# Quantum and classical molecular dynamics

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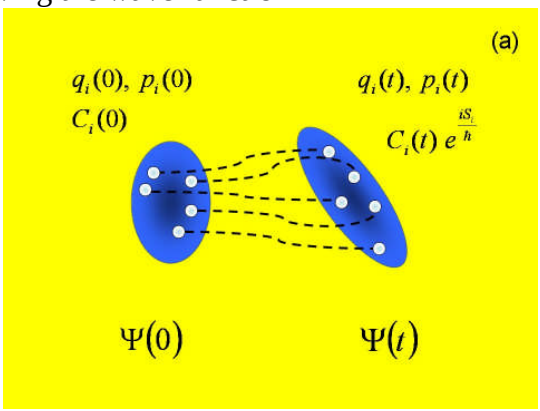
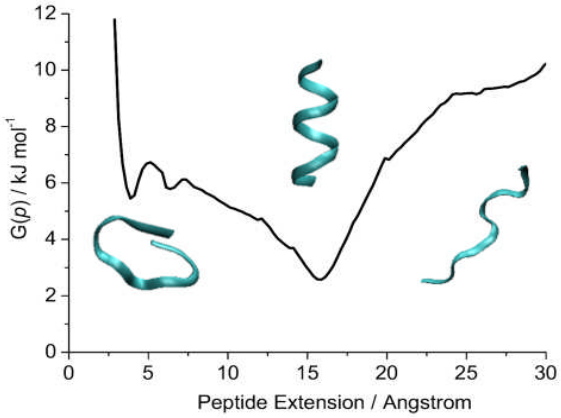
The goal of our research is to develop new computational methods for atomistic simulations in chemistry and physics. These methods should allow us to treat bigger molecular systems faster and more accurately. There are two main areas of research in the Leeds Quantum and Classical Molecular Dynamics group.

First project is focused on ***quantum wave packet dynamics***. Chemical dynamics is about rearranging nuclei whose motion is often nonclassical. Such effects as tunnelling, zero point energy, and quantization of vibrational and rotational motions are crucial for understanding chemical dynamics. Although the lows of quantum mechanics are known quantum equations for realistic systems with many degrees of freedom are very difficult to solve even with the fastest computers. The central problem is that complicated quantum wave functions are always represented as a superposition of a large number of simple basis functions and the size of the basis grows extremely fast with the number of degrees of freedom. We develop new techniques which speed up quantum simulations and allow to treat larger molecular systems[1-3]. The main idea is to use classical mechanics to guide quantum basis is illustrated on the figure below which shows a trajectory guided grid following the wave function




We developed several methods which exploit this very simple idea and applied them to many interesting problems in chemistry and physics which range from chemical dynamics[4] and spectroscopy to dynamics of electrons in laser field[5] and even quantum computers[6].

Second project is focused on ***classical molecular dynamics of biological molecules*** such as proteins for example. Here we disregard quantum effects and only consider classical dynamics. The molecules we are simulating are often comprised of thousands of atoms, which are viewed almost as classical balls connected by springs. The problem with classical molecular dynamics is that for molecules of this size atomistic simulations can be done on the time scale of picoseconds but the time scale of important biological processes such as protein folding for example is microseconds or longer so that at least 6 orders of magnitude has to be bridged. We developed efficient methods which allow to solve this problem by viewing long time dynamics as a set of short time processes. Therefore one very long simulation is replaced by a number of short ones. An example of such study can be found in ref[7] where we reproduced experimental data on peptide cyclization shown below




With our new methods of accelerated classical dynamics we are looking now at protein folding, drug binding and other problems important in biochemistry in which we reach microsecond time scale[7]. .

Our research is very mathematical and involves the use of powerful computers. Both projects are suited not only for chemists but also for physics and mathematics graduates

## References

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