The Computational Difficulty of Quantum Mechanics

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It suffices to consider a non-relativistic mechanics formulated through a potential function, V. In classical mechanics, the quantities to be computed are the position vectors of all N_p interacting particles at each time t. The position vector of the ith particle is written $\bar{r}_i(t)$. The classical equations of motion to be solved are thus,

$$m_i \frac{d^2\bar{r}_i}{dt^2} = -\frac{\partial V(\bar{r}_1, \bar{r}_2, \bar{r}_3, ...)}{\partial \bar{r}_i} \tag{1}$$

There is a separate equation for each particle. Assuming that V is a given function, these (ordinary) differential equations can be computed numerically by using a discrete grid of time points (say the interval [0, T] divided into N_t equal steps, $\tau = T/N_t$, so that the jth time is $t = j\tau$). A number of different numerical algorithms could be used, but they all come down to finding the position vectors $\bar{r}_i(j\tau)$ in terms of the positions at the previous two time points and in terms of the corresponding values of the RHS of (1). If we assume that V depends, in general, on all the particle distances, i.e. all the $|\bar{r}_i - \bar{r}_j|$, then evaluation of the RHS of (1) for any given i and at any given time may be proportional, at worst, to the number of pairs times the dimensionality of space, $3N_p(N_p - 1)/2$. The same procedure is followed for each particle, i, and each direction separately giving potentially another factor of $3N_p$ computation time Hence the computation time is proportional to the number of particles cubed, proportional to the dimensionality of space squared, and proportional the number of time steps, $3^2 N_p^3 N_t$.

The quantum mechanical equivalent of (1) can be formulated using the Schrodinger equation, Equ.(2):-

$$\left\{-\left(\frac{\hbar^2}{2m_1}\nabla_1^2 + \frac{\hbar^2}{2m_2}\nabla_2^2 + \frac{\hbar^2}{2m_3}\nabla_3^2 + ...\right) + V(\bar{r}_1, \bar{r}_2, \bar{r}_3, ...)\right\}\psi(t, \bar{r}_1, \bar{r}_2, \bar{r}_3, ...) = i\hbar\frac{\partial\psi(t, \bar{r}_1, \bar{r}_2, \bar{r}_3, ...)}{\partial t}$$

There is now just one, partial differential, equation for the whole N_p-particle system. Whereas the classical state was defined by $3N_p$ real variables at each time point, the quantum mechanical problem involves a complex field defined over a $3N_p$ dimensional space at each time point. Crudely speaking, the number of degrees of freedom in the quantum mechanical problem exceeds that in the classical problem by a factor equal to the indenumerable infinity of the continuum raised to the power $3N_p$. Therein lies the problem.

As a computational problem, this is an overstatement. Considered as a computational problem we must agree to work to some finite accuracy. This also applies to the classical problem. Finding even a single real degree of freedom precisely would require infinite information and infinite computation. The accuracy of the numerical solution to the

Schrodinger equation will depend upon how many discrete spatial points are used in the numerical algorithm. We shall assume that using N_s spatial points per direction is equivalent to the accuracy of the classical problem solved numerically using N_t time steps. If we consider the solution inside some finite cube of side L, then the spatial grid size is $\varepsilon = L/N_s$. Each $\bar{r}$ can take N_s^3 different values. So the number of different values of $(\bar{r}_1, \bar{r}_2, \bar{r}_3, ...)$ is $N_s^{3N_p}$.

The Schrodinger equation can be solved in essentially the same time-stepping manner as Equ.(1), but the quantity being calculated is now the complex-valued ψ at each of the $N_s^{3N_p}$ different values of its parameters, at each time point. Hence, the computational time is proportional to $2.3^2.N_t\left(N_s^{3N_p}\right)^3$. (The factor of 2 is because it's a complex quantity).

The numerical solution of the quantum problem therefore takes a factor $\sim(N_s^{3N_p} / N_p)^3$ longer to solve than the classical problem (ignoring the numerical factor). This increases exponentially with the number of particles, N_p. In practice this means that the quantum problem is essential incomputable.

One could object that the above computing times have been rather exaggerated in that all $N_p\left(N_p - 1\right)/2$ pairs of interactions have been taken into account. In practice such a computation would be carried out by assuming interactions were negligible beyond, say, the nearest neighbours. In this case the computation becomes proportional to the number of particles in the classical case, $3N_pN_t$, and proportional to the number of discrete spatial points in the QM case, $2.3.N_t N_s^{3N_p}$. Hence, the factor by which the time of the QM computation exceeds the classical computation reduces to $\sim N_s^{3N_p} / N_p$. However, this still increases exponentially with the number of particles, N_p, so it makes no essential difference, as illustrated by the following examples:-

Example 1: Take $N_s \sim 100$ for a reasonably accurate solution. Consider the 3-body problem ($N_p = 3$). Then the quantum problem takes $\sim 10^{18}$ times longer than the classical problem. Thus, if the latter took 0.1 sec, the former would take the order of the age of the universe.

Example 2: Take $N_s \sim 100$ for a reasonably accurate solution. Consider $N_p = 7$. Then the quantum problem takes $\sim 10^{41}$ times longer than the classical problem. Thus, if the latter were so fast that it took only the order of the strong nuclear timescale, 10^{-23} sec, the former would still take the order of the age of the universe.

Example 3: Take the smallest possible N_s, i.e. $N_s = 2$, though this could hardly give an accurate solution. Consider $N_p = 26$. Then the quantum problem takes $\sim 10^{22}$ times longer than the classical problem. Thus, if the latter took a millisecond, the former would still take the order of the age of the universe.

Example 4: Take the smallest possible N_s, i.e. $N_s = 2$, though this could hardly give an accurate solution. Consider $N_p = 46$. Then the quantum problem takes $\sim 10^{40}$ times longer than the classical problem. Thus, if the latter were so fast it took only the order of the strong nuclear timescale, 10^{-23} sec, the former would still take the order of the age of the universe.

Example 5: Take the smallest possible N_s, i.e. $N_s = 2$, though this could hardly give an accurate solution. Consider $N_p = 69$. Then the quantum problem takes $\sim 10^{60}$ times longer than the classical problem. Thus, if the latter were so fast it took only the order of the Planck timescale, $\sim 10^{-43}$ sec, the former would still take the order of the age of the universe.

The universe is effectively computing its own future. The last example shows that it is inconceivable that any classical computer could perform the required computation to follow the evolution of just 69 particles, even in the age of the universe. Of course, what is actually happening is that the universe is simulating the quantum mechanics by *being* quantum mechanical, not a classical computer.

Imprecise Corollary: Something called a quantum computer exists because the universe must be one. It is massively faster than a classical computer.

A very reasonable objection to this conclusion is that the real world is unlikely to work in a manner analogous to solving the equations of either classical or quantum physics. It may be that reality has a wholly different way of continuously computing its future which is far more efficient. But if so, could we not in principle discovery what this process is and replicate it mathematically? In other words, if reality has such an alternative, vastly more efficient, algorithm, this would constitute an improved theory of physics. Let's call this hypothetical theory IM (Improved Mechanics). Moreover, we could, in principle, build a computing device to exploit this. So we again conclude the existence of a far-faster-than-classical computing device, based now on IM. The above corollary is therefore correct so long as we interpret a "quantum computer" to be any computer based on the real world's own secret efficient algorithms. Hence,

Better Corollary: Far faster computing devices than classical computers exist because the universe is one.

However, for the rest of this Note we shall assume that conventional quantum mechanics ***is*** the correct theory, and that the universe is therefore a quantum computer, as would then be necessary in order for it to keep up with itself!

The oddest conclusion follows from considering what resources this quantum computer called the universe needs to carry out its continuous simulation. At each time it needs to store the $N_s^{3N_p}$ complex numbers representing the quantum state. Even if N_s were as small as 2, for $N_p = 99$ this is $2^{297} \sim 10^{89}$ numbers. This is approximately the total number of photons plus fundamental particles in the whole of the observable universe. Let's say we use the spin states of these 10^{89} particles as a binary storage device. So, even if the whole of the universe were used as RAM in this way, the maximum number of particles for which a simulation of the quantum mechanical evolution could be carried out would be just 99 particles. But the universe is carrying out this computation, without noticeable hesitation, for ~10^{89} particles.

So how does the universe actually do it? One possibility is that quantum mechanics is just wrong. However, if the Schrodinger equation is correct then there must be some enormous resource available – other than this universe.

This is Deutsch's challenge to Penrose: "where is the calculation (of a quantum computer) carried out?"

It appears that quantum mechanics, if correct, requires the multiverse. The above argument shows that this follows quite independently of the usual arguments based on interference.

A more general formulation of quantum mechanics uses the $3N_p$ dimensional Hilbert space spanned by vectors which may be written $\left|\xi_1, \xi_2, \xi_3, ...\right\rangle$, which are just direct products of single particles states,

$$\left|\xi_1, \xi_2, \xi_3, ...\right\rangle = \left|\xi_1\right\rangle\left|\xi_2\right\rangle\left|\xi_3\right\rangle... \qquad (3)$$

and where each ξ is a label for the possible one-particle states. Let's say there are N_{states} such one-particle states. For example, for spin-½ particles restrained to lie at one fixed position we would have $N_{states} = 2$, i.e. two spin states only. Or, for a free particle in a box in 3D space, the quantum states would be labelled by three positive integers n_x, n_y, n_z. Restricting the maximum energy per particle, $E_{max} = \left(\frac{\pi\hbar}{L}\right)^2 \frac{n_{max}^2}{2m}$, would yield a finite, but possibly very large, value for N_{states} of the order of $n_{max}^3 / 2$. In the previous Schrodinger equation case we had $N_{states} = N_s^3$, so we see that N_s is essentially the same thing as n_{max}. Equ.(3) implies that the number of N_p-particle states is $N_{states}^{N_p}$ (strictly with a correction for identical particles). For $N_{states} = N_s^3$ this reproduces the same number of states obtained from the Schrodinger formulation, i.e., $N_s^{3N_p}$. So the formulation chosen for quantum mechanics makes no difference.

Finally, it is tempting to think that ~99 particles (atoms?) might be the boundary between quantum and classical behaviour. But it does not seem to be. Zeilinger's team (Hackermuller et al, 2003, quant-ph/0309016) have demonstrated interference in beams of fluorofullerene $C_{60}F_{48}$ containing 108 atoms and some 1632 atomic mass units (i.e. protons and neutrons) plus 792 electrons. But it might be, indeed almost certainly is, the case that almost all the internal degrees of freedom of this molecule are unexcited in order to permit the interference to be coherent.