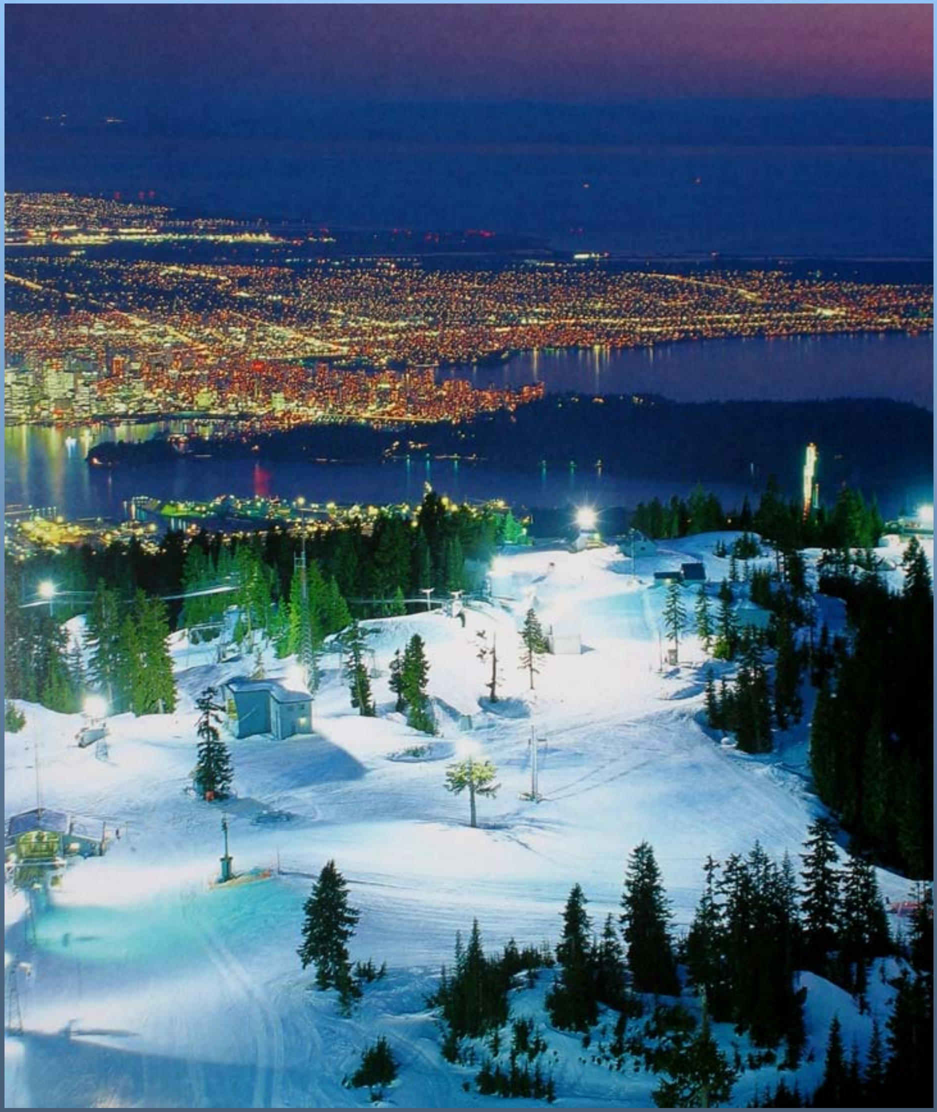
PCE STAMP

DECOHERENCE AROUND LOOPS: Polarons with a twist

(Vancouver, Dec 04, 2009)

Physics & Astronomy
UBC
Vancouver



Pacific Institute for Theoretical Physics

DECOHERENCE AROUND LOOPS: Polarons with a twist

Work done with: Zhen Zhu, Eric Mills (UBC); Andrew Hines (formerly UBC)
Amnon Aharony, Ora Entin-Wohlman (Beersheva)

I WILL TALK ABOUT: A problem in which a particle moves around a closed loop, which has a flux through it. This particle is coupled to a bath , which may be either a bosonic bath (the traditional polaron problem) or a spin bath. We will study a spin bath in this talk.

FOR FURTHER INFORMATION:

Email: stamp@physics.ubc.ca
Web: http://www.physics.ubc.ca/~berciu/PHILIP/index.html

SUPPORT FROM:

UBC

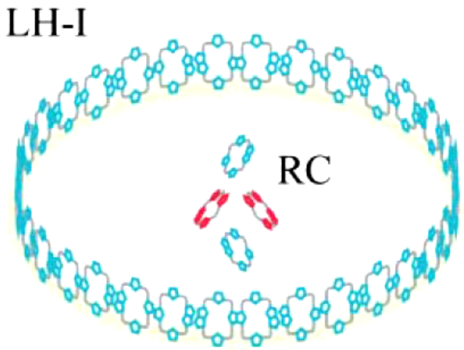
PiTP

25 years cifar
Canadian Institute for Advanced Research

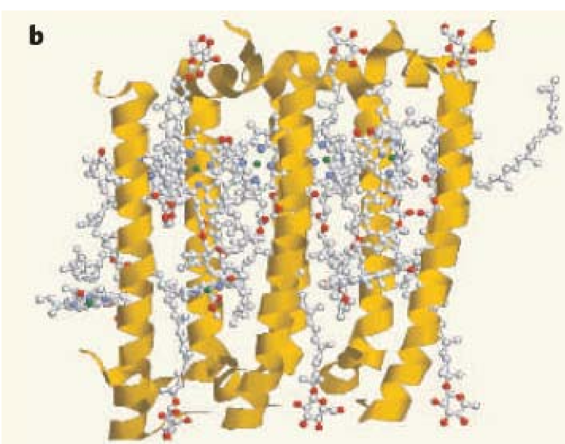
MOLECULAR LOOPS

1) LIGHT-HARVESTING PROTEINS

These have a ring structure:



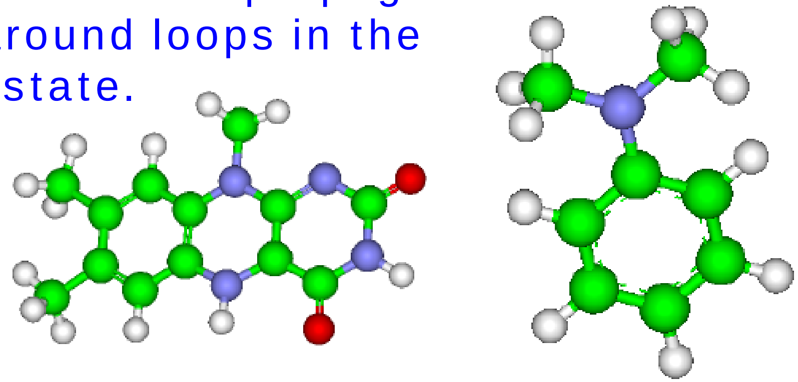
They also show coherent exciton dynamics at 77K. Dephasing by local & extended phonons, & defects.



Engels et al., Nature 446, 782 (2007)

2) CHEMICAL COMPASSES

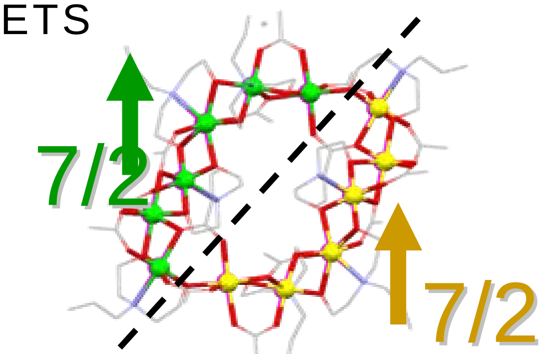
Increasing evidence for role of nuclear spin bath in avian guidance systems. These switch on propagation of radical pairs around loops in the triplet state.



Rodgers & Hore, PNAS 106, 353 (2009)

3) MOLECULAR MAGNETS

Wherein one has the propagation of information around EXCHANGE loops.



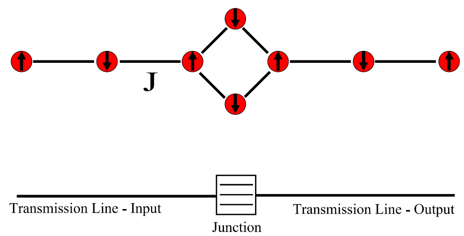
A key role is played by Dzyaloshinski-Moriya interactions in these systems (phase rotation along links). Decoherence is caused by nuclear spins and phonons.

CM Ramsey et al., Nat. Phys 4, 277 (2008)

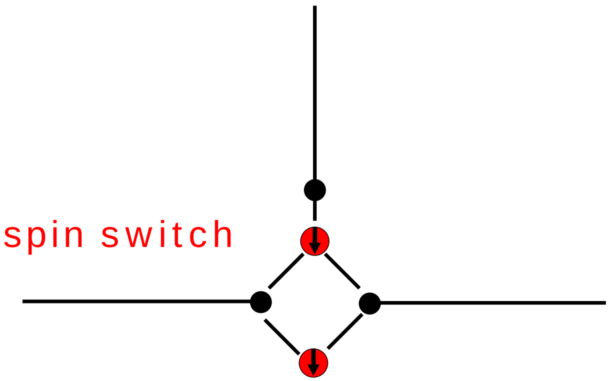
"TOP-DOWN" LOOPS

1) SPIN LOOPS: This is an advertisement for work by myself & Eric Mills, inspired by experiments of the Eigler group

A spin junction



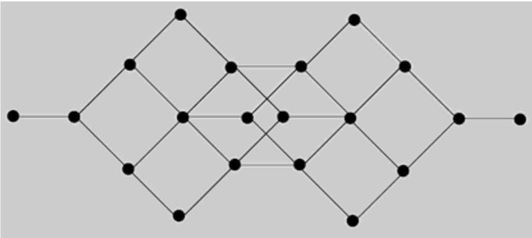
A spin switch



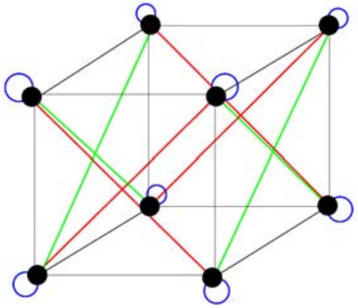
Hirjibehedin et al., Science **312**, 1021 (2006)

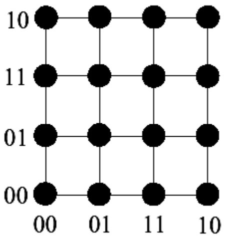
2) ELECTRONIC LOOPS: These are of course very familiar; eg., quantum dot loops, normal and superconducting rings, etc., etc.

QUANTUM INFORMATION LOOPS



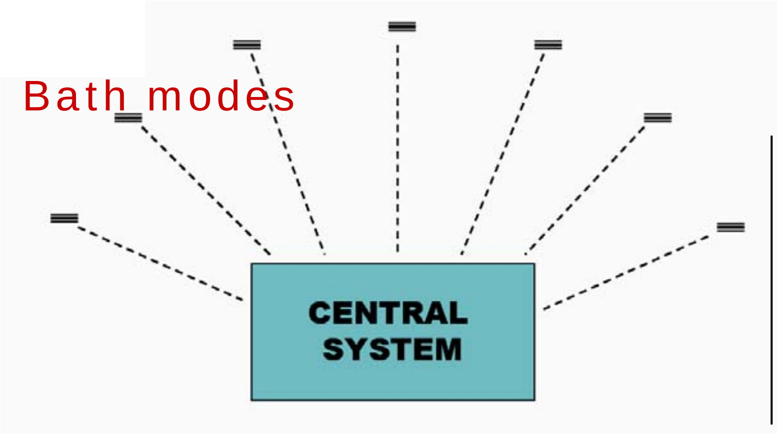
Underlying all of these specific applications is the role of loops in general QM systems, & which is crucial in Q Info processing. This is most easily seen in the Quantum Walk formulation of Quantum info processing. A set of N interacting qubits is then an N-dimensional hypercube. One can study many other topologies, but in all of them, loops play the central role.





A: DECOHERENCE at NANOSCALE in SOLID STATE

Decoherence in subtle because it has many sources; eg.,



(1) OSCILLATOR BATHS

Environment: $$H_{env} = \frac{1}{2}\sum_{q=1}^{N}\left(\frac{p_q^2}{m_q} + m_q\omega_q^2 x_q^2\right)$$

Coupling to environment:

$$H_{int} = \sum_{q=1}^{N}[F_q(P,Q)x_q$$

Feynman & Vernon, Ann. Phys. 24, 118 (1963)

Caldeira & Leggett, Ann. Phys. 149, 374 (1983)
AJ Leggett et al, Rev Mod Phys 59, 1 (1987

(2) SPIN BATHS

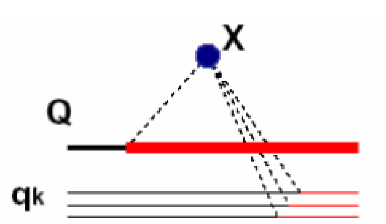
Environment: $$H_{env}^{sp} = \sum_{k}^{N_s}\mathbf{h}_k\cdot\boldsymbol{\sigma}_k + \sum_{k,k'}^{N_s}V_{kk'}^{\alpha\beta}\sigma_k^{\alpha}\sigma_{k'}^{\beta}$$

P.C.E. Stamp, PRL 61, 2905 (1988)
NV Prokof'ev, PCE Stamp, J Phys CM5, L663 (1993)
NV Prokof'ev, PCE Stamp, Rep Prog Phys 63, 669 (2000)

Coupling to environment:

$$H_{int}^{sp} = \sum_{k}^{N_s}\boldsymbol{F}_k(P,Q)\cdot\boldsymbol{\sigma}_k$$

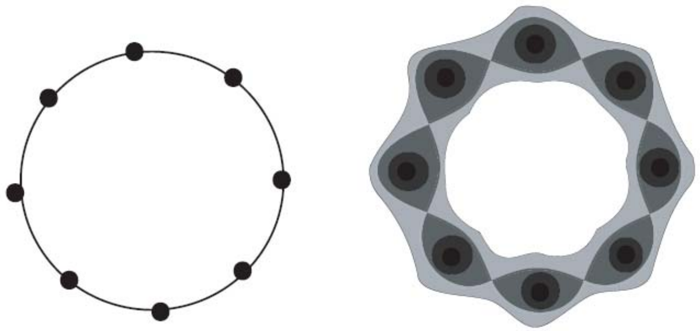
(3) 3RD PARTY DECOHERENCE



However, one can have decoherence even without direct coupling to an environment, via a "3rd party"

PCE Stamp, Stud. Hist Phil Mod Phys **37**, 467 (2006)

The “BARE LOOP”



We consider the ring geometry shown at right. The bare Hamiltonian is

$$H_V \;=\; \frac{1}{2M}(\mathbf{P} - \mathbf{A}(\mathbf{R}))^2 + U(\boldsymbol{R})$$

Let’s truncate this to a site basis, with N sites:

$$H_o \;=\; \sum_{ij}\left[t_{ij}c_i^\dagger c_j\, e^{iA^o_{ij}} + H.c.\right] + \sum_j \varepsilon_j c_j^\dagger c_j$$

where for a constant uniform field we have: $A^o_{ij} = \frac{e}{2}\mathbf{H}\cdot\mathbf{R}_i \times \mathbf{R}_j \;=\; \Phi/N$

All we have done here is truncate to the lowest band; if we define the operators: $c_j^\dagger = \sqrt{\frac{1}{N}}\sum_{k_n} e^{ik_n j} c_{k_n}^\dagger$

Then we have:

$$\begin{aligned} H_o \;&=\; \sum_n \epsilon^o_{k_n} c_{k_n}^\dagger c_{k_n} \\ &=\; 2\Delta_o \sum_n \cos(k_n - \Phi/N) c_{k_n}^\dagger c_{k_n} \end{aligned}$$

COUPLING to a SPIN BATH

Without specifying which of the many applications we are working on, we can give a general form for the coupling of the ring particle to a spin bath:

Position coupling: $$H_{int}(\mathbf{R}) = \sum_k \boldsymbol{F}(\boldsymbol{R} - \boldsymbol{r}_k) \cdot \boldsymbol{\sigma}_k$$

Momentum coupling: $$H_{int}(\mathbf{P}) = \sum_k \boldsymbol{G}(\boldsymbol{P}, \boldsymbol{\sigma}_k)$$

If we now truncate to the lowest band, we get: $$H = H_{band} + H_{SB}$$

where $$H_{band} = \sum_{ij} [t_{ij} c_i^\dagger c_j e^{iA^o_{ij} + i\sum_k (\boldsymbol{\phi}_k^{ij} + \boldsymbol{\alpha}_k^{ij} \cdot \boldsymbol{\sigma}_k)} + H.c.] + \sum_j (\varepsilon_j + \sum_k \boldsymbol{\gamma}_k^j \cdot \boldsymbol{\sigma}_k) c_j^\dagger c_j$$

Most of these terms are fairly obvious, except for one. Consider what happens when the particle hops between 2 sites; a spin bath wave-function will also change: $$|\boldsymbol{\sigma}_k^f\rangle = \hat{T}_{ij}^k \, |\boldsymbol{\sigma}_k^{in}\rangle = e^{i(\phi_k^{ij} + \boldsymbol{\alpha}_k^{ij} \cdot \boldsymbol{\sigma}_k)} |\boldsymbol{\sigma}_k^{in}\rangle$$

where: $$\hat{T}_{ij}^k = \exp\left[-i/\hbar \int_{\tau_{in}(\mathbf{R}_i)}^{\tau_f(\mathbf{R}_j)} d\tau \; H_{int}^k(\mathbf{R}, \sigma_k)\right]$$

Typically $|\boldsymbol{\alpha}_k^{ij}| \sim \pi |\boldsymbol{\omega}_k^{ij}| / 2\Omega_o$ where $\boldsymbol{\omega}_k^{ij} = \boldsymbol{\gamma}_k^j - \boldsymbol{\gamma}_k^i$

The MODEL WE WANT TO SOLVE: POLARON in a SPIN BATH

So, we now have the Hamiltonian $H \;=\; H_{band} + H_{SB}$

where:
$$H_{band} = \sum_{ij} [t_{ij} c_i^\dagger c_j e^{iA^o_{ij} + i\sum_k (\boldsymbol{\phi}_k^{ij} + \boldsymbol{\alpha}_k^{ij} \cdot \boldsymbol{\sigma}_k)} + H.c.]$$
$$+ \sum_j (\varepsilon_j + \sum_k \boldsymbol{\gamma}_k^j \cdot \boldsymbol{\sigma}_k) c_j^\dagger c_j$$

$$H_{SB} \;=\; \sum_k \mathbf{h}_k \cdot \boldsymbol{\sigma}_k \;+\; \sum_{k,k'} V_{kk'}^{\alpha\beta} \sigma_k^\alpha \sigma_{k'}^\beta$$

This is actually just a new kind of polaron problem – we will be looking at it on a ring

Now actually the general solution of this problem is exceedingly complicated. So in this talk I will focus on a special case, in which we look at pure phase decoherence. The model is

$$H_\phi \;=\; \sum_{<ij>} [\Delta_o c_i^\dagger c_j e^{i(A^o_{ij} + \sum_k \boldsymbol{\alpha}_k^{ij} \cdot \boldsymbol{\sigma}_k)} + H.c.]$$

METHODS

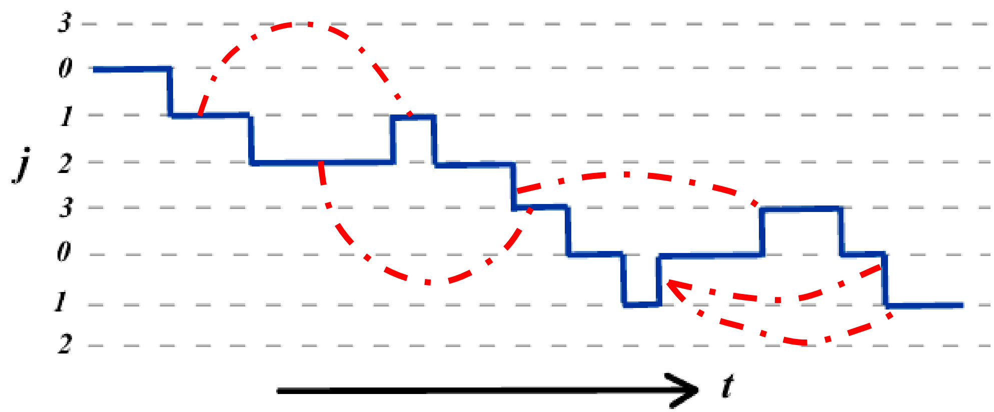
The propagator of the reduced density matrix for the particle:

$$\mathcal{K}(1,2) = \int_{\Theta_1}^{\Theta_2} d\Theta \int_{\Theta_1'}^{\Theta_2'} d\Theta' \; e^{-\frac{i}{\hbar}(S_o[\Theta]-S_o[\Theta'])} \mathcal{F}[\Theta,\Theta']$$

$$\mathcal{F}[\Theta,\Theta'] = \prod_k \langle \hat{U}_k(\Theta,t)\hat{U}_k^\dagger(\Theta',t)\rangle$$

For our model, the effect of transitions in the spin bath can be entirely summarized in phase factors associated with each hop:

$$\exp\{-ip\sum_k \left(\sum_{\langle mn\rangle=\langle 01\rangle}^{\langle N0\rangle} - \sum_{\langle mn\rangle=\langle l,l+1\rangle}^{\langle j-1,j\rangle} \right) (\boldsymbol{\alpha}_k^{mn}\cdot\boldsymbol{\sigma}_k)\}$$



The reduced density matrix is then give by a sum over winding number:

$$\rho_{jj'}(t) = \sum_{l,l'} \mathcal{K}_{jj',ll'}(t)\rho_{l,l'}^{(in)} \qquad \mathcal{K}_{jj',ll'}(t) = \sum_{pp'} K^o_{jj',ll'}(p,p';t)F_{jj'}^{ll'}(p,p')$$

Where we are simply weighting over the free particle propagator:

$$K^o_{jj',ll'}(t) = G^o_{jl}(t)G^o_{j'l'}(t)^\dagger \qquad K^o_{jj',ll'}(t) = \sum_{pp'} K^o_{jj',ll'}(p,p';t)$$

With: $$G^o_{jj'}(t) = \sum_{p=-\infty}^{+\infty} J_{Np+j'-j}(2\Delta_o t)e^{-i(Np+j'-j)(\Phi/N+\pi/2)}$$

AVERAGING OVER THE BATH

We will actually perform two kinds of average over the environment. One is an average over the states of the individual bath states (this becomes a thermal average if the bat is in equilibrium). The second is an "ensemble average", where we average over a large number of baths. This is done when for example, we have an ensemble of different couplings to the bath (appropriate, eg., for a large biomolecule).

1) AVERAGE OVER BATH STATES

One has:
$$F_{jj'}^{ll'}(p,p') = \langle e^{i(\mu+N\bar{p})\sum_k \boldsymbol{\alpha}_k \cdot \boldsymbol{\sigma}_k} \rangle$$
$$\rightarrow \prod_k \cos((N\bar{p}+\mu)|\boldsymbol{\alpha}|) \quad \text{(symmetric ring)}$$

where: $\mu = j' - j + l' - l$, $\bar{p} = p' - p$

2) ENSEMBLE AVERAGE

One has:
$$\bar{F}_{jj'}^{ll'}(p,p') \equiv \langle\langle e^{i(\mu+N\bar{p})\boldsymbol{\alpha}\cdot\boldsymbol{\sigma}} \rangle\rangle = \int d\boldsymbol{\alpha} P(\boldsymbol{\alpha}) \langle e^{i(\mu+N\bar{p})\boldsymbol{\alpha}\cdot\boldsymbol{\sigma}} \rangle$$

where we also average over a distribution of couplings with a weighting function. An example – a Gaussian average:

$$P(|\boldsymbol{\alpha}|) = e^{-|\boldsymbol{\alpha}|^2/2\lambda_o} / \sqrt{2\pi\lambda_o}$$

Then one finds:
$$\langle\langle e^{i(\mu+N\bar{p})\boldsymbol{\alpha}\cdot\boldsymbol{\sigma}} \rangle\rangle \rightarrow \exp[-\lambda(\bar{p}+\mu)^2/2]$$

RESULTS for the FREE PARTICLE

To give you some idea of the results, we plot all the analytic results for a simple 3-site ring.

At right, the probability to go from site *0* to site *j* in time *t*.

$$P^o_{j0}(t) = \frac{1}{3}\Big(1 + (3\delta_{j,0} - 1)\Big[J_0(2\Delta_o\sqrt{3}t) + 2\sum_{p=1}^{\infty} J_{6p}(2\Delta_o\sqrt{3}t)\cos(2p\Phi)\Big] + (\delta_{j,1} - \delta_{j,2})2\sqrt{3}\sum_{p=1}^{\infty} J_{6p-3}(2\Delta_o\sqrt{3}t)\sin((2p-1)\Phi)\Big)$$

We can also look at the current around the ring:

$$I^o_{0,1} = \frac{2}{3}\Delta_o \sum_{p=-\infty}^{\infty} J_{3p+1}(2\Delta_o\sqrt{3}t)K(p,\Phi) \ ,$$

$$K(p,\Phi) = \sin(p\Phi) \quad \text{if} \quad p = \text{odd} \ ,$$

$$K(p,\Phi) = \sqrt{3}\cos(p\Phi) \quad \text{if} \quad p = \text{even}$$

The key thing for you to take from these figures is that the flux threading the ring controls the current (a consequence of quantum non-locality)

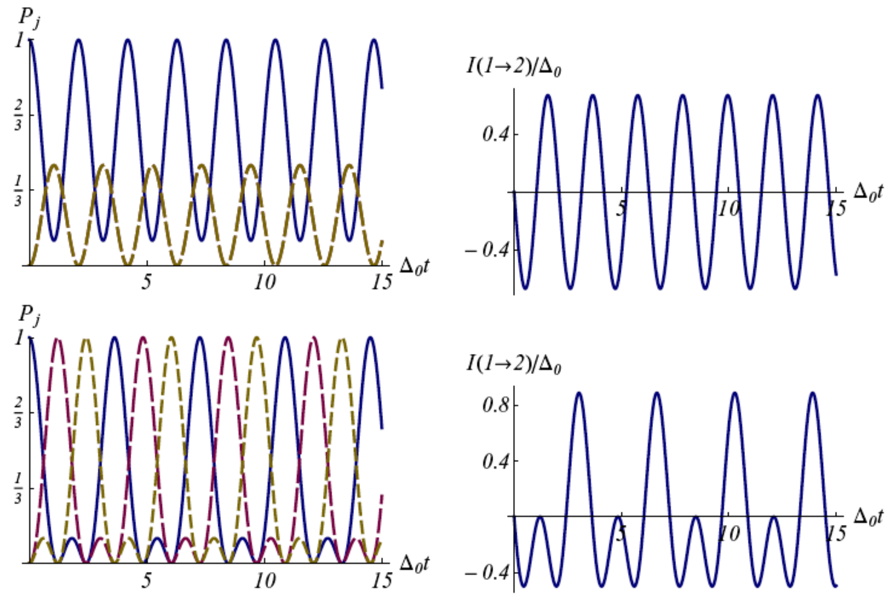


FIG. 3: Results for the free particle for $N = 3$ and for a particle initially on site 1. Left: The probabilities to occupy site 1 (full line), 2 (large dashes), and 3 (small dashes). Right: the current from site 1 to site 2. Top: $\Phi = 0$. Bottom: $\Phi = \pi/2$.

ROLE of DECOHERENCE

We can also get analytic results for the case where the bath is coupled in (which I don't show here).

The results for strong decoherence (below) simply show that all influence of the external flux has disappeared. One gets a power law decay of all correlations.

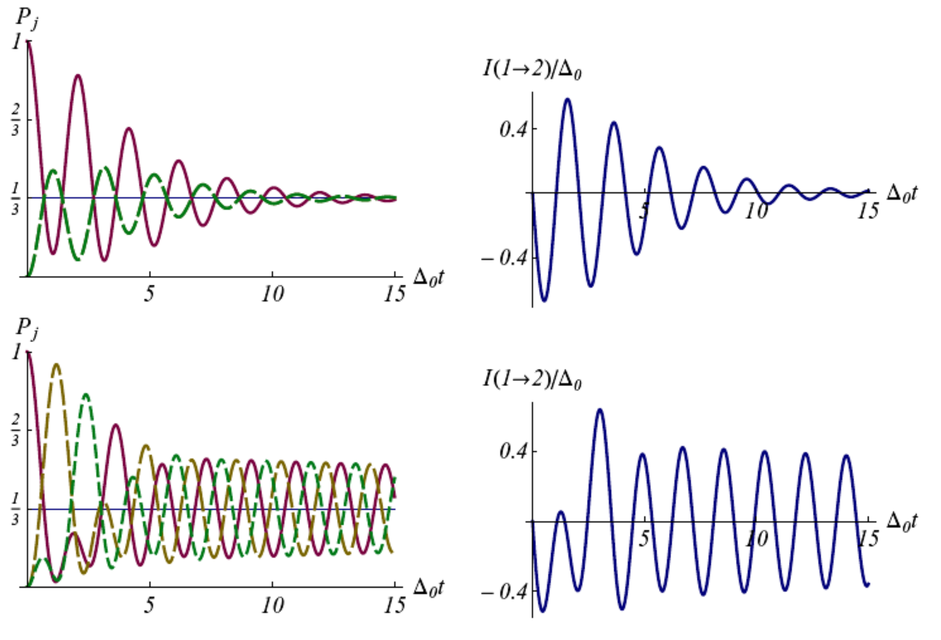


FIG. 4: Plot of $P_{j0}(t)$ for a 3-site ring, for a particle initially on site 1, in the intermediate decoherence limit, with $\lambda = .02$. Left: The probability to occupy site 0 (full line), 1 (large dashes), and 2 (small dashes). Right: the current from site 0 to site 1. Top: $\Phi = 0$. Bottom: $\Phi = \pi/2$.

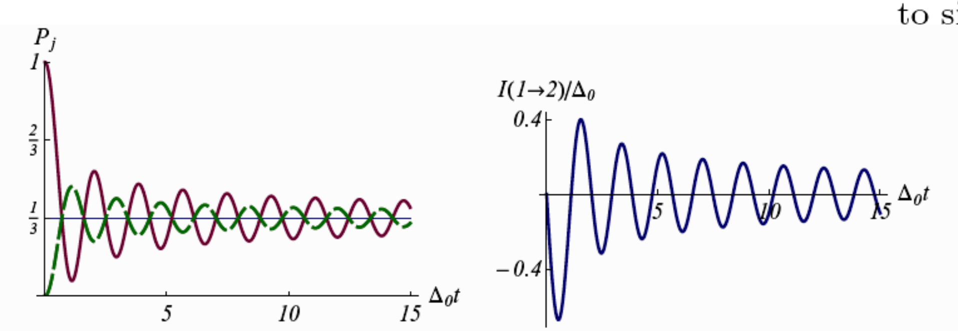


FIG. 5: Plot of $P_{j0}(t)$ for a 3-site ring, for a particle initially on site 1, in the strong decoherence limit. Left: The probability to occupy site 0 (full line), 1 (large dashes), and 2 (small dashes). Right: the current from site 0 to site 1 (compare Fig. 3). The results do not depend on Φ.

Things get very interesting in the intermediate decoherence regime (above). The decay becomes extremely unconventional, and moreover one gets 'Hofstadter' like patterns in the results as a function of the flux.

INTERFERENCE AROUND the RING

Suppose we have an initial state with 2 wave-packets: $\Psi(t) = \frac{1}{\sqrt{2}}(\psi_1(t) + \psi_2(t))$

We pick 2 Gaussian packets:

$$|\psi_1(t)\rangle = \frac{1}{Z} \sum_{n=0}^{N-1} e^{-(k_n - \pi/2)^2 D/2} \times e^{-ij_0 k_n - i2\Delta_0 t \cos(k_n - \Phi/N)} |k_n\rangle$$

$$|\psi_2(t)\rangle = \frac{1}{Z} \sum_{n=0}^{N-1} e^{-(k_n - \pi/2)^2 D/2} \times e^{-i2\Delta_0 t \cos(k_n - \Phi/N)} |2\pi - k_n\rangle$$

So, now let's see how these evolve in the presence of a bath. We give the wave-packets a relative velocity v, and watch how the OFF-DIAGONAL matrix elements of the density matrix evolve.

The results are fascinating (no time to show them here). One sees Hofstadter interference, and long time tails, and recurrence phenomena.

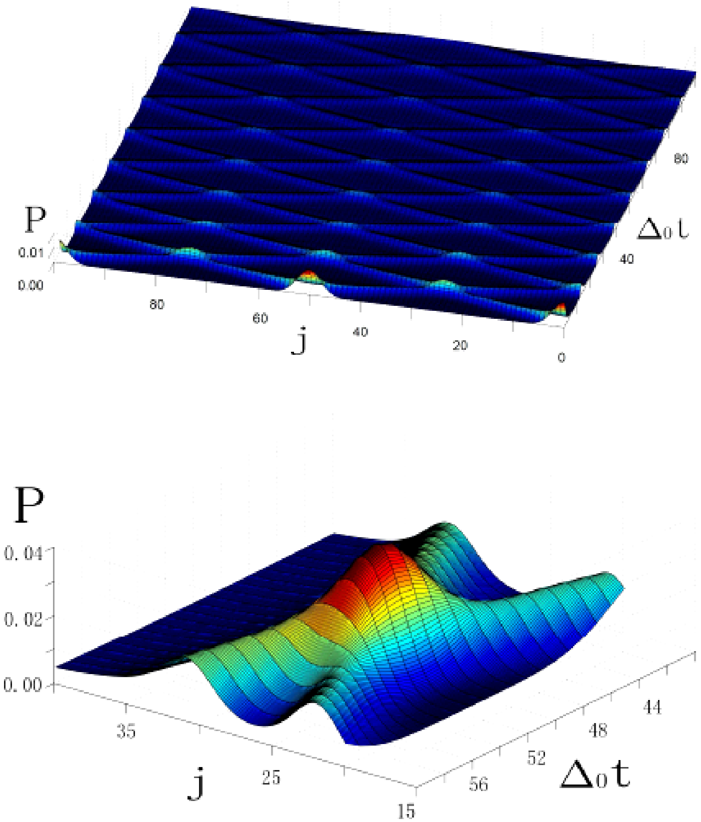
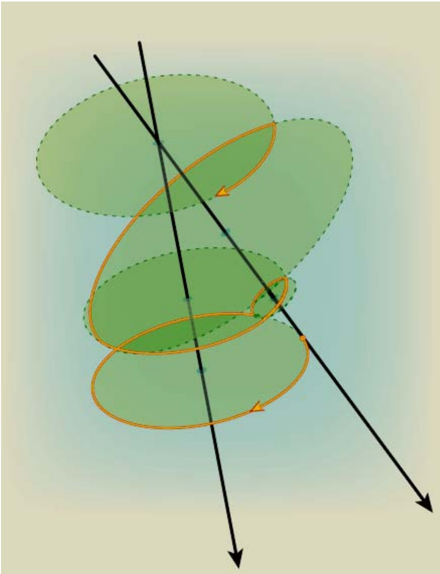


FIG. 6: Plot for $P_j(t)$ as a function of both j and $\Delta_o t$ in the strong decoherence limit. $j_o = 50$ and $N = 100$. The relative velocity is $\frac{\pi}{2}$, in phase units. Top: global view. Bottom: a particular peak

SUMMARY of the PHYSICS



Path followed by a bath spin as the particle hops

An important remark – the dynamics of the particle in this problem is entirely non-dissipative. The main effect of the bath is to cause polaronic band-narrowing, and to cause decoherence.

The decoherence operates as shown at left; each time the particle moves, the axis about which each bath spin precesses will change. The accumulated phase of each bath spin is then conditional on the path followed by the particle – this is a path integral way of saying that the spin bath is entangling with the particle. Hence we get decoherence, but with no energy relaxation.

It turns out that there quite a few applications of these results, simply because physicists are trying very hard these days to make systems where the dissipative coupling to bosonic modes is very small.

What is much more surprising is that biological systems should be able to take advantage of this. How and why this happens is still somewhat mysterious. Most of the decoherence is probably cuased in these systems by coupling to either localised defects or to real spins (paramagnetic, or nuclear), ie., to a spin bath.

THANKS FOR YOUR TIME!

Z Zhu, A Aharony, O Entin-Wohlman, PCE Stamp, /condmat 0909.4098