Physics 127c: Statistical Mechanics

Application of Path Integrals to Superfluidity in He^4

The path integral method, and its recent implementation using quantum Monte Carlo methods, provides both an intuitive understanding and a computational approach to Bose condensation and superfluidity in strongly interacting Bosons such as liquid He^4. I will briefly discuss Feynman's calculation of the λ-transition from the early 1950s, and how to formulate the condensate density and superfluid density in the path integral approach. See the references in "Further Reading" for more details. This application provides a nice illustration of the use of the path integral method in quantum statistical mechanics.

Feynman's Theory of the λTransition

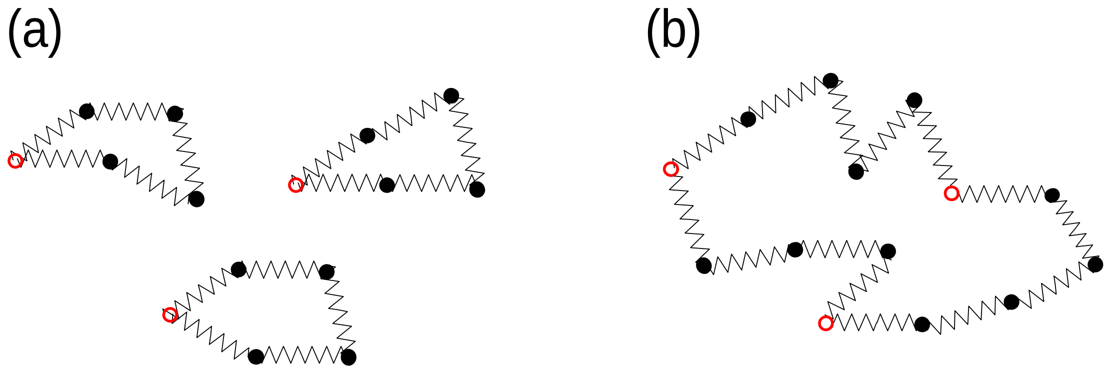

Figure 1: Paths contributing to the partition function for 3 particles. The red, hollow circles denote the initial and final position of each particle, and the black filled circles are the intermediate positions. For Bosons we must include paths such as in (b) which result in exchanges amongst the particles. (For Fermions paths would conetribute with a sign depending on the order of the permutation.)

For a Bose system of N particles the partition function is

$$Z = \bar{\rho}_B(\mathbf{x}, \mathbf{x}; \beta) = \int d^{3N}x \frac{1}{N!} \sum_P \bar{\rho}(\mathbf{x}, P\mathbf{x}; \beta) \tag{1}$$

so that the path integrals contributing to Z must include *exchange loops* in which the path results in permutations of the particles, Fig. 1. In terms of the paths

$$Z = \int_{\mathbf{x}(0)=P[\mathbf{x}(\beta\hbar)]} \mathcal{D}\mathbf{x}(t) \exp\left\{-\frac{1}{\hbar}\int_0^{\beta\hbar} d\tau \left[\frac{m}{2}\dot{\mathbf{x}}^2 + V\left(\mathbf{x}(\tau)\right)\right]\right\}. \tag{2}$$

When do the exchanges become important? Long paths are costly because of the $\dot{\mathbf{x}}^2$ term in the exponential. At best, ignoring any potential cost and supposing two particles each move the nearest neighbor separation d the weight of an exchange path is of order (estimating $\dot{\mathbf{x}}$ from a straight path)

$$\exp\left[-\frac{2}{\hbar}\frac{m}{2}\left(\frac{d}{\beta\hbar}\right)^2 \beta\hbar\right] \sim \exp\left[-\frac{md^2k_BT}{\hbar^2}\right] \sim \exp\left[-\left(\frac{d}{\lambda}\right)^2\right] \tag{3}$$

with λ the thermal de Broglie wave length. The result $d \sim \lambda$ is the basic criterion we have arrived at before for the importance of quantum effects. At high temperatures the paths contributing to Z will typically involve

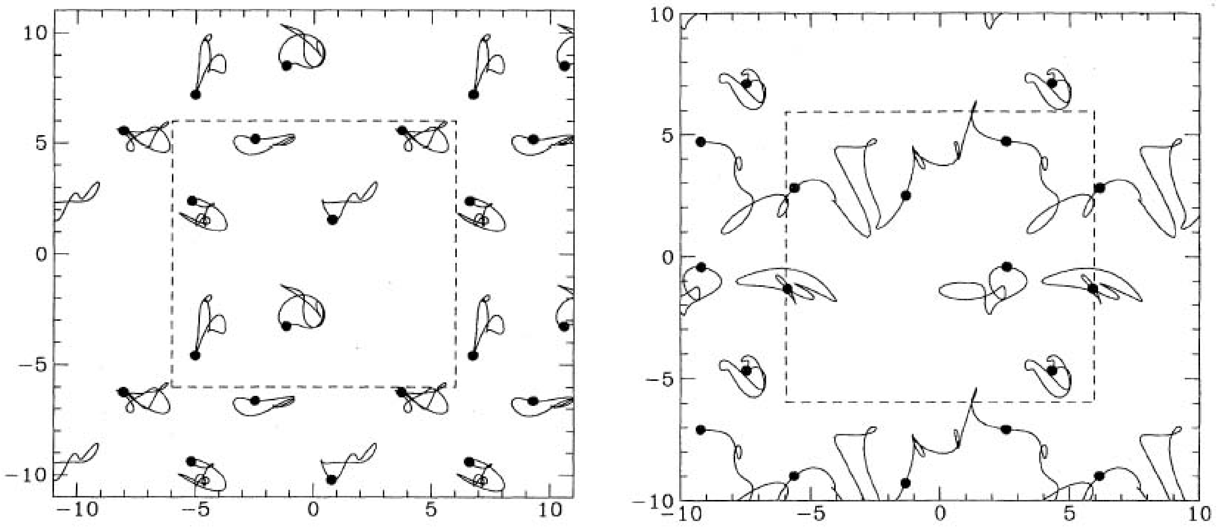

Figure 2: Typical paths from Monte Carlo calculations of the partition function of 6 He^4 at liquid densities. The first panel is at $2K$ and the second at $0.75K$. The paths have been smoothed (80 and 53 imaginary time slices were used in the actual calculations) and the simulation region is copied 4 times in the figure to make the geometry clearer. Axes labels are in Angstrom. [From Ceperley (1995)]

only small excursions of each particle. At low temperatures, when $\lambda \gtrsim d$ there is little cost from longer paths, and exchanges become possible. This is shown in actual Monte Carlo calculations on He^4 in Fig. 2.

Feynman suggested that the λ-transition, and the onset of Bose condensation and superfluidity, could be understood as the proliferation of infinite (or system spanning) exchange loops.

First he wanted to take into account the strong interaction. If the strongly repulsive cores overlap along the path, there is an enormous penalty from the potential term. Thus Feynman suggested the particles avoid each other, and the cost is less if the other particles move out the way (the cost Δx^2 is less than $(d+\Delta x)^2 - d^2$). He supposed that for a leg of the exchange loop of length r a number of order r/d particles must move a distance d'out of the way in an imaginary time $\beta\hbar/n$. The value of d' depends on the separation d and the hard core radius. Thus the contribution to the quantity in the exponential is

$$\frac{mr^2 k_B T}{2\hbar^2} \tag{4}$$

from the particle in the exchange loop and

$$\frac{n}{\hbar}\frac{m}{2}\left(\frac{d'}{\beta\hbar/n}\right)^2 \frac{\beta\hbar}{n} = \frac{md'^2 k_B T}{2\hbar^2} n^2 = \frac{mr^2 k_B T}{2\hbar^2}\left(\frac{d'}{d}\right)^2 \tag{5}$$

from the particle moving out the way. The correction Eq. (5) can be taken into account by replacing the mass in Eq. (4) by an effective mass

$$m' = m\left[1 + \left(\frac{d'}{d}\right)^2\right]. \tag{6}$$

Then the integral along the exchange path can be calculated for free particles of mass m', which is given by the diffusion expression. This leads to the estimate of the free energy

$$e^{-\beta F} = \int \frac{1}{N!} \sum_P \left(\frac{m'}{2\pi\hbar^2\beta}\right)^{3N/2} \exp\left[-\frac{m'}{2\hbar^2\beta}\sum_i (\mathbf{x}^{(i)} - P\mathbf{x}^{(i)})^2\right] f(\mathbf{x}^{(1)}, \mathbf{x}^{(2)} \ldots \mathbf{x}^{(N)}) d^3x^{(1)} \ldots d^3x^{(N)} \tag{7}$$

where $\mathbf{x}^{(i)} - P\mathbf{x}^{(i)}$ is the distance between the initial and final position of particle i in the permutation P, and f is a function that weights the initial configurations (e.g. something like $e^{-\beta U}$ with U the potential energy).

The weight function f will give configurations where the particles are separated by distance d. For a given size loop, the exponential suppression is less if each leg is between nearest neighbors with separation d rather than having fewer, longer legs. Thus Feynman supposes only nearest neighbor loops are important, and then each $(\mathbf{x}^{(i)} - P\mathbf{x}^{(i)})^2$ is about d^2. Then

$$e^{-\beta F} = \frac{1}{N!} \left(\frac{m'}{2\pi\hbar^2\beta}\right)^{3N/2} \sum_P y^{n(P)}, \tag{8}$$

where

$$y = \exp\left(-\frac{m'd^2k_BT}{2\hbar^2}\right), \tag{9}$$

and $n(P)$ is the total number of sides of the polygons forming all the exchange loops in the permutation P. The problem is reduced to loop counting in a random liquid like configuration. Feynman argues that there is a transition involving the importance of large loops: "A single large polygon of r sides contributes a very small amount y^r with $y < 1$. But a large polygon can be drawn in more ways than a small one. Increasing the length r by one increases the number of polygons available by a factor say s (perhaps 3 or 4) although the contribution of each is multiplied by y. Thus if $sy < 1$ (high T) large polygons are unimportant. As T falls, suddenly when $sy = 1$ the contributions from very large polygons (limited by the size of the container) begin to be important." He then went on using various tricky arguments to attempt to solve the statistical mechanics of loops given by Eq. (8), for which I refer you to his original paper, or his book *Statistical Mechanics*.

Expressions for thermodynamic quantities can be calculated from Eq. (7) by differentiation in the usual way, supposing f does not depend on temperature. For the internal energy

$$U = U_0 + \frac{3}{2}Nk_BT - \frac{m'}{2\hbar^2}(k_BT)^2\left\langle R^2\right\rangle \tag{10}$$

with $R^2 = \sum_i (\mathbf{x}^{(i)} - P\mathbf{x}^{(i)})^2$, and for the specific heat

$$\frac{C}{Nk_B} = \frac{3}{2} - 2\frac{m'k_BT}{2\hbar^2}\left\langle R^2\right\rangle + \left(\frac{m'k_BT}{2\hbar^2}\right)^2\left\langle R^4 - \left\langle R^2\right\rangle^2\right\rangle. \tag{11}$$

Elser evaluated these expressions for loops on a cubic lattice using Monte Carlo methods, and, after choosing m' to match the transition temperature, obtained quite good agreement with experimental measurements, Fig. 3.

Condensate Density

The condensate fraction is N_0/N where $N_\mathbf{p}$ is the number of particles in momentum state $\mathbf{p}$. For a many particle wavefunction in the momentum representation $\tilde{\Psi}$ the probability of finding a particular particle in state $\mathbf{p}$ is given by summing $\left|\tilde{\Psi}\right|^2$. Thus

$$N_\mathbf{p} = N \sum_{\mathbf{p}_2,\mathbf{p}_3\cdots\mathbf{p}_N} \left|\tilde{\Psi}(\mathbf{p}, \mathbf{p}_2 \ldots, \mathbf{p}_N)\right|^2. \tag{12}$$

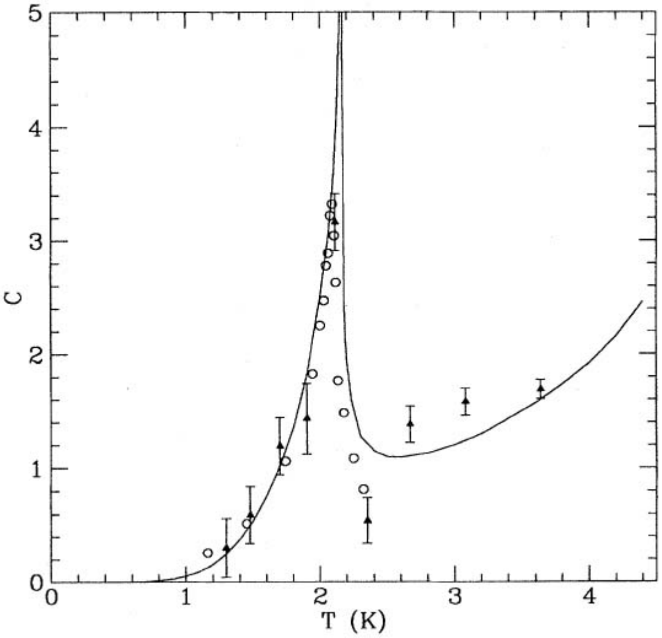

Figure 3: Calculations of the specific heat from the flucutation term in Eq. () for 20^3 atoms on a cubic lattice (open circles) by Elser. Also shown are full path integral Monte Carlo calculations (triangles), and experimental results (solid line). [From Ceperley (1995)]

Returning to the coordinate representation by Fourier transforming

$$\tilde{\Psi}(\mathbf{p}_1, \mathbf{p}_2 \ldots, \mathbf{p}_N = (V)^{-N/2} \int \Psi(\mathbf{x}_1, \mathbf{x}_2 \ldots \mathbf{x}_N) e^{-i(\mathbf{p}_1\cdot\mathbf{x}_1 + \cdots + \mathbf{p}_N\cdot\mathbf{x}_N)/\hbar}, \tag{13}$$

and using

$$\sum_{\mathbf{p}} e^{i\mathbf{p}\cdot\mathbf{x}/\hbar} = \frac{V}{(2\pi\hbar)^3} \int d^3p\, e^{i\mathbf{p}\cdot\mathbf{x}/\hbar} = \delta(\mathbf{x}) \tag{14}$$

gives

$$\frac{N_{\mathbf{p}}}{N} = \frac{1}{V} \int d^3x\, e^{-i\mathbf{p}\cdot\mathbf{x}/\hbar} \left[\int \cdots \int \Psi^*(\mathbf{x}_1, \mathbf{x}_2 \ldots \mathbf{x}_N) \Psi(\mathbf{x}_1 + \mathbf{x}, \mathbf{x}_2 \ldots \mathbf{x}_N) d^3x_1 \ldots d^3x_N \right], \tag{15}$$

and so the condensate density

$$\frac{N_{\mathbf{0}}}{N} = \frac{1}{V} \int d^3x \left[\int \cdots \int \Psi^*(\mathbf{x}_1, \mathbf{x}_2 \ldots \mathbf{x}_N) \Psi(\mathbf{x}_1 + \mathbf{x}, \mathbf{x}_2 \ldots \mathbf{x}_N) d^3x_1 \ldots d^3x_N \right]. \tag{16}$$

At nonzero temperature the $\Psi^*\Psi$ is replaced by the density matrix $\rho_B = \bar{\rho}_B / Tr\bar{\rho}_B$, so that

$$\frac{N_{\mathbf{0}}}{N} = \frac{1}{V} \int d^3x \frac{\int \cdots \int \bar{\rho}_B(\mathbf{x}_1, \mathbf{x}_2 \ldots \mathbf{x}_N; \mathbf{x}_1 + \mathbf{x}, \mathbf{x}_2 \ldots \mathbf{x}_N)\, d^3x_1 \ldots d^3x_N}{\int \cdots \int \bar{\rho}_B(\mathbf{x}_1, \mathbf{x}_2 \ldots \mathbf{x}_N; \mathbf{x}_1, \mathbf{x}_2 \ldots \mathbf{x}_N)\, d^3x_1 \ldots d^3x_N}. \tag{17}$$

(This is the off-diagonal element of the one particle density matrix—the density matrix integrated over $N-1$ coordinates, and the existence of the condensate was described as off-diagonal long range order (ODLRO)

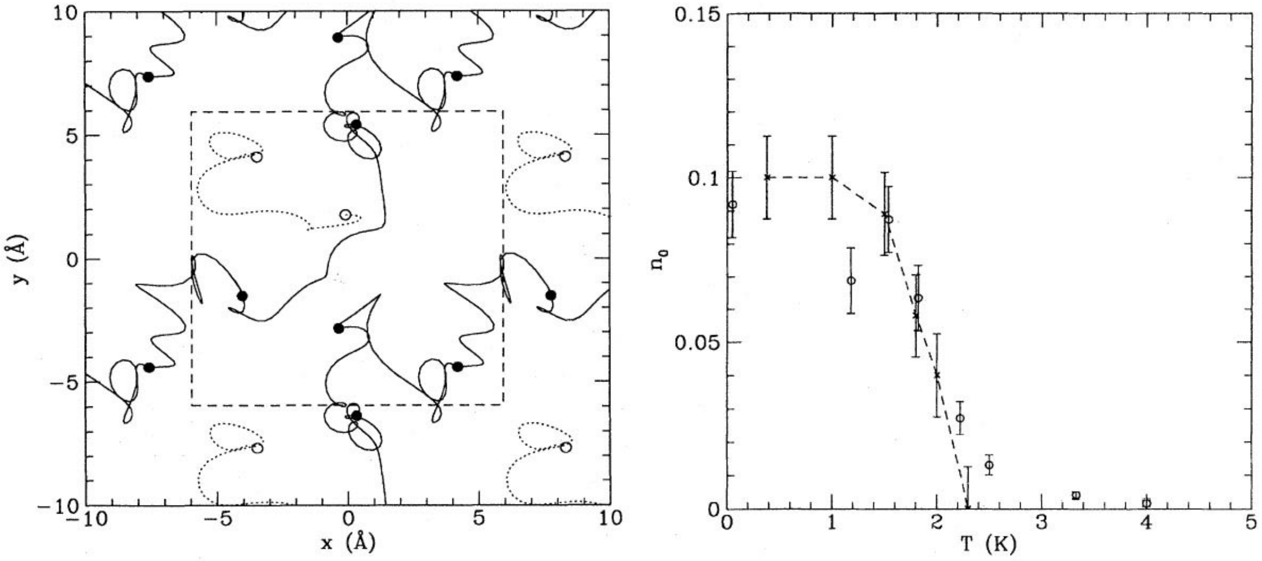

Figure 4: Left panel - sample configuration of one "cut" chain given by QMC for Helium at $0.75K$; right panel - condensate fraction given by such calculations (open circles) and neutron scattering experiments (crosses and dashed line). [From Ceperley (1995)]

by Penrose and Onsager in their pioneering early work on the subject.) In terms of paths, Eq. (17) is the path integral for paths with ends separated by $\mathbf{x}$ relative to the path integral for closed paths, averaged over all $\mathbf{x}$. In a Monte Carlo calculation this is given by the fraction of the volume covered by the separation of the ends of a cut chain. For V large, the average is dominated by large separations, and so it is the probability of macroscopic end separations.

Superfluid Density

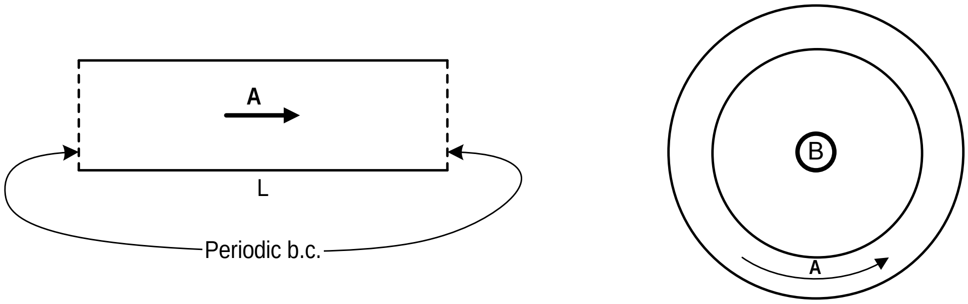

Figure 5: Periodic geometry for calculating the superfluid density.

Pollock and Ceperley and Ceperley derive a nice expression for the superfluid density in terms of the *winding number* of paths. I find their derivation hard to follow, so this is my version. You might prefer the originals! The problem can be formulated in terms of the statistical mechanics with moving walls, or in a rotating system, but I find it cleaner to imagine a vector potential **A** coupling to a fictitious charge q on each Boson, which makes the calculation analogous to the ones we did in superconductivity.

With a constant vector potential the Hamiltonian takes the form

$$H = \sum_{i=1}^{N} \frac{(\mathbf{p}_i - q\mathbf{A}/\mathbf{c})^2}{2m} + V(\mathbf{x}_i) \tag{18}$$

$$= \sum_{i=1}^{N} \left[\frac{\mathbf{p}_i^2}{2m} + V(\mathbf{x}_i) \right] - \frac{q}{mc}\mathbf{P}\cdot\mathbf{A} + \mathbf{O}(\mathbf{A}^2) \tag{19}$$

with **P** the total momentum.

Consider a periodic geometry with **A** along the periodic direction. Physically this would correspond to a torus of superfluid with a "solenoid" at the center acting as the source of **A**. Note that there is no $\mathbf{B} = \nabla\times\mathbf{A}$ at the torus, so for a normal fluid there would be no dependence of the free energy on **A**. The superfluid shows the effect of **A** in an analogy with the Aharanov-Bohm effect. The expression for the superfluid momentum density (mass times velocity) is

$$\mathbf{g}_s = n_s\hbar(\nabla\phi - \frac{q}{\hbar c}\mathbf{A}) \tag{20}$$

with n_s the superfluid (number) density. With the chosen gauge the phase gradient $\nabla\phi$ remains zero when small **A** is switched on since the circulation $\oint \nabla\phi\cdot\mathbf{dl}$ is fixed. Thus there is a superflow, and a corresponding increase in the free energy $\Delta F \propto A^2$. The total momentum can be calculated by taking derivatives with respect to **A** of $F = -k_B T \ln Tr e^{-\beta H}$ with H given by Eq. (18) in the usual way

$$\mathbf{P} = \frac{-mc}{q}\frac{\partial F}{\partial\mathbf{A}} = -Vn_s\frac{q}{c}\mathbf{A}. \tag{21}$$

Hence

$$n_s = \frac{1}{V}\frac{mc^2}{q^2}\frac{\partial F}{\partial(\frac{1}{2}A^2)}. \tag{22}$$

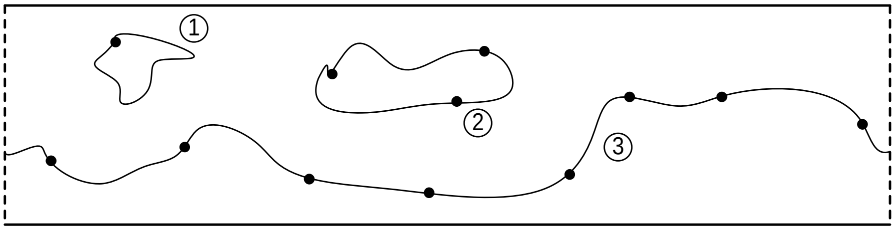

Figure 6: Path integral calculation of n_s. The dots represent the intial (and final) positions of the particles. The phase Φ(path) from the vector potential is only nonzero for paths such as (3) which wind around the torous.

Now we calculate F from the path integral expression. We know from standard quantum mechanics, or by direct calculation, that the effect of the vector potential in the Hamiltonian is to multiply each path contribution by the phase factor given by integrating **A** along all the particle paths, i.e.

$$e^{i\Phi(\text{path})} = \exp\left[\frac{iq}{\hbar c}\sum_{i=1}^{N}\int_{\mathbf{x}'(i)}^{\mathbf{x}(i)} \mathbf{A}\cdot\mathbf{dl}\right]. \tag{23}$$

In the free energy $\mathbf{x} = \mathbf{x}'$ or $\mathbf{x} = P\mathbf{x}'$, and the integral reduces to the integral of $\mathbf{A}$ along the exchange loops. For constant $\mathbf{A}$ this integral is zero unless the path winds around the torus, and then

$$\Phi(\text{path}) = \frac{q}{\hbar c} L A W, \tag{24}$$

with W the *winding number* equal to the number of times the path winds around the torus in the direction of $\mathbf{A}$.

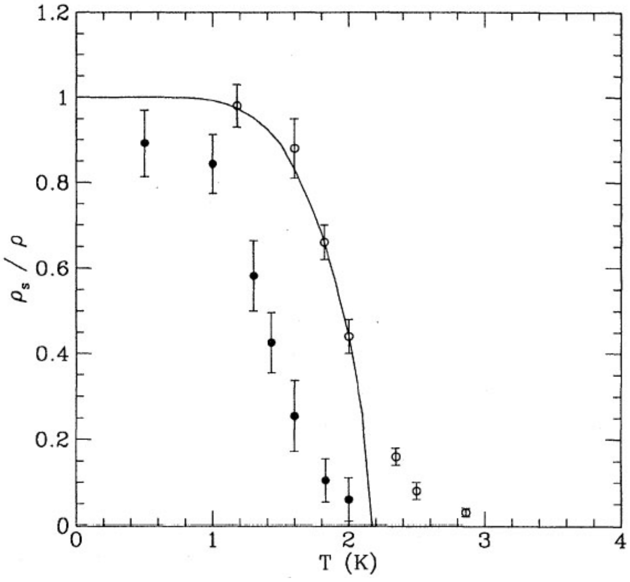

Figure 7: Calculation of n_s/n using the mean square winding number from path integral Monte Carlo calculations (open circles). The solid circles are from a different method for finite droplets of He^4. [From Ceperley (1995)]

The free energy is given by

$$F = -k_B T \ln \sum_{\text{paths}} e^{i\Phi(\text{path})} \times (\text{path integral})_{A=0}, \tag{25}$$

and the difference from the $A = 0$ free energy is

$$\Delta F = -k_B T \ln \left[\frac{\sum_{\text{paths}} e^{i\Phi(\text{path})} \times (\text{path integral})_{A=0}}{\sum_{\text{paths}} (\text{path integral})_{A=0}} \right] == -k_B T \left\langle e^{i\Phi(\text{path})} \right\rangle_0, \tag{26}$$

where the average is over the paths for $A = 0$. Expanding to second order

$$\Delta F = \frac{1}{2} k_B T \left\langle \Phi(\text{path})^2 \right\rangle_0 = \frac{m k_B T}{2\hbar^2} L^2 \left\langle W^2 \right\rangle_0 . \tag{27}$$

And so the superfluid density is given in terms of the mean square winding number of the paths

$$\frac{n_s}{n} = \frac{1}{N} \frac{m k_B T L^2}{\hbar^2} \left\langle W^2 \right\rangle_0 . \tag{28}$$

If the geometry is periodic in all three dimensions, then replace $\left\langle W^2 \right\rangle_0 \to \left\langle W^2 \right\rangle_0 /3$ with $\left\langle W^2 \right\rangle_0$ the mean square winding number summed over all directions. Results for Monte Carlo calculations of liquid He^4 are shown in Fig. 7.

References

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[2] D. M. Ceperley, Rev. Mod. Phys. **67**, 279 (1995)

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