A Local Approach for Interacting Electrons

Roger Haydock

3 July 2013

Electronic Structure Discussion Group

(Analytic and computational linear and moment methods, electronic structure, colloidal forces)

Plan

- Black Body Theorem and Projected Density of States
- The Problem with Interactions
- Excitations and the Projected Density of Transitions
- Computational Issues
- Binding in the Heisenberg Spin Chain
- What's Next

Max von Laue
1879 - 1960

X-Ray Diffraction

Black-body theorem, 1914

The effect of the boundary on the intensity of modes inside a cavity decreases exponentially with its distance in wavelengths

The Local Density of Modes or States, PDoS

The PDoS converges in the Mean

Jacques Friedel
1921 -

Friedel Oscillations …

von Laue's theorem applies to the electronic Schrödinger equation

Moments of the PDoS are expectation values of powers of the electronic Hamiltonian

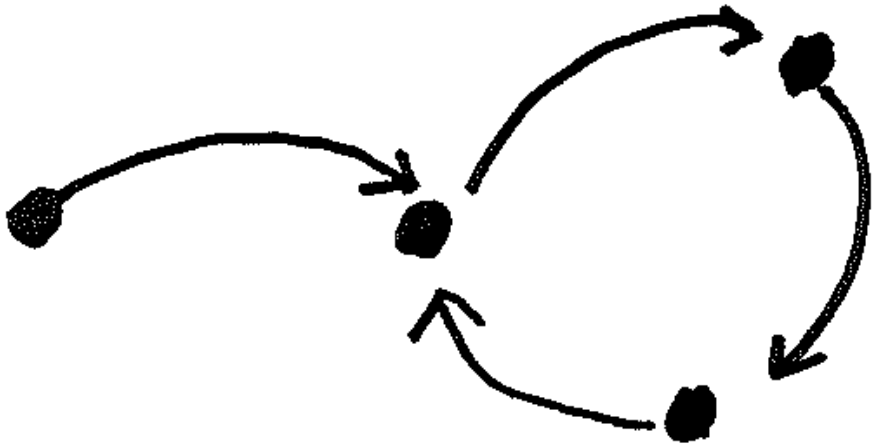
Liquid Transition Metals with Françoise Cyrot-Lackmann

The Problem with Interactions

- States are not local, the PDoS only exists for special states - infinities
- Need something local, an excitation
- Describe excitations by adding and multiplying operators (creation, annihilation, …)
- Excitations propagate by super-operators $\boldsymbol{\Lambda}$ – left and right multiplication like commutators (Heisenberg's equation)

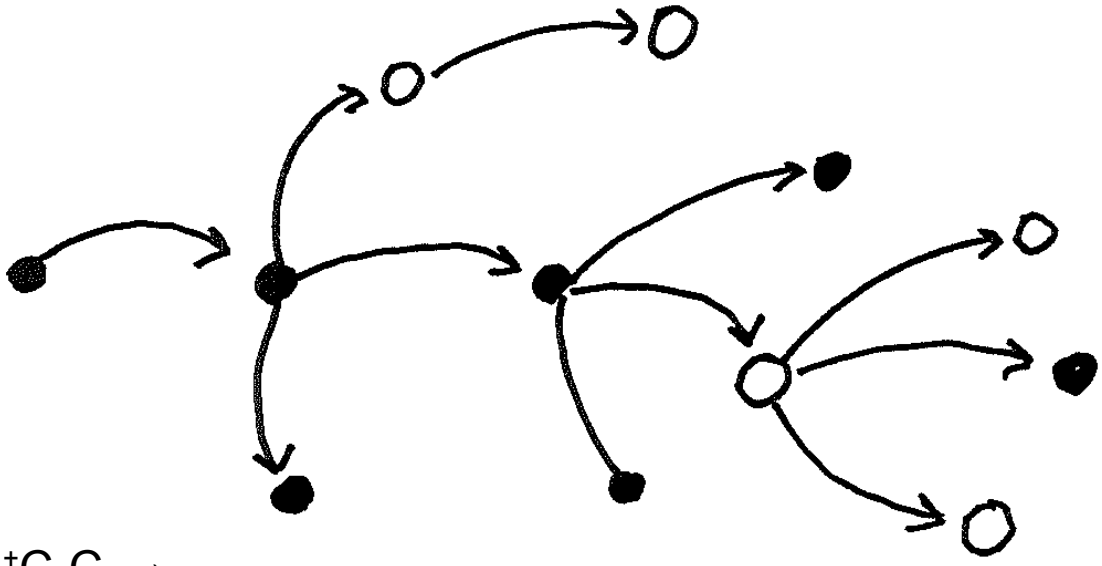
Evolution of Excitations

- Independent



$C_0^\dagger \rightarrow C_1^\dagger \rightarrow C_2^\dagger \rightarrow C_3^\dagger \rightarrow \ldots$

- Interacting



$C_0^\dagger \rightarrow C_1^\dagger\, C_2^\dagger\, C_3 \rightarrow C_4^\dagger\, C_5^\dagger\, C_6^\dagger C_7 C_8 \rightarrow \ldots$

The Local Expansion

- The initial excitation $c^\dagger$ is the most local operator
- Then $\Lambda c^\dagger$ is the next most local, and so on
- $\Lambda^m c^\dagger$ is the m-th most local
- It is convenient to orthogonalize each new operator to previous ones
- Produces a structure of 'shells' around $c^\dagger$
- Moments are the local expansion

Projected Density of Transitions PDoT

The PDoT is the probability density that an excitation ($c^\dagger$) will induce a transition (Ψ) with energy E

$$n(E) = \sum_\alpha |tr\{c,\Psi_\alpha\}|^2 \, \delta(E-E_\alpha)$$

$$n(E) = (1/\pi) \, Im[tr\{c(E-\boldsymbol{\Lambda})^{-1}c\dagger\}]$$

This has a local expansion – a continued fraction

Physical Meaning of the PDoT

- Energy distribution of stationary transitions (stationary states) induced by a disturbance
- Stationary states are equilibrium states with definite temperatures if interacting
- Excitation added at equilibrium so the energy is the chemical potential
- The most localized transitions dominate the PdoT at each energy

Moment Relations for the PDoT

- $\int E^m\, n(E)\, dE = tr\{c\Lambda^m c\dagger\}$ power moments
- $U_m = P_m(\Lambda)c\dagger$ Polynomial operator
- Orthonormal U_m tridiagonalize Λ

  b_m if k=m-1, or b_k if m=k-1
- $Tr\{U_k\dagger \Lambda U_m\} =$ a_m if k=m

  0, otherwise
- $Tr\{c(E-\Lambda)^{-1}c\dagger\} = 1/\ E-a_0-b_1^2/\ E-a_1-b_2^2/\ E-\ \ldots$

Degeneracy of Transitions

- If different transitions have the same energy, the most localized is in the PDoT
- The logarithm of the normalization of a transition is entropy of the transition
- Adding an electron with minimal entropy induces a transition from the N-electron ground state to the N+1 electron ground state

Computing the Local Expansion

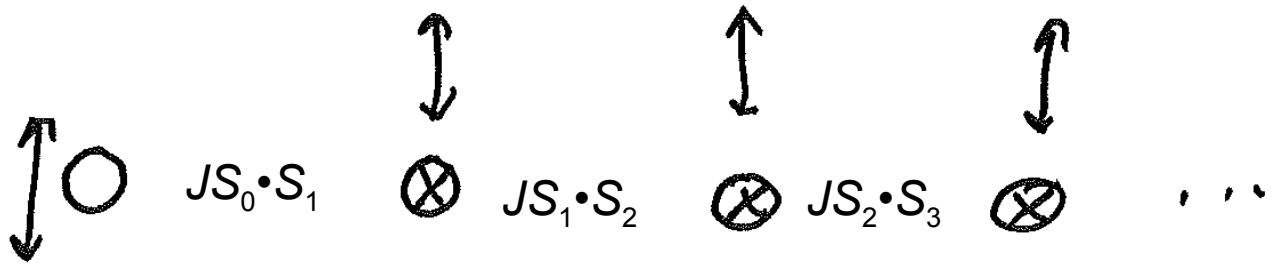
- Construct a tridiagonal matrix for $\boldsymbol{\Lambda}$
- First basis element is $c^\dagger$, which determines the rest
- Super-operating with $\boldsymbol{\Lambda}$ generates sums of products of operators ($c_\alpha^\dagger$, $c_\beta^\dagger c_\gamma^\dagger c_\delta$, …)
- The number of products in the basis grows as the exponential/factorial of the power of $\boldsymbol{\Lambda}$

Sparse Vectors

- If the interactions are local Λ is very sparse in space of operator products
- Store only non-zero coefficients of operator products – sparse vector representation
- Array structure – index for operators in a product followed by the coefficient

- An index of 64 bits spans 2^{64} products or vectors of dimension about 10^{19}
- Still limited to order 10^{9} non-zero components
- Can calculate tridiagonal matrices of dimension 20-30 (40 to 60 moments of the PdoT)
- Time and Memory scale with resolution of the PDoT not size of the System

The Semi-Infinite Spin ½ Heisenberg Chain



- Good for development because well studied
- Initial excitation is to add spin-0 to the chain
- The Hamiltonian is $\boldsymbol{H} = JS_0 \cdot S_1 + JS_1 \cdot S_2 + JS_2 \cdot S_3 + \ldots$
- $\boldsymbol{\Lambda}$ is left multiplication by $\boldsymbol{H}$ minus right multiplication by $\boldsymbol{H}$ - $JS_0 \cdot S_1$
- Excitations generated by $\boldsymbol{\Lambda}$ take the form $S_a \cdot S_b x(S_c x \ldots (S_y x S_z) \ldots)$
- This choice of $\boldsymbol{\Lambda}$ makes the transition energies the binding energies of the chain

The Sparse Basis

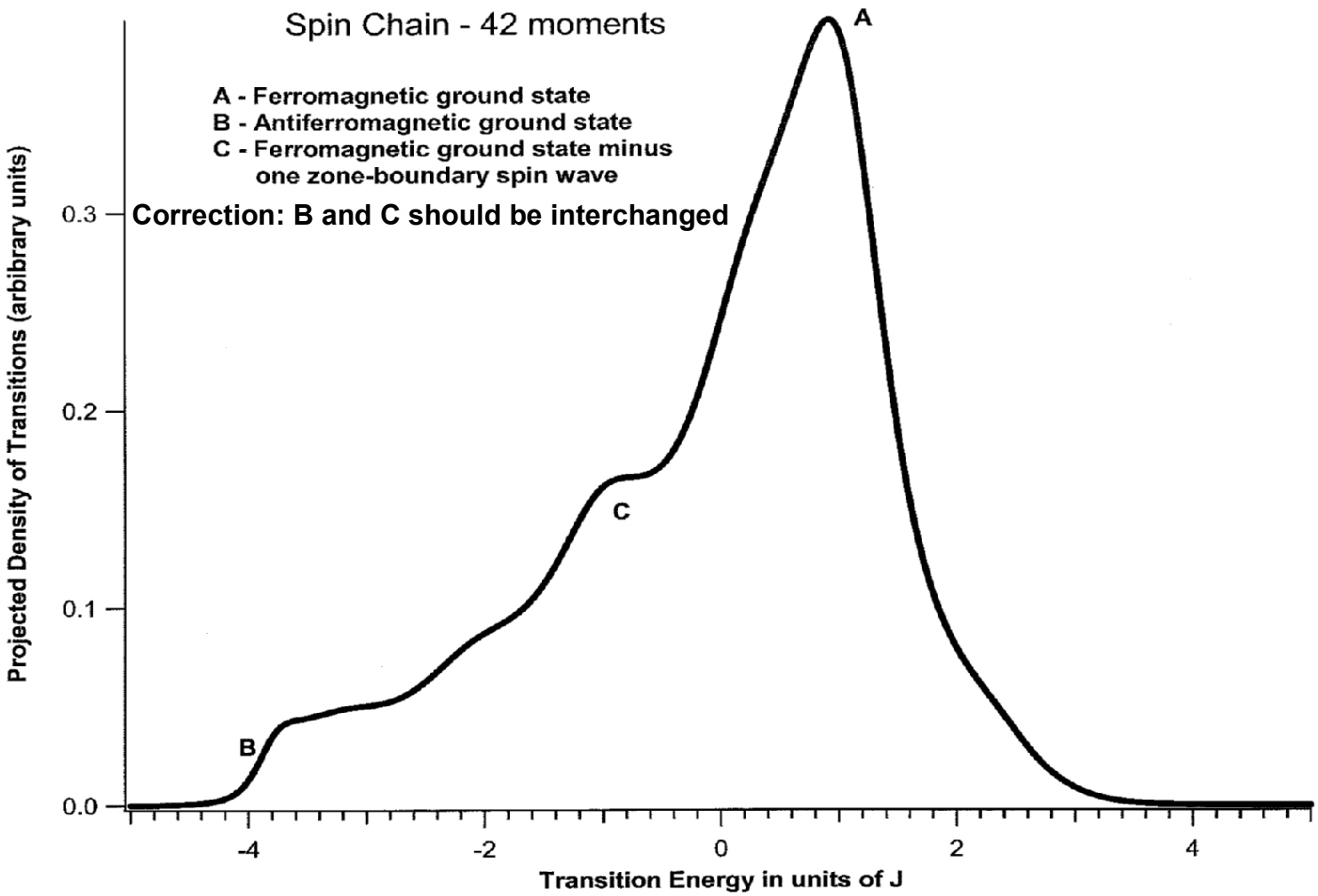
- Each multiplication by $\boldsymbol{\Lambda}$ only creates excitations on neighbors of existing excitations – Locality of $\boldsymbol{\Lambda}$

- For N ions, there are in principle 4^N operators I, S_x, S_y, S_z on each ion

- Only include in the index the non-identity operators

- Because $\boldsymbol{\Lambda}$ is local, it only triples the number of excitations with each application

PDoT for the Spin Chain



Basis 'Degeneracy'

- Tridiagonal basis has exponentially growing degeneracy – many operator products with the same coefficient
- Why?
- Can we reduce basis set growth with a symmetrized basis?
- Have found products of spin operators which reduces 3^N to 2^{N-3} (beats states)

Adding an Electron to an Orbital

- For independent electrons this is the density of states
- Changes smoothly as interactions turned on; acquires a tail
- Interpret as including interaction energies when electron added
- Can get total binding energies by adding electrons in order of increasing energy

Band-Structures for Interacting Electrons

- Add an electron with wave-number **k**
- PDoT has singularity at the Fermi energy $\varepsilon(\mathbf{k})$ for **k** on the Fermi surface

Conclusions

- Generalize independent electronic structure to interacting electronic excitations and transitions
- Projected Density of Transitions gives thermodynamic quantities due to interactions
- Sparse Vector computational methods and other tricks are required