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RESTRICTED FERMION PATH INTEGRALS

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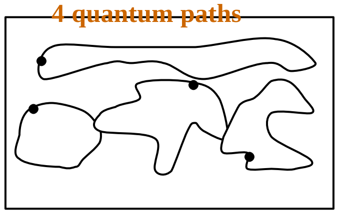
Fermion Path Integrals

1. Direct Fermion Path Integrals: *“the sign problem”*
2. Restricted Path Integrals
   - A. Restricted Path Identity
   - B. Para/ortho hydrogen example
   - C. The reference point
   - D. Free particle nodes
   - E. Nodal Action
   - F. Momentum distribution
   - G. Superfluidity

“Direct” Fermion Path Integrals

- Path integrals map quantum mechanics into a system of cross-linking closed “polymers.”



$$Z = \sum_{p=1}^{N!} \frac{(-1)^P}{N!} \int dR_1 ... dR_M \, e^{-\sum_{i=1}^{M} S(R_i, R_{i+1})}$$

$R_0 = PR_M$, P permutation,
$S(R_i, R_{i+1})$ is “boltzmannon action”

- Bosons are easy: simply sample **P**.
- Fermions: sample the “action” and carry $(-1)^P$ as a weight.
- Observable is **even P - odd P.** scales exponentially in N and T^{-1}!

$$\text{CPUtime} \propto e^{-2} e^{2N[F_F - F_B]/k_B T}$$

Importance Sampling

Given the integral $I = \int dx f(x)$

How should we sample x to maximize the efficiency?

Transform the integral to:

Estimator

$$I = \int dx p(x) \left[\frac{f(x)}{p(x)} \right] = \left\langle \left[\frac{f(x)}{p(x)} \right] \right\rangle_p$$

The variance is:

$$u = \left\langle \left[\frac{f(x)}{p(x)} - I \right]^2 \right\rangle_p = \int dx \frac{f(x)^2}{p(x)} - I^2$$

Optimal sampling: $\frac{du}{d\,p(x)} = 0$ with constraints

Parameterize as: $$p(x) = \frac{q^2(x)}{\int dx q^2(x)}$$

Solution: $$p^*(x) = \frac{|f(x)|}{\int dx |f(x)|}$$

Estimator:

$$f(x)/p^*(x) = \frac{sign(f(x))}{\int dx |f(x)|}$$

If f(x) is entirely positive or negative, estimator is constant. "zero variance principle."

We can't sample $p^*(x)$, but its form can guide us.

Importance sampling is a general technique: it works in many dimensions.

Fermion variance

- Compute a fermion observable by sampling the boson probability and taking the sign as a weight

$$\langle O \rangle_F = \frac{\langle s(P) O(R) \rangle_B}{\langle s(P) \rangle_B} \quad s(P) = (-1)^P$$

- The variance of O for this choice can be separated into a bosonic and fermionic contribution.

$$u_F(O) = u_B(O) \left[\frac{Z_B}{Z_F} \right]^2$$

- The fermion efficiency is

$$x = \left[\frac{Z_F}{Z_B} \right]^2 = \left[\frac{M_+ - M_-}{M} \right]^2 = e^{-2b N (m_F - m_B)}$$

- Big problem once N becomes large OR temperature becomes low-precisely when fermi statistics matter.

The Sign Problem

The expression for Fermi particles, such as He^3, is also easily written down. However, in the case of liquid He^3, the effect of the potential is very hard to evaluate quantitatively in an accurate manner. The reason for this is that the contribution of a cycle to the sum over permutations is either positive or negative depending on whether the cycle has an odd or even number of atoms in its length L. At very low temperature, the contributions of cycles such as L=51 and L=52 are very nearly equal but opposite in sign, and therefore they very nearly cancel. It is necessary to compute the difference between such terms, and this requires very careful calculation of each term separately. It is very difficult to sum an alternating series of large terms which are decreasing slowly in magnitude when a precise analytic formula for each term is not available. Progress could be made in this problem if it were possible to arrange the mathematics describing a Fermi system in a way that corresponds to a sum of positive terms. Some such schemes have been tried, but the resulting terms appear to be much too hard to evaluate even qualitatively.
The (explanation) of the superconducting state was first answered in a convincing way by Bardeen, Cooper, and Schrieffer. The path integral approach played no part in their analysis, and in fact has never proved useful for degenerate Fermi systems.

Feynman and Hibbs,1965.

Fixed-Node method

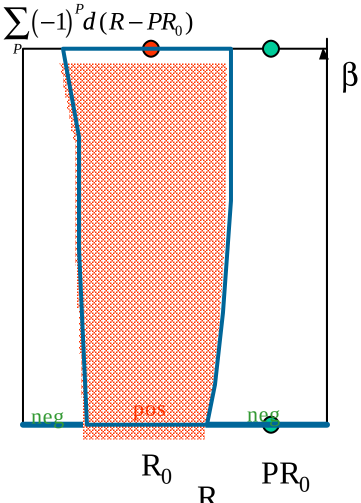
- Get rid of negative walks by canceling them with positive walks. We can do this if we know where the density matrix changes sign. Restrict walks to those that stay on the same side of the node.
- Fixed-node identity. Gives exact solution if we know the places where the density matrix changes sign: the nodes.

$$r_F(R_b, R_*; b) = \frac{1}{N!}\sum_P (-1)^P \int_{r_F(R_t, R_*; t)>0} dR_t e^{-S(R(t))} \text{ with } R_0 = \mathrm{P}R_*$$

- Classical correspondence exists!!
- Problem: fermion density matrix appears on both sides of the equation. We need nodes to find the density matrix.
- But still useful approach. (In classical world we don't know V(R).)

Proof of the fixed node method

1. The density matrix satisfies the Bloch equation with initial conditions.
$$\frac{\partial r(R,t)}{\partial t} = l\nabla^2 r(R,t) - V(R)\, r(R,t) \qquad r(R,0) = \frac{1}{N!}\sum_P (-1)^P d(R - PR_0)$$
2. One can use more general boundary conditions, not only initial conditions, because solution at the interior is uniquely determined by the exterior-just like the equivalent electrostatic problem.
3. Suppose someone told us the surfaces where the density matrix vanishes (the nodes). Use them as boundary conditions.
4. Putting an infinite repulsive potential at the barrier will enforce the boundary condition.
5. Returning to PI's, any walk trying to cross the nodes will be killed.
6. This means that we just restrict path integrals to stay in one region.



Ortho-para H_2 example

In many-body systems it is hard to visualize statistics.

- The simplest example of the effect of statistics is the H_2 molecule in electronic ground state.
- Protons are fermions- must be antisymmetric.

1. Spins symmetric (↑↑). spatial wf antisymmetric (ortho) "fermions"
2. Spins antisymmetric (↓↑- ↑↓). spatial wf symmetic (para) "bosons"
3. Non symmetrical case (HD) "boltzmannons"

All 3 cases appear in nature!

- Go to relative coordinates: $r = r_1 - r_2$
- Assume the bond length is fixed $|r|=a$. Paths are on surface of sphere of radius a.

PIMC task is to integrate over such paths with given symmetries.

For a single molecule there is no potential term, a "ring polymer" trapped on the surface of a sphere.

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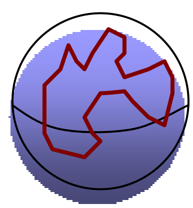
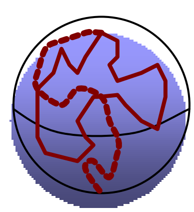
Paths on a sphere

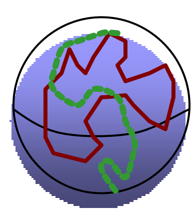
1. "boltzmannons" Ring polymers on sphere
   $O(r \rightarrow r)$



2. "bosons" 2 types of paths allowed.
   $O(r \rightarrow r) + O(r \rightarrow -r)$



3. "fermions" 2 types of paths allowed
   $O(r \rightarrow r) - O(r \rightarrow -r)$
   Low efficiency as $\beta \rightarrow \infty$



$$z = e^{-b(E_1 - E_0)}$$

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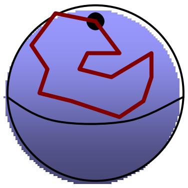
Restricted paths for ortho H_2

- Fix origin of path: the reference point.
- Only allow points on path with a positive density matrix. paths staying in the northern hemisphere: $r(t) \cdot r(0) > 0$
- Clearly negative paths are thrown out.
- They have cancelled against positive paths which went south and then came back north to close.
- The symmetrical rule in "t": $r(t) \cdot r(t') > 0$ is incorrect.
- Spherical symmetry is restored by averaging over the reference point: the north pole can be anywhere.
- Can do many H_2 the same way.
- Ortho H_2 is much more orientable than either HD or para H_2.



Reference Point

- New feature compared with boson path integrals.
- Scalar averages can only be taken at the reference point.
- However partition function and all derivatives (energy) use information from the whole path.
- We lose time slice symmetry if nodes are time dependent. But this is probably necessary to fix phase of density matrix.
- Reference point moves are expensive and ultimately cause RPIMC to get "stuck" for $T < E_F/10$.
- One can use a 2 reference points. This restores time-reversal symmetry and means we only need nodes for $t < \beta/2$.
- Unfortunately, more than 2 reference points brings back the "sign" problem.

RPIMC with approximate nodes

- In almost all cases, we do not know the “nodal” surfaces.
- We must make an an ansatz.
- This means we get a fermion density matrix (function with the right symmetry) which satisfies the Bloch equation at all points except at the node.
- That is: it has all the exact “bosonic” correlation
- However, there can be a derivative mismatch across the nodal surface.
- We expect that there is a free energy bound. (proved at high temperature and at zero temperature)
- Maybe one can find the best nodes using the variational principle. (variational density matrix approach)

Free particle nodes

- For non-interacting (NI) particles the nodes are the finite temperature version of a Slater determinant:

$$\rho_F^{NI}(R', R; \tau) = \frac{1}{N!}\det\left[g\left(r'_i, r_j; \tau\right)\right]$$

where $g\left(r'_i, r_j; \tau\right)$ is the single particle density matrix.

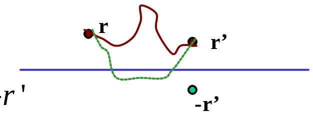
$$g(r', r; \tau) = (4\pi\lambda\tau)^{-3/2} e^{-\frac{(r-r')^2}{4\lambda\tau}} + \text{periodic images}$$

- At high T, nodes are hyperplanes.
- At low T they try to minimize kinetic energy.
- There is “time dependence”.
- Problem: no spin-coupling in nodes
- Militzer-Pollock chose g(r,r’;t) with Hartree eqs.
- Can also add backflow to nodes.

Nodal action

- "Primitive Rule:" simply reject paths if they cross a node.
- Will lead to an error proportional to $\sqrt{l t} / r_{nn}$
- Improved nodal action:solve for a particle next to a planar node. Use method familiar from electrostatics, the method of images:

$$r(r',r;t) = e^{-\frac{(r-r')^2}{4lt}} - e^{-\frac{(r-r^*)^2}{4lt}} \qquad r^* = -r'$$



$$dS(r',r;t) = -\ln\left(1 - \mathrm{e}^{-\frac{dd'}{lt}}\right) \quad \text{d=distance to node} \approx \left|\nabla \ln\left(r\left(R,R';t\right)\right)\right|^{-1}$$

- Determine nodal distance using "Newton estimate."
- As paths approach within a thermal wavelength of the node, we get a repulsion, to account for the probability that a path could have crossed and recrossed within τ.

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Practical fermion issues

- Bosonic methods are applicable! Fermion code is built on top of bosonic code.
- Add a "gate" in multilevel Metropolis where:
  - Sign of density matrix is checked
  - Nodal action is computed and used
- Reference point moves are expensive: all slices must be checked for nodal violations.
- Permutations are still needed! However, 2 particle exchanges will always be rejected. Only odd particle cyclic exchanges (3,5,...) allowed as updates.
- Determinantal updates
  - Full determinant evaluation takes N^3 operations
  - However row/column updates take only N^2.
- Use inverse of Slater matrix to compute derivative needed for the gradient in the nodal action.

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Momentum distribution

- For bosons the momentum distribution shows evidence of BEC.
  - Long exchange cycles⇒n(r) long range ⇒ n_0 >0
- What is effect for fermions? Run logic in reverse.
  - For NI fermions, n(k) has discontinuity at k_F.
  - Hence $n(r) \propto \cos(k_F r)/(k_F r)^2$
  - We must have cancellation of long-range positive and negative exchanges!
  - Negative permutations allowed/required off-diagonal.
- Algorithm recently tested by Militzer: *cond-mat/0310401*
- Exchanges are needed to get a Fermi-liquid.
- Long exchanges do not lead to a phase transition or superfluidity.

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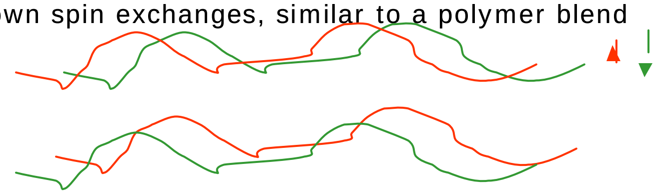
Fermion superfluidity

- Liquid ^{3}He becomes superfluid at very low temperatures (T_c ~ 1mK).
- With the exact nodal restriction this must also happen within RPIMC, because we can calculate the free energy.
- What happens to the paths at this phase transition?
- SPECULATION: there is a "Cooper" pairing of up and down spin exchanges, similar to a polymer blend



- Not tried in ^{3}He because of formidable practical difficulties (length, temperature scale) and lack of knowledge of nodal topology required.

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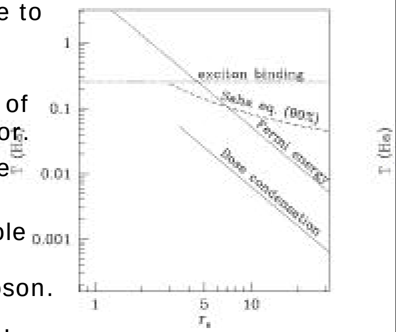
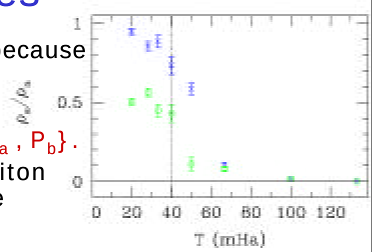
Exciton superfluidity

- What system is the most appropriate to observe superfluidity of fermions? (strongest pairing)
- Consider the simplest 1-band model of particles and holes in a semiconductor.
- Assume masses are isotropic and the same; only the charge is different.
- At low temperature a particle and hole can bind together to form an *exciton* (like a hydrogen atom) which is a boson.
- If the exciton density is high enough, they can bose condense.: $T\rho^{3/2} < 2.7$
- Shumway-Ceperley (1999) observed this transition for excitons.
- What do the paths look like?

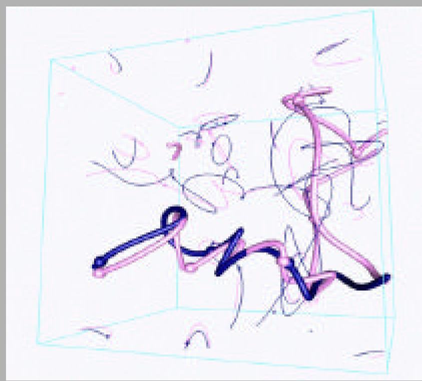


Pairing Nodes

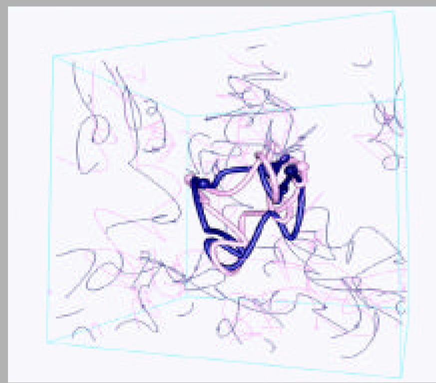
- Free fermion nodes does not allow pairing because nodes of two species are independent.
  - Consider two pairs of fermions.
  - Possible exchanges are $\{I, P_aP_b\}$ and $\{P_a, P_b\}$.
  - The permutation P_aP_b represents an exciton exchange but it is forbidden if nodes are independent since the path will cross "a" nodes or "b" nodes first.
- Instead we used paired nodes: ***A{*** $g(a_1-b_1)g(a_2-b_2)$…..***}*** where g(r) is a pairing function (we used a Gaussian).
- Nodes are time-independent ⇒ winding number formula for superfluid response.
- We can define 2 different responses. Let W_x be winding number of species x.
  - movement of walls: $<(W_a+W_b)^2>$
  - magnetic field: $<(W_a-W_b)^2>$



Excitonic Paths $[r_s=6 \quad T<T_c]$



Winding exchange (3,6)



Pair exchange (2,2)

Blue=electron lavendar=hole

Path Integral Applications

Bosons

- Superfluid ^4He
- Solid ^4He
- BEC in traps
- Superfluidity on surfaces (H_2 on silver)
- Helium droplets
- …….

Fermions

- Homogenous electrons/plasma
- High Temperature hydrogen/helium (interior of planets)
- Liquid/solid ^3He
- Electron-hole liquid
- BEC of fermions
- …….

Summary

- Restricted paths allow realistic calculations of many fermion systems
- Makes a nodal assumption which is only controlled for $T>T_F$.
- Paths get stuck at low temperature $T<10T_F$ unless you make other assumptions (e.g. ground state nodes.)
- Generalization of method for bosonic PI
- Unifies theory of bose and fermi systems
- Proof that stable fermion methods can exist.

DANGER: you can find in the literature solutions to the "fermion sign problem" several times a year.

In all known cases these either:

–have a serious error

–are known not to work

–work only in special cases (1D, HO, lattice models,..)

–cannot scale at large N or low temperature.

–Have uncontrolled approximations.

–……

(these are the opinions of DMC)