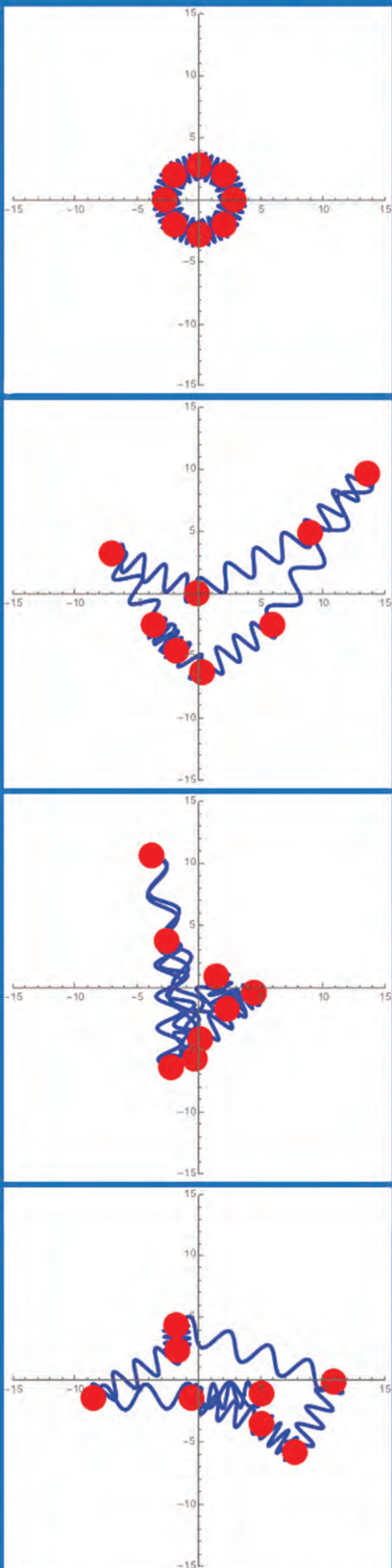
MODELLING QUANTUM MECHANICS: THE RING POLYMER METHOD

INTRO

"Anyone not shocked by Quantum Mechanics has not yet understood it" – Niels Bohr

The Ring Polymer Method is a method of modelling Quantum Mechanical Particles in a general potential. The method makes use of an analogy between the general problem of a quantum particle in a thermal bath and a classical system which we can, with relative ease, simulate the dynamics of. The method is an excellent tool to allow us to visualise more intuitively the non-localised quantum mechanical behaviours that we would otherwise have little direct comprehension of due to the inherent strangeness of quantum mechanics.



METHOD

The quantum particle in a thermal bath has a mathematical mirror image with a particular classical system. That system consists of a set of masses connected in circular fashion by spring-like forces, which are suspended in an external harmonic potential and exposed to ambient thermally excited gas-like particles that drive the elements of the ring of masses in a Brownian motion by collisions with them. These random impulses cause fluctuations of position of the ring polymer ensemble. After enough time iterations a histogram of the positions of each mass in the ring can be built up and analysed. By equations 5-9, one can retrieve the QM kernel using a wick rotation.

RESULTS

Observations from the results include the distinctive Gaussian Normal Distribution of the positions of the connected masses, as shown by Figure 2. This histogram represents the wave function of the quantum particle we hoped model the behaviour of via the Ring Polymer Method. Figure 2 also confirms that the ground state solution of the time-independent Schrödinger equation, shown by the red line, agrees precisely with the results.

CONCLUSION

This method correctly implements the path integral formulation of quantum mechanics and yields the behaviour of the quantum particle in a thermal bath. Note that we never had to computationally sum over all paths explicitly using Eqns. 1, 2 & 3, nor did we have to find wave equations for all energy levels of the particle, which involves simply changing the temperature in this approach.

Eqn. 1

$$K(x_a,t;x_b,t') = \int \mathcal{D}[x(t)]\, e^{(i/\hbar)S[x(t)]}$$

Eqn. 2

$$\mathcal{D}[x(t)] = \frac{1}{A}\prod_{k=1}^{N-1}\left\{\frac{dx_k}{A}\right\}$$

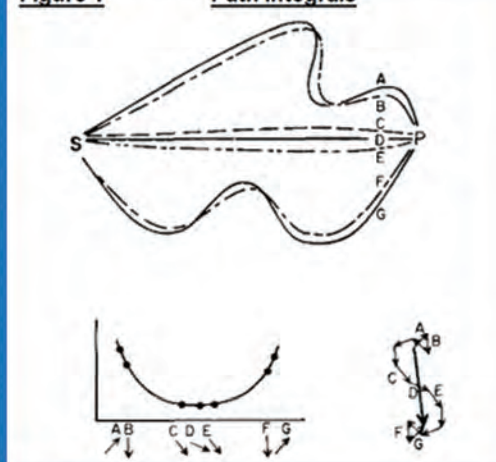
Eqn. 3

$$S[x(t)] = \int_t^{t'} \mathcal{L}(p,q,t)\, dt$$

Eqn. 4

$$\frac{\delta F}{\delta f(x)} = \frac{\partial F}{\partial f} - \frac{d}{dx}\frac{\partial F}{\partial f'}$$

Figure 1 **Path Integrals**



Eqn. 5

$$\langle x'|e^{-i\hat{H}t/\hbar}|x\rangle = \int \mathcal{D}[x(t)]\, e^{(i/\hbar)S[x(t)]}$$

Eqn. 6

$$Z = \mathrm{Tr}\left(e^{-\beta\hat{H}}\right) = \int_{-\infty}^{\infty} \langle x|e^{-\beta\hat{H}}|x\rangle\, dx$$

Eqn. 7

$$\hat{U}(t) = e^{-i\hat{H}t/\hbar}$$

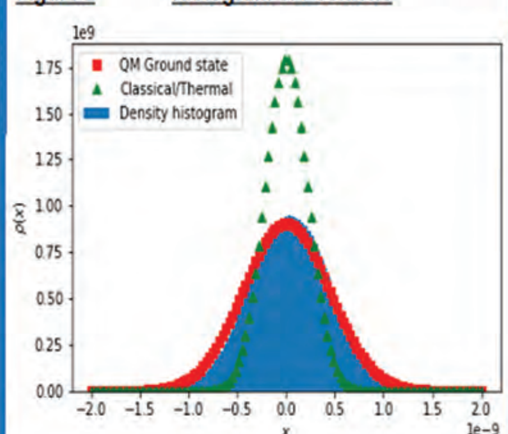
Eqn. 8

$$\beta = (i/\hbar)t$$

Eqn. 9

$$\langle x|e^{-\beta\hat{H}}|x\rangle \xrightarrow[\textit{Wick rotation}]{} \langle x|e^{-i\hat{H}t/\hbar}|x\rangle$$

Figure 2 **Histogram of Positions**



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