumulated knowledge – from thousands of experimental observations– was pulled together with a combination of rules-of-thumb and a special kind of chemical intuition. While this approach is still useful, over the last forty years
or so there has been a quiet revolution. It is now possible to predict the properties (energetics, shape, reactivity etc.) of most molecules in a completely quantitative fashion, from many-electron quantum mechanics. The only inputs are the specification of the kinds of atom present, plus some information to select amongst the many possible structures. This has become so successful that most experimental chemists now run commercial quantum-chemistry computer packages such as “Gaussian” to simulate the properties their desired products, before performing costly experiments and synthesis. Similar progress has been made in solid-state physics.

In 1998 John Pople of Northwestern University shared the Chemistry Nobel Prize for his successful implementation of variational and perturbational many-electron quantum mechanics to predict molecular properties, culminating in the computer package “Gaussian” that is now familiar to many chemists. The Prize recognised the considerable conceptual, mathematical and computational difficulties involved, which are typical in many-particle physics. This work also showed that chemistry and physics are not really disjoint disciplines.

**DENSITY FUNCTIONAL THEORY: QUANTUM CHEMISTRY AND SOLID STATE PHYSICS BY THE “BACK DOOR”**

Pople’s 1998 Chemistry prize was shared by another theorist, Walter Kohn, now at the University of California, Santa Barbara. Kohn until that point was known principally as a solid state physicist, and expressed some bemusement at receiving a chemistry prize. His contribution to chemistry was an approach to the many-electron problem termed “Density Functional Theory” (DFT). His approach contrasted with Pople’s frontal approach based on construction of approximate many-body wavefunctions $\psi_N$. Kohn started by proving, with Pierre Hohenberg, the subtle Hohenberg-Kohn (HK) theorem showing that all information about a many-electron system is encoded in a quantity, the one-electron number density $n(x)$, that is vastly more compact than the many-electron wavefunction $\psi_N(x_1,x_2,x_3,\ldots,x_N)$. The quantity $n(x)$ is just the density, at space position $x$, of the “fuzzy cloud” that represents the quantal electrons in popular chemistry diagrams of atoms and molecules.

“Short-sighted” physics: the Local Density Approximation

Unfortunately the HK theorem gives no information telling how to unlock the information contained in $n(x)$. In 1965, however, Kohn and Lu Sham of UC San Diego found a practical way to implement these ideas. At the time the Hartree and Hartree-Fock theories were popular, respectively, for solids/large molecules and for small molecules/atoms respectively. These are mean-field theories. That is, they describe the motions of one electron at a time using the one-particle Schrodinger
equation, but moving in a *mean field* containing approximate information about interactions with all the other electrons. The Kohn-Sham formalism shows that the *exact* groundstate energy $E_0$ and number density $n(x)$ can be found from equations of the same simple mathematical *form* as the Hartree equations. The only difference is that the Hartree mean field is augmented by an *exchange-correlation potential* $v_{xc}(x)$ that depends only on the number density distribution $n(x')$, and converts mean-field theory to a formally exact groundstate theory. Luckily it was found that the dependence of $v_{xc}(x)$ on $n(x')$ is often “local” (short-sighted, determined mainly by $n(x')$ for $x'$ close to $x$). Thus we have $v_{xc}(x) \approx w_{xc}(n(x))$, and the local function $w_{xc}(n)$ was taken from numerically exact Diffusion Monte Carlo calculations on a simple, solved model system, the uniform electron gas ("jellium": see above).

The resulting Kohn-Sham Local Density Approximation (KS-LDA) was, for more than thirty years, the only practical way to predict the energetics, and hence the geometrical structure, of solids from first principles. For small-molecule chemistry, it was not as accurate as Pople’s methods, and so it was largely ignored by chemists, though some employed it for very large molecules where the Gaussian computer code could not cope.

The KS local density approximation was shown to be exact in the limit of slowly-varying electron densities $n(x)$, but it was inaccurate for small molecules because their density varies too rapidly in space. This situation changed with the work of Perdew, Parr, Lee, Yang, Becke and others in the 80s and early 90s. They introduced the “Generalized Gradient Approximation” (GGA), working within the density functional formalism but allowing for the gradient of the density function $n(x)$ in a simple and still computable way. Now a useful chemical accuracy was available for molecules of all sizes, and DFT is now one of the most widely-used chemical tools.

**TIME DEPENDENT DENSITY FUNCTIONAL THEORY – AN ONGOING RESEARCH FOREFRONT**

Kohn-Sham theory is justified only for analysing *groundstate* properties of the electronic system. For *time-dependent* electronic properties such as the response of matter to high-frequency electromagnetic radiation, one requires *time-dependent density functional theory (TDDFT)*. Its general formulation started with the *Runge-Gross theorem*, a kind of time-dependent Hohenberg-Kohn theorem introduced in 1984 by Eberhard Gross, now working in Berlin. It is still actively under development and is presently being used for a wide range of problems.
MY OWN CONTRIBUTIONS

In an Inaugural Professorial Lecture it is customary to say something about one’s own contributions since arriving at one’s institution. In 1977, after undergraduate studies in Melbourne and a PhD and postdoctoral research in the USA, I took up a position at Griffith. There I worked initially on nuclear magnetic resonance with colleague David Doddrell and student Kerwin Kleinschmidt.

**Metal surface physics from groundstate DFT**

In the early 80s I began a collaboration with Jim Rose at Michigan and later at Iowa State, trying to understand surface properties of metals and obtaining the best description at that time of the variation of surface properties between different exposed crystallographic faces [1,2]. The main tool of my reductionist approach was groundstate DFT, and accordingly no experimental data were required as input, but output numbers agreed well with experiment. Such numbers are required, for example, to explain facetting of real metal surfaces. In the course of this work, with student Geoff Harris I obtained [3] the first evaluation of the linear response function of metallic surface electrons including the exchange-correlation potential. This work also permitted benchmarking of some ideas concerning direct local density approximations for response functions, rather than for the xc potential as in the usual DFT. That approach is now proving useful in new work that I will describe below.

**Electronic excitations at metal surfaces**

In the late 80s, with student Geoff Harris, I was the first to show [4] that microscopic theory (adiabatic LDA) implies the existence of multipole surface plasmons (a type of surface charge density wave) on the bare surface of simple metals, without any overlayers present. Previous hydrodynamic theories had suggested that an overlayer of a lower-density metal would be required in order for these waves to exist. Experiments involving electron energy loss clearly show the presence of these multipole surface plasmons on clean surfaces without overlayers.

I also worked out [5] one of the first applications, in the surface plasmon field, of a new version of Time Dependent Density Functional Theory, the Dynamic Local Density Approximation proposed by Gross and Kohn in 1985.

My interest in density functional theory took me to Santa Barbara for two sabbaticals, in 1989 and 1993. There I met Walter Kohn and interacted with his group, especially with Hardy Gross, the inventor of the modern form of Time Dependent DFT. I also worked on collective electronic excitations in semiconductor quantum wells, to match the experiments of Prof. Beth Gwinn [6]. Santa Barbara is an amazing place with a close nexus between the departments of Physics,
Materials Engineering and Chemistry. There, as well as Walter Kohn, I met several other current and future Nobel Prize winners.

**Conceptual Developments in Time-dependent Density Functional Theory**

My work on the surface plasmon problem started me thinking about time dependent DFT from a more theoretical point of view. In particular, the Dynamic LDA of Gross and Kohn made a local approximation in the space domain but allowed for memory (nonlocality) in the time domain (much like some elderly humans, who are nearsighted but remember long-past events). This seemed a little unsymmetrical to me, and in order to test its validity I found a system where an exact solution of the many-body problem could be given for a particular type of plasmon motion. The system was a harmonically confined electron gas, realised in the experiments of Beth Gwinn, and for this system I proved a new result that I termed the Harmonic Potential Theorem. I was able to show that the Dynamic LDA violated this theorem, as did various types of hydrodynamics in common use for solid state electron gases. I guessed a fairly simple general remedy by putting together classical ideas about memory and fluid elements, together with quantum mechanical ideas from TDDFT. This was possibly my most influential solo paper. In particular the idea was taken up by Walter Kohn (the founder of DFT) and Giovanni Vignale. They rewrote the theory of linear TDDFT response, this time as a current density functional theory rather than a density functional theory. This allowed them to satisfy my Harmonic Potential Theorem. It also produced a very general theory that is now starting to be used for other purposes such as a partial solution of the notorious polarisation puzzle in the first-principles theory of semiconductor dielectric response. I had intended to develop my ideas further myself, but I guess it’s no disgrace to be outpaced by a Nobel laureate, and it does feel good to have initiated a path that has been so fruitful! In a subsequent paper with Hardy Gross I showed that my original partial solution gave the same results as the more sophisticated Kohn-Vignale work, for the special case of one-dimensional motion. That paper also gave a nonlinear version of my theory. On the basis of these results and some related work, I contributed to a longer paper with Hardy Gross and his student Martin Petersilka that has become my most-cited work.

**The problem of dispersion forces in nanostructures and soft condensed matter generally**

Most well bound molecules and strong/hard solids are held together by the traditional types of strong chemical bonds – ionic, covalent and metallic. These bonds are not fundamental types of force, but are emergent properties arising from the Coulomb force plus the quantum mechanics of electron motion. They are well understood and quantitatively predictable via existing quantum chemical and DFT packages as discussed above. Weaker emergent forces can be important, however. These include hydrogen bonds and the weakest of all, the dispersion force (the outer attractive part of the van der Waals force). These weaker forces are important in “soft matter”
including many biological systems, polymers (plastics) and the case of greatest current interest to me, nanostructures such as carbon nanotube arrays. These last are based on graphitic bonding, and have strong binding within a sheet of carbon atoms but much weaker binding between the sheets. The storage of hydrogen between the sheets in graphitic structures is one of the most promising strategies for greenhouse-friendly mass transportation fuel, and the US Department of Energy has issued a target of 6.5 atomic weight percent reversible storage, for a viable technology. Unfortunately various experiments make widely different claims about the percentage of hydrogen that will go into graphite. Theory does no better, with very different estimates based on different methods of calculation.

A major difficulty is the prediction of the energy required to stretch graphene planes apart. This depends on the dispersion force between the planes. The distant dispersion force is completely missed by the Local Density and Generalized Gradient Approximations of standard DFT. The quantum chemical methods employed in the standard Gaussian package cannot be used for such large systems. Some workers have therefore resorted to empirical fitted force laws between carbon atoms. The problem there is that, unlike the underlying fundamental Coulomb force, these emergent forces are not simply additive. A different fitted force-law is required for each new situation, despite claims in the literature of (e.g.) a “universal graphitic C-C force”.

It therefore seems that some new theory is required, and it is necessary to go right back to first principles. This has been one of my projects for some time. I have aimed for a fully reductionist theory, free from the empirical fits that have been popular recently.

I will first describe pictorially how the attractive dispersion force arises as an emergent property from quantum mechanics plus the repulsive Coulomb force between electrons. (For this brochure I have summarised, in words, the animated picture shown in the oral presentation).

A word-picture of the origin of the attractive van der Waals (vdW, dispersion) force. The simplest case is that of two rare-gas atoms, far enough apart that there is no overlap of the electron density clouds. These atoms are spherical, in their ground state. In the usual mean-field theory, and also in the local and Generalized Gradient approximations of DFT, there is no force between the atoms: the positive nuclear and negative electron charges cancel perfectly. Although the time-averaged electronic charge distribution of each atom is spherical, the quantum mechanical zero-point fluctuations imply that for short times each atom can have a non-spherical charge corresponding, for example, to the electron on one atom being more on the left side than the right. This asymmetric charge distribution creates an electric dipole $d$ and hence an electric field $E = -d/R^3$ at the second atom, where $R$ is the distance between the atoms. The second atom responds by forming its own dipole $d_2 = E\alpha = (-d/R^3)\alpha$ where $\alpha$ is the polarisability of the second atom. This
then creates an electric field \( E_2 = \frac{d_2}{R^3} = -\frac{\alpha}{R^6} \) back at the first atom. This field creates an energy \( U \sim dE_2 = -\frac{d^2 \alpha}{R^6} \). Although the original dipole \( d \) is a fluctuation and averages to zero over time, its square \( d^2 \) has a nonzero average value. Thus we obtain a net time-averaged interaction energy \( U \) between the atoms, proportional to \(-R^{-6}\). This yields an attractive van der Waals (dispersion) force proportional to \( 1/R^7 \).

The table below summarises certain aspects of the dispersion (vdW) force, in comparison with some other types of force.

<table>
<thead>
<tr>
<th>Bare coulomb</th>
<th>vdW (dispersion)</th>
<th>Gravity</th>
</tr>
</thead>
<tbody>
<tr>
<td>1/R^2</td>
<td>1/R^7 for two SMALL OBJECTS. Other laws for other geometries. (falls off less rapidly than covalent but more rapidly than bare Coulomb)</td>
<td>1/R^2</td>
</tr>
<tr>
<td>Attractive or repulsive</td>
<td>Always attractive for two objects in their electronic groundstate.</td>
<td>Always attractive</td>
</tr>
<tr>
<td>Quite strong</td>
<td>Fairly weak</td>
<td>Extremely weak</td>
</tr>
<tr>
<td>Tends to cancel between charge-neutral objects</td>
<td>Does not cancel : ubiquitous</td>
<td>Does not cancel – ubiquitous</td>
</tr>
<tr>
<td>Additive for &gt; 1 source</td>
<td>NOT ADDITIVE</td>
<td>Additive</td>
</tr>
<tr>
<td>Fundamental</td>
<td>EMERGENT (from long-ranged correlation of electron motions).</td>
<td>Fundamental</td>
</tr>
<tr>
<td>Known exactly</td>
<td>GOOD THEORY LACKING. LDA/GGA misses it entirely. QC methods fail for large systems. Empirical pair forces are not universal.</td>
<td>Known exactly</td>
</tr>
</tbody>
</table>

My contributions to the basic theory of vdW forces.

In 1994 I published a paper [10] establishing that the essential vdW force can be obtained from a time-dependent mean field theory followed by use of a standard theorem, the fluctuation-dissipation theorem. This is in sharp contrast to static mean-field theory, which misses the vdW interaction completely, as discussed above. The advantages of obtaining the vdW force this way are as follows:
The same formalism also obtains the other chemical forces (covalent, metallic) in a “seamless” fashion;
this is free of the “overcounting” problems of methods that attempt to add vdW forces to LDA;
it does not assume additivity;
the time dependent approach involves response functions: local approximations often apply for these;
this gives great flexibility and leads to new types of density functional

The simplest form of this class of theory is the so-called RPA correlation energy, but I have recently shown how the more general time dependent density functional theory can give better answers [11,12]. I also showed how to derive and motivate some simple approximations [13]. While having the advantages listed above, this class of theory is computationally formidable when applied without approximation to three-dimensional structures of interest in (e.g.) graphitic hydrogen storage systems.

Recent success with our methods.

Therefore, with postdoctoral fellow Jun Wang, I first applied this method to a simple model of the vdW attraction between two thin metal slabs [14]. This is a simpler problem than graphite from a geometric point of view, but is somewhat similar in that there is higher conductivity within a plane than between planes. This is still, however, a case where quantum chemical methods and other forms of perturbation theory both fail. The LDA was once believed to describe this essentially metallic bonding situation quite well, at least near the equilibrium separation. Our work called this into question, and turned out to be something of a benchmark for future work. Using our more accurate microscopic method we obtained, as expected, the correct asymptotic vdW force, proportional to $D^{-7/2}$, at large separations $D$ between the slabs. We also verified that the LDA gave essentially no force at large distance, thus failing as expected. Our method also gave the first believable results ever, for the intermediate range of separations $D$. Perhaps surprisingly, we found that although the LDA did give rather good results for the energy near the equilibrium point, it was in error by up to 20% for the maximum force of attraction. These errors made by the LDA would be disastrous if translated to the related problem of the structure and energetics in layered graphite hydrogen storage systems.

Current work in my group.

My current work on this problem is supported by a joint ARC Discovery Grant shared with experimentalist A/Prof. Evan Gray. Also involved are postdoctoral fellow Hung Le, former student
Tim Gould (presently at York University, UK), and colleague Prof. Angel Rubio of San Sebastian, Spain. We are seeking an “honest” and seamless treatment of the energetics of graphite and its intercalates via extended RPA methods, with a view to the problem of clean energy storage. This is a formidable computational task, but we know that our approach contains all of the needed physics.

In the last few weeks I have made what I believe is a breakthrough. This takes the form of an approximation for the dynamic response functions that naturally yields the LDA if applied to the whole of the response. Thus all the good features of the LDA are recovered at small separations between the graphite sheets. I have realised, however, that this approximation can be made selectively, so that the long-ranged (small-wavenumber) correlations responsible for the vdW interaction are treated fully while the short-ranged correlations are given an LDA-like treatment, saving an enormous amount of computation. The final form of the theory, in fact, is a correction to the LDA energy. The theory is still “seamless” because the two approximations still come from the same basic theory, and we will be able to test directly that our numbers are insensitive to our choice of changeover wavenumber. This is in sharp contrast to previous work by other groups, in which an empirical long-ranged tail is added to the LDA energetics: there the results are extremely sensitive to the distance at which this correction is cut off, and it has to be determined empirically.

If successful, our new theory will be used to obtain reliable predictions for the absorption energetics of hydrogen in graphite and nanostructures involving carbon nanotubes. Meanwhile Dr. Gray and co-workers will be using their state-of-the-art hydrogenation apparatus to try to remove some of the experimental uncertainties seen in the literature to date.

*Future prospects within my group.*

Some of the same difficulties also apply to the van der Waals forces that bind other technologically important forms of “soft condensed matter” such as polymers and polymer-metal interfaces. I am hoping that my methods can be usefully applied there as well. It is not yet clear whether the ab initio prediction of tertiary and quaternary structures of biomolecules might not also require these methods.

In the longer term, I believe the insights I have gained into response functions can fruitfully be combined with other modern theoretical methods such as Dynamical Mean Field Theory. This should shed some light on the properties of so-called “strongly correlated” solids such as organic conductors, high-temperature superconductors and “heavy-Fermion” systems. These are all problems at the forefront of condensed matter theory.
SUMMARY

So what is the answer to the question posed in the title of this talk? We have seen that “the whole” is often precisely “the sum of its parts”, in the sense that large complex systems are accurately described by mathematical equations. These equations are built “bottom-up” by understanding the basic forces of Nature, plus the classical or quantal equations of motion of the many individual particles present.

On the other hand, the accurate solution of these equations (reductionism) is often difficult or impossible in practice. When sufficiently accurate solutions are possible, these solutions often exhibit “emergent” properties that one could scarcely have guessed, by understanding only the motion of the particles one at a time. The search for these solutions, and the emergent properties that they explain, has been the central theme of my life as a theoretical physicist. This has taken me into various related areas including materials science, surface science, chemistry, nanoscience and clean energy studies.

Examples of emergent properties discussed in the talk included the sausage and kink instabilities that ruined the early experiments on clean fusion energy production, and the phenomenon of superconductivity.

Another emergent property discussed in some detail was the creation of the attractive van der Waals interaction as a result of correlated motions of electrons, plus the purely repulsive Coulomb force between electrons. The present theory of this phenomenon in graphitic clean-energy storage nanosystems seems to be in some disarray, and theoretical elucidation of this problem is my largest current project. This is being undertaken in collaboration with experimentalist Evan Gray. With luck we may be able to help in the quest for a “greenhouse-friendly” hydrogen energy economy.

The title “The whole is more than the sum of its parts” can be given a further significance. One can view the formerly separate disciplines Physics, Chemistry and Biology as “parts” of Science. Then, as the barriers between these disciplines become blurred through the increasing success of a quantitative, reductionist approach, we may indeed see in the twenty-first century a broader holistic Science emerge, that is indeed more than the sum of its parts.

Whatever one’s view on the title of this talk, one thing is guaranteed: the quantum many-body problem is at the heart of the theory of condensed matter and nanostructures, and it is not in general exactly soluble. I thus expect that there will be no lack of fascinating and useful phenomena for theorists like myself to tinker with, into the foreseeable future.
PUBLICATIONS CITED


ACKNOWLEDGMENTS

I would first like to thank all of the students, collaborators and colleagues mentioned in the text above.

The School of Science at Griffith University has been a wonderful place to work. Where else would a theoretical physicist regularly share a coffee table with chemists, biologists, engineers and mathematicians, to the great benefit of his breadth of view?

I am also very grateful to my wife, Astrid, for her support and for giving me the confidence to pursue my longer-term goals. She and my children, William and Sarah, have also been very good-natured about my sometimes odd working hours and my various solo overseas research trips.

My thanks also go to Carmel Johnson, who ably took care of the practical arrangements for this Lecture.

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