Many Particle Systems

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The Classical Problem

How To Model This Why Doesn't This Work?

How Do We Solve This?

Master Equation Second Quantization The Black Box Conclusion

The Future

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How To Model This Why Doesn't This Work?

The Classical Problem

- ▶ We are for the purposes of this talk interested in the reaction $A + A \rightarrow A$
- ▶ We start with a large, but finite number of dust particles.
- After a finite time they all react leaving us with a single particle.

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How To Model This Why Doesn't This Work?

How To Model This

The usual rate equation for this reaction is the Smoluchowski equation.

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- The usual rate equation for this reaction is the Smoluchowski equation.
- $\blacktriangleright \ \frac{dc}{dt} = -\kappa c^2$
- c is the mean particle population and κ is the rate coefficient

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How To Model This Why Doesn't This Work?

Why Doesn't This Work?

The Smoluchowski equation is only valid in the thermodynamic limit.

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Why Doesn't This Work?

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- When our particle population starts to fall rapidly we are no longer in this limit.

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How To Model This Why Doesn't This Work?

Why Doesn't This Work?

- The Smoluchowski equation is only valid in the thermodynamic limit.
- When our particle population starts to fall rapidly we are no longer in this limit.
- ► This gives odd and unrealistic results when modelling.

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Master Equation Second Quantization The Black Box Conclusion

The Master Equation

• First we must write a master equation for this reaction.

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Master Equation Second Quantization The Black Box Conclusion

The Master Equation

▶ First we must write a master equation for this reaction. ▶ $\frac{dP(N,t)}{dt} = \frac{\kappa}{2V}[(N+1)NP(N+1,t) - N(N-1)P(N,t)]$

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Master Equation Second Quantization The Black Box Conclusion

The Master Equation

- First we must write a master equation for this reaction. $\frac{dP(N,t)}{dt} = \frac{\kappa}{2V} [(N+1)NP(N+1,t) - N(N-1)P(N,t)]$
- Then we embark on obscure and lengthy process of second quantization.

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Master Equation Second Quantization The Black Box Conclusion

Second Quantization

 We create a Hilbert Space, with the usual notion of annihilation and creation operators.

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Master Equation Second Quantization The Black Box Conclusion

Second Quantization

- We create a Hilbert Space, with the usual notion of annihilation and creation operators.
- We define a wave equation to describe our system for any given time

$$|\Psi\rangle_{A+A\to A} := \sum_{N} P(N,t)(a^+)^N |0\rangle$$

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Second Quantization

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$$|\Psi\rangle_{\mathcal{A}+\mathcal{A}\to\mathcal{A}} := \sum_{N} P(N,t)(a^+)^N |0\rangle$$

► We can then write down the evolution operator, $H_{A+A\to A}[a^+, a^-] = -\frac{\kappa}{2V}(a^+ - a^{+^2})a^{-^2}$, that satisfies the imaginary time Schödinger equation. $\frac{d}{dt}|\Psi\rangle_{A+A\to A} = -H_{A+A\to A}[a^+, a^-]|\Psi\rangle_{A+A\to A}$

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Master Equation Second Quantization The Black Box Conclusion

The Black Box

The next stage is to define a general observable.

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Master Equation Second Quantization The Black Box Conclusion

The Black Box

- The next stage is to define a general observable.
- Write down the full expression of the expectation value of this observable

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Master Equation Second Quantization The Black Box Conclusion

The Black Box

- The next stage is to define a general observable.
- Write down the full expression of the expectation value of this observable
- We then split the time into small compartments, rearrange and finally convert it to a continous system.

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- This leaves us with a Path Integral to solve.

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- Write down the full expression of the expectation value of this observable
- We then split the time into small compartments, rearrange and finally convert it to a continous system.
- This leaves us with a Path Integral to solve.
- Solving this partly gives us a constraint equation which looks identical to the original Smoluchowski equation with an additional term.

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Master Equation Second Quantization The Black Box Conclusion

The Final Result

$$\triangleright \ \partial_t \bar{\Phi}(t) = -\bar{\kappa} \bar{\Phi}^2(t) + i\eta \sqrt{2\bar{\kappa}} \bar{\Phi}$$

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Master Equation Second Quantization The Black Box Conclusion

The Final Result

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The η represents a white noise, which when a simulation is down it should be averaged over.

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- $\Phi(t)$ is the now complex population variable.

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- The η represents a white noise, which when a simulation is down it should be averaged over.
- $\Phi(t)$ is the now complex population variable.
- Taking the averaging over several noises and only looking at the real part of Φ gives a matching to the results expected from Monte Carlo Simultions.

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$A + B \rightarrow C$

The next step is to calculate a reaction where a single "super" dust particle forms.

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$A + B \rightarrow C$

- The next step is to calculate a reaction where a single "super" dust particle forms.
- Maybe we will find a general form of the complex noise term.
- Is it possible to show that if we average over the complex term an infinite number of times the Im(Φ(t)) → 0?

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