**Title:** Quantum reconstruction in terms of imaginary time

**Speakers:** Russell Thompson

**Collection/Series:** Lee's Fest: Quantum Gravity and the Nature of Time

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**Abstract:**

Modern quantum simulations methods often use a fictitious imaginary time introduced by Feynman to exactly transform static quantum problems to dynamic imaginary time classical ones [1]. In addition to imaginary time simulation methods such as centroid molecular dynamics and path integral Monte Carlo, one can apply this quantum-classical isomorphism to self-consistent field theory (SCFT). An advantage of the field-theoretic perspective is that it can be exactly transformed into quantum density functional theory (DFT), meaning that the theorems of DFT (Hohenberg-Kohn and Mermin theorems) prove an equivalence between classical imaginary time SCFT dynamics and static quantum results [2]. Since imaginary time is assigned the same properties as regular time, one can replace the imaginary time in the SCFT equations with real time (a Wick rotation), which gives the equations of time-dependent DFT. The time-dependent DFT theorem (Runge-Gross theorem) then proves that one obtains all results of standard quantum mechanics from this imaginary time classical starting point. These results make it very tempting to consider treating imaginary time as an element of reality. This quantum reconstruction from imaginary time will be discussed, including a speculative look at treating imaginary time in the context of special relativity, with a preliminary comparison to the deformed special relativity of Magueijo and Smolin.

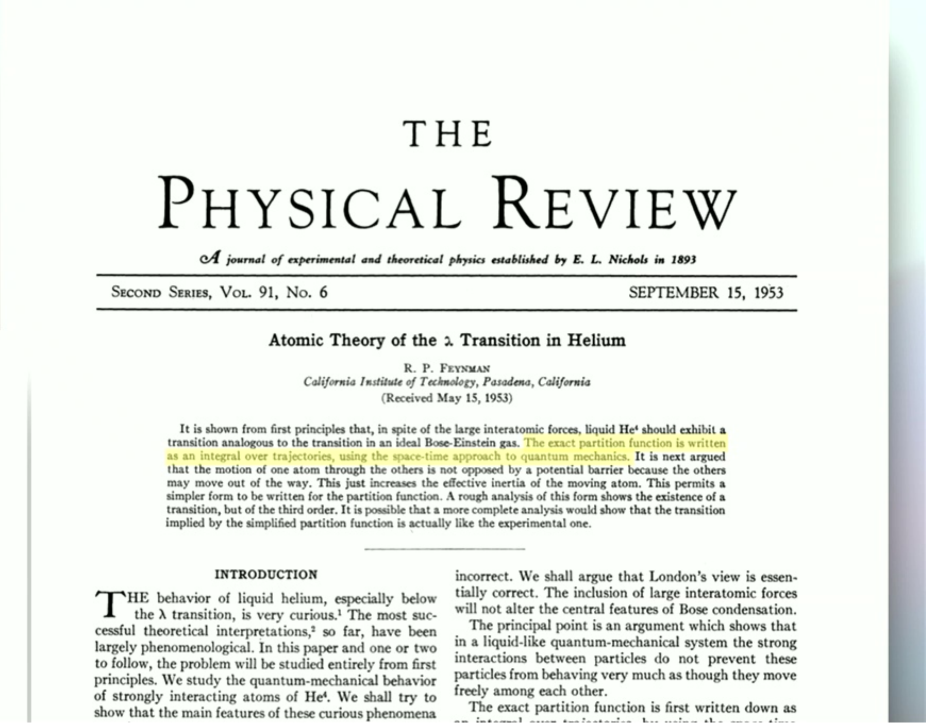
[1] D. M. Ceperely, Reviews of Modern Physics 67, 279 (1995)
[2] R. B. Thompson, Journal of Chemical Physics 150, 204109 (2019)
[3] J. Magueijo and L. Smolin, Physical Review D 67, 044017 (2003)

# Quantum reconstruction using imaginary time

**Russell Thompson**
Department of Physics & Astronomy
University of Waterloo

# The ring polymer quantum-classical isomorphism

- In 1953, Richard Feynman showed that the path integral action describing a quantum particle is isomorphic with the ***classical*** partition function of a ring polymer
- This concept forms the basis of modern quantum simulations methods such as Centroid Molecular Dynamics, Ring Polymer Molecular Dynamics and Path Integral Monte Carlo



THE

PHYSICAL REVIEW

*A journal of experimental and theoretical physics established by E. L. Nichols in 1893*

SECOND SERIES, VOL. 91, No. 6 SEPTEMBER 15, 1953

## Atomic Theory of the λ Transition in Helium

R. P. FEYNMAN
*California Institute of Technology, Pasadena, California*
(Received May 15, 1953)

It is shown from first principles that, in spite of the large interatomic forces, liquid $He^4$ should exhibit a transition analogous to the transition in an ideal Bose-Einstein gas. The exact partition function is written as an integral over trajectories, using the space-time approach to quantum mechanics. It is next argued that the motion of one atom through the others is not opposed by a potential barrier because the others may move out of the way. This just increases the effective inertia of the moving atom. This permits a simpler form to be written for the partition function. A rough analysis of this form shows the existence of a transition, but of the third order. It is possible that a more complete analysis would show that the transition implied by the simplified partition function is actually like the experimental one.

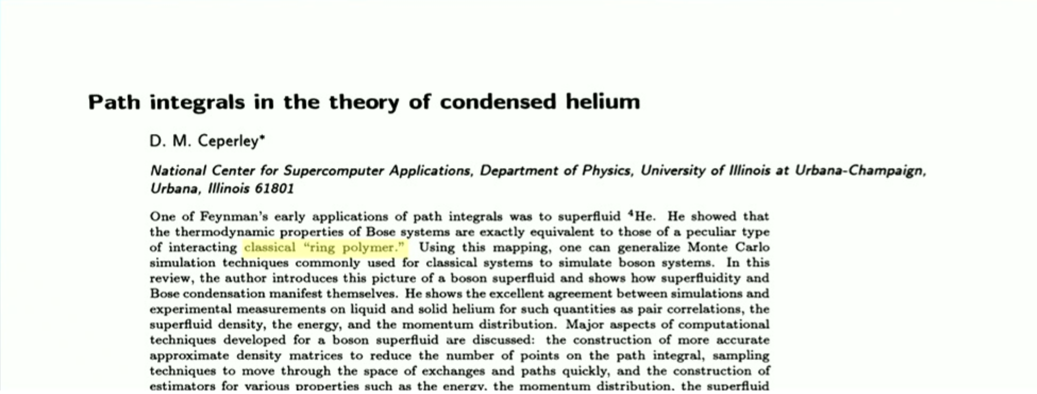
### INTRODUCTION

THE behavior of liquid helium, especially below the λ transition, is very curious.[1] The most successful theoretical interpretations,[2] so far, have been largely phenomenological. In this paper and one or two to follow, the problem will be studied entirely from first principles. We study the quantum-mechanical behavior of strongly interacting atoms of $He^4$. We shall try to show that the main features of these curious phenomena

incorrect. We shall argue that London's view is essentially correct. The inclusion of large interatomic forces will not alter the central features of Bose condensation.

The principal point is an argument which shows that in a liquid-like quantum-mechanical system the strong interactions between particles do not prevent these particles from behaving very much as though they move freely among each other.

The exact partition function is first written down as



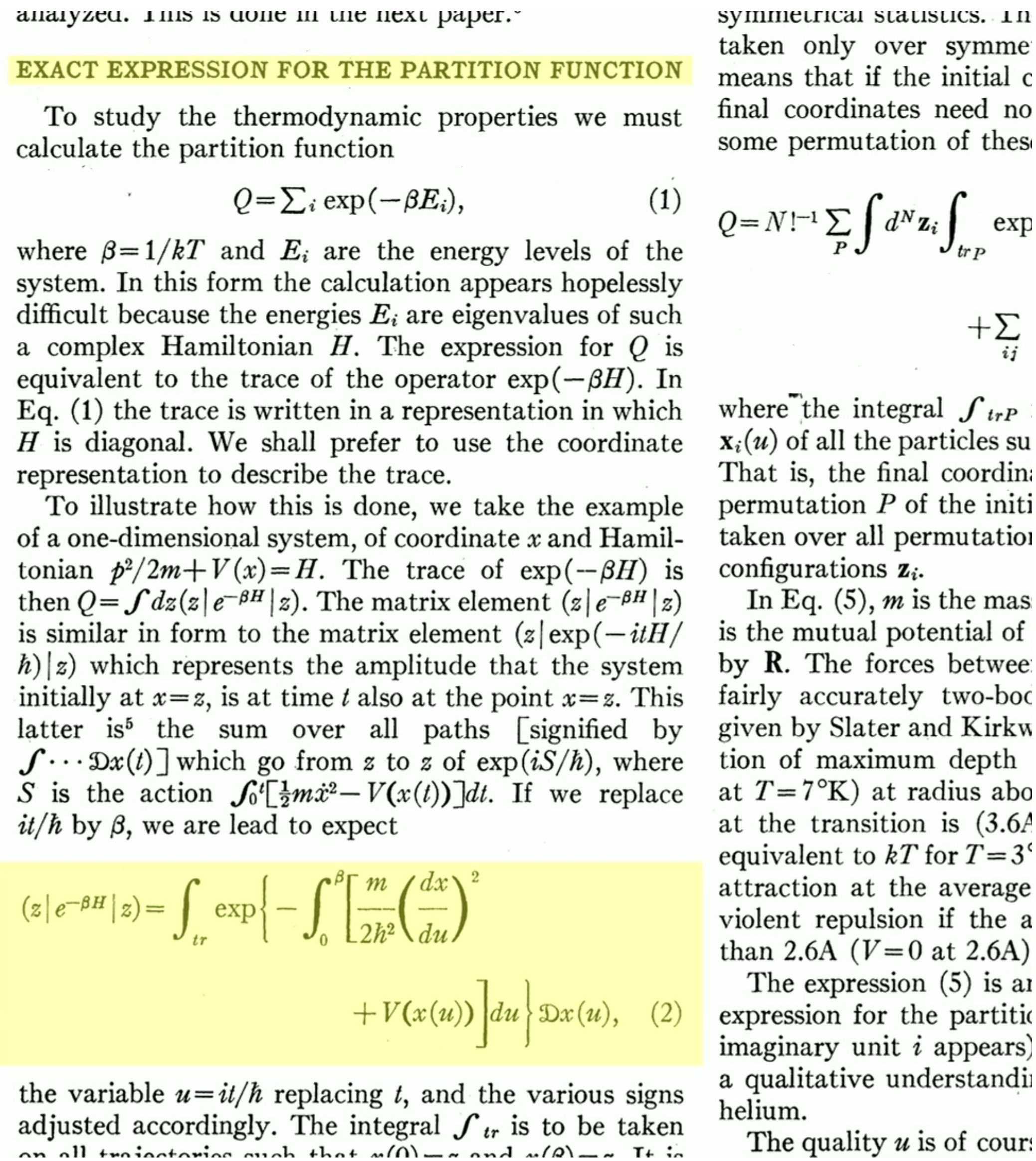
## Path integrals in the theory of condensed helium

D. M. Ceperley*

*National Center for Supercomputer Applications, Department of Physics, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801*

One of Feynman's early applications of path integrals was to superfluid $^4He$. He showed that the thermodynamic properties of Bose systems are exactly equivalent to those of a peculiar type of interacting classical "ring polymer." Using this mapping, one can generalize Monte Carlo simulation techniques commonly used for classical systems to simulate boson systems. In this review, the author introduces this picture of a boson superfluid and shows how superfluidity and Bose condensation manifest themselves. He shows the excellent agreement between simulations and experimental measurements on liquid and solid helium for such quantities as pair correlations, the superfluid density, the energy, and the momentum distribution. Major aspects of computational techniques developed for a boson superfluid are discussed: the construction of more accurate approximate density matrices to reduce the number of points on the path integral, sampling techniques to move through the space of exchanges and paths quickly, and the construction of estimators for various properties such as the energy, the momentum distribution, the superfluid

- For $u = s$ (where $s$ is the contour describing the coarse-grained path of a polymer), this is the ***classical*** partition function of a **ring polymer**



analyzed. This is done in the next paper.

EXACT EXPRESSION FOR THE PARTITION FUNCTION

To study the thermodynamic properties we must calculate the partition function

$$Q=\sum_i \exp(-\beta E_i), \tag{1}$$

where $\beta=1/kT$ and $E_i$ are the energy levels of the system. In this form the calculation appears hopelessly difficult because the energies $E_i$ are eigenvalues of such a complex Hamiltonian $H$. The expression for $Q$ is equivalent to the trace of the operator $\exp(-\beta H)$. In Eq. (1) the trace is written in a representation in which $H$ is diagonal. We shall prefer to use the coordinate representation to describe the trace.

To illustrate how this is done, we take the example of a one-dimensional system, of coordinate $x$ and Hamiltonian $p^2/2m+V(x)=H$. The trace of $\exp(-\beta H)$ is then $Q=\int dz(z|e^{-\beta H}|z)$. The matrix element $(z|e^{-\beta H}|z)$ is similar in form to the matrix element $(z|\exp(-itH/\hbar)|z)$ which represents the amplitude that the system initially at $x=z$, is at time $t$ also at the point $x=z$. This latter is[5] the sum over all paths [signified by $\int\cdots\mathfrak{D}x(t)$] which go from $z$ to $z$ of $\exp(iS/\hbar)$, where $S$ is the action $\int_0^t[\frac{1}{2}m\dot{x}^2-V(x(t))]dt$. If we replace $it/\hbar$ by $\beta$, we are lead to expect

$$(z|e^{-\beta H}|z)=\int_{tr}\exp\left\{-\int_0^\beta\left[\frac{m}{2\hbar^2}\left(\frac{dx}{du}\right)^2+V(x(u))\right]du\right\}\mathfrak{D}x(u), \tag{2}$$

the variable $u=it/\hbar$ replacing $t$, and the various signs adjusted accordingly. The integral $\int_{tr}$ is to be taken on all trajectories such that $x(0)=z$ and $x(\beta)=z$. It is

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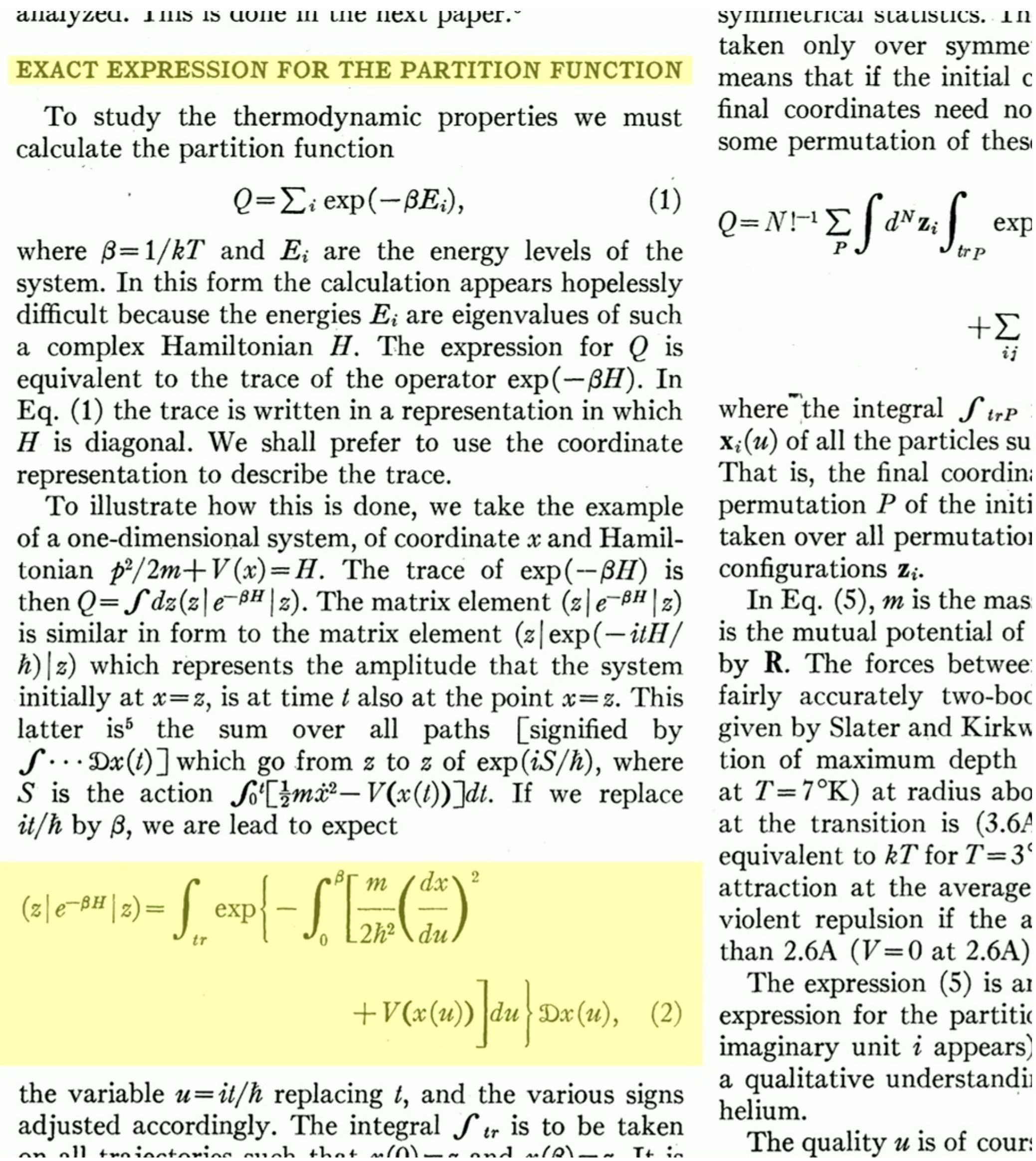

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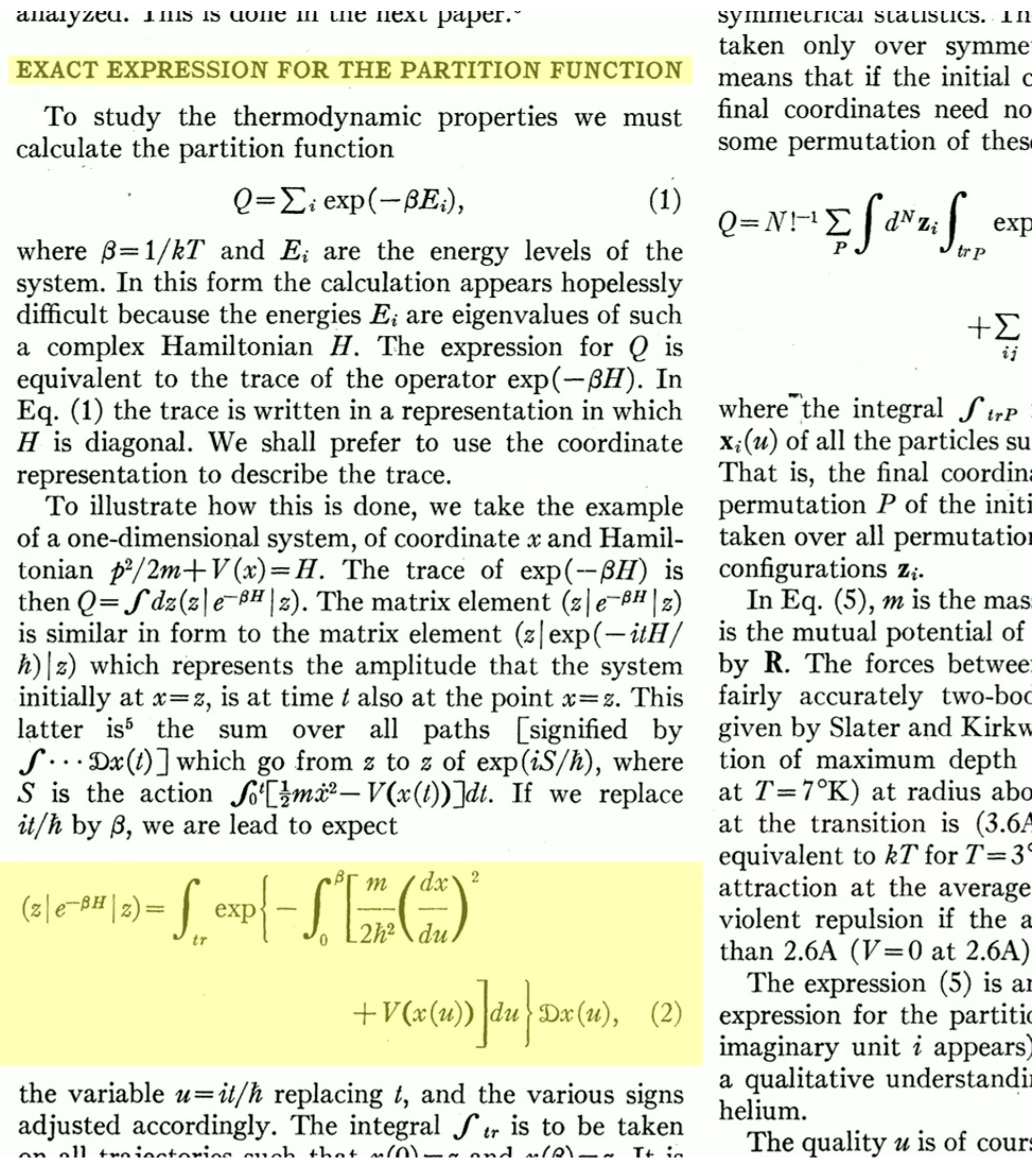
- $\beta$ is called the "imaginary time"
- For $u = it/\hbar$, this is the matrix element of the quantum action



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- Instead of polymer-based simulations, one can use polymer self-consistent field theory (SCFT)
- SCFT is a well known methodology (thousands of papers published on it) which uses the same Feynman path integral
- ***Advantage of SCFT:*** The equations of SCFT can be converted exactly into those of quantum density functional theory (DFT)
- DFT is an even better known methodology (hundreds of thousands of papers published on it)
- The Hohenberg-Kohn theorems and the Mermin theorem of DFT prove that SCFT derived from the classical path integral partition function reproduces all of static quantum mechanics (QM)

- ***What about time?***
- Reconstruct QM by starting with assumption of classical, distinguishable trajectories for particles, although not obeying Newtonian dynamics
    - ***Example:*** de Broglie-Bohm theory
- ***Postulate*** thermal “dimension” that behaves exactly like time dimension, except for being cyclic and imaginary.
- The principle of indifference, or equivalently extending classical concept of structureless particle to structureless “threads” (imaginary time trajectories) means that “classical” partition function must be given by Feynman’s path integral

- SCFT, and thus DFT, drop out of path integral
- Since cyclic imaginary time was assumed to behave just like real time, we also automatically have the dynamics
    - Wick rotate SCFT equations and turn off cyclicity
    - We get expression for the quantum weak value and the equations of time-dependent DFT
    - The Runge-Gross theorem of TDDFT guarantees this reproduces all of non-relativistic QM
- We have reconstructed a de Broglie-Bohm related/inspired theory using one assumption (cyclic imaginary time) in addition to classical concepts
- Only get TDDFT equations if time has a direction — incompatible with illusory time or block universe

- ***Can this be tested?***
- DFT theorems mean there is a one-to-one mapping between QM and "classical" imaginary time rings
- Ring polymer SCFT can make no predictions within QM that can distinguish the "classical" 5D picture from 4D QM
- ***Speculation:***
  - Special relativity: $ds^2 = -c^2dt^2 + dx^2 + dy^2 + dz^2 + \hbar^2c^2d\beta^2$

**Immediate problem: variable speed of light!**

- Special relativity: $ds^2 = -c^2dt^2 + dx^2 + dy^2 + dz^2 + \hbar^2c^2d\beta^2$

Immediate problem: variable speed of light!

- Passing resemblence to doubly special (or deformed) relativity of Amelino-Camelia; Magueijo and ***Smolin***
- Has ***two*** maximal quantities: on both velocity and energy

Magueijo, J.; ***Smolin, L.*** (2002). "Lorentz invariance with an invariant energy scale". *Physical Review Letters*. **88** (19): 190403

Thank you!