Some Ideas for Calculating Phase Diagrams for Interacting Electrons

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- Local, Variational Approach
- Heisenberg's Equation
- Densities of transitions
- Bands of excitations

Heisenberg instead of Schrödinger

$$i \hbar \, \partial/\partial t \, \vartheta = \mathscr{L} \, \vartheta$$

- Evolve operator 'waves' ϑ rather than states
- For operators use disturbances – spin flip or electron creation
- Such operators are local
- Microscopic instead of macroscopic energies

Projected Density of Transitions

$$n(E) = \Sigma_\alpha \, |tr\{\vartheta_0^\dagger \vartheta_\alpha|^2 \, \delta(E-E_\alpha)$$

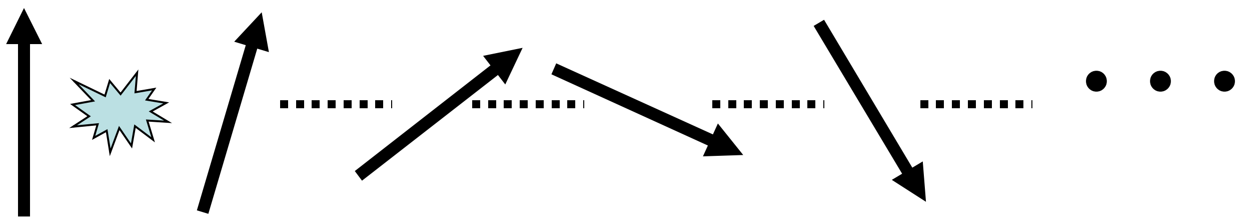
- Probability density that ϑ_0 induces the transition ϑ_α which has energy E_α
- Smooth bands with singularities at edges – qualitative or discontinuous changes
- Examples: s to p symmetry, surface or bulk normalization

Interpretation of Singularities in the Density of Transitions

- Operators for microscopic, local disturbances are non-singular
- The singularities arise from projection of operators on states – structure of Liouvillian
- Singularities are phase boundaries – where phase is taken to mean qualitative or discontinuous change in the states

Example – Heisenberg Chain

$$H = J\,(S_0 \bullet S_1 + S_1 \bullet S_2 + S_2 \bullet S_3 + \ldots)$$

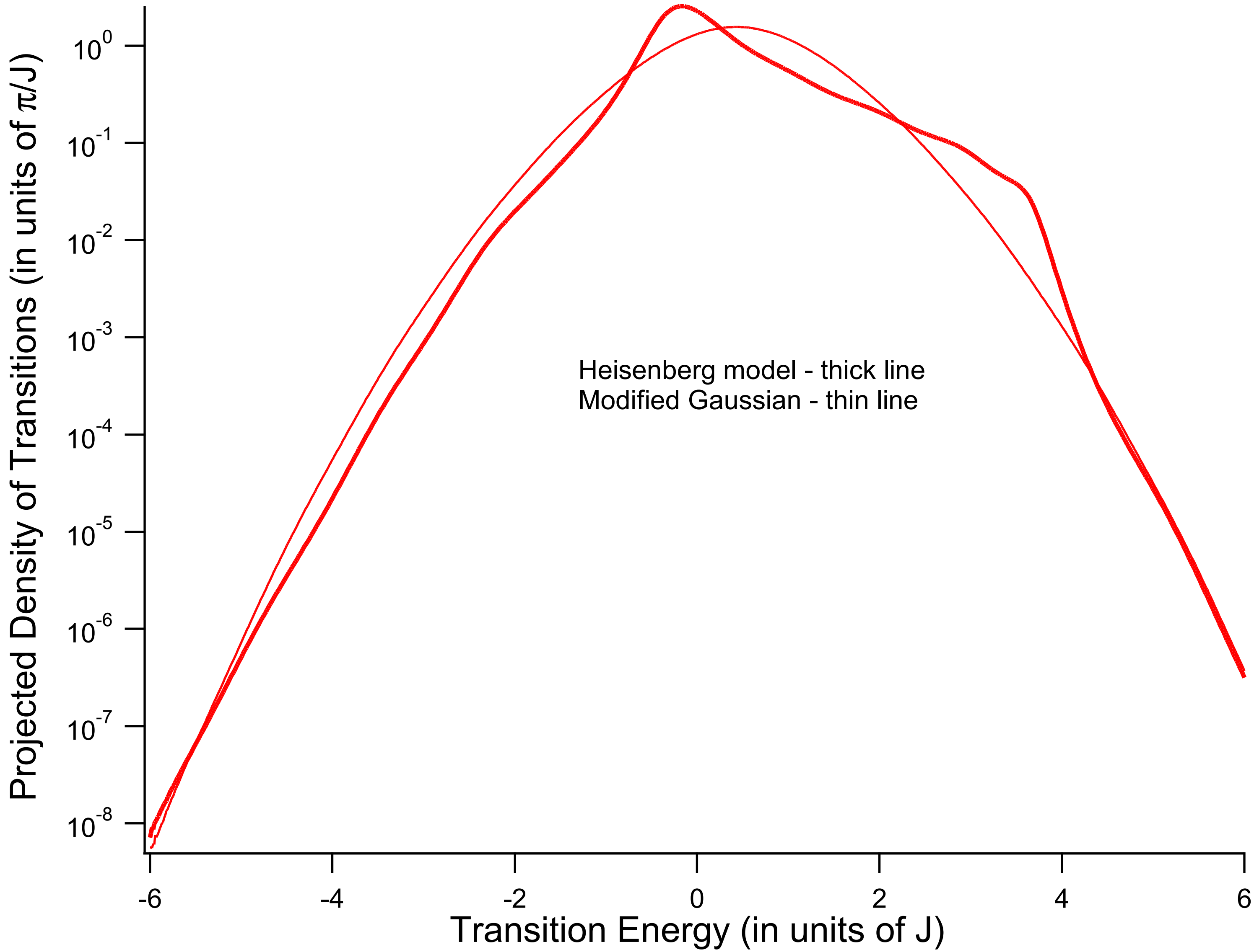


The bond break couples to other transitions represented as linear combinations of products of Pauli spin matrices

Local calculation of binding energy

Tridiagonalize the equations of motion for the bond break

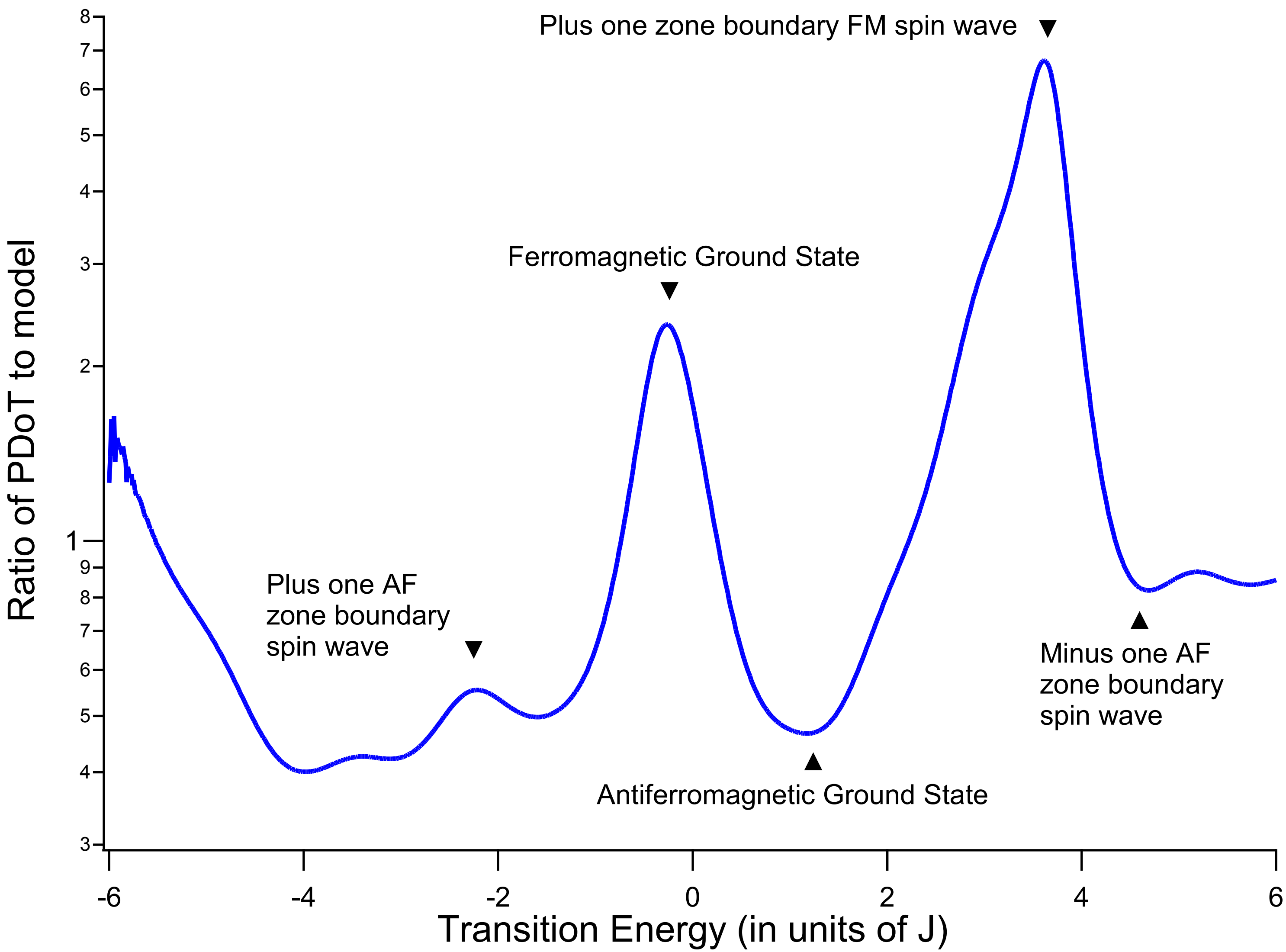
10^{10} by 10^{10} sparse matrix goes to 17 by 17 tridiagonal matrix



Projected Density of Transitions (in units of π/J)
10^0
10^-1
10^-2
10^-3
10^-4
10^-5
10^-6
10^-7
10^-8
Heisenberg model - thick line
Modified Gaussian - thin line
-6
-4
-2
0
2
4
6
Transition Energy (in units of J)

Mössbauer-type Effect

- Singularities on a Gaussian background
- Transitions with few degrees of freedom in foreground
- Infinite temperature background
- Why Gaussian not hyperbolic secant
- Take ratio of spectrum to background to make singularities clearer – like differentiating data



Plus one zone boundary FM spin wave
Ferromagnetic Ground State
Plus one AF
zone boundary
spin wave
Antiferromagnetic Ground State
Minus one AF
zone boundary
spin wave
Ratio of PDoT to model
Transition Energy (in units of J)
-6
-4
-2
0
2
4
6

Summary

- Heisenberg rather than Schrödinger for interacting electrons
- Find bands and 'van Hove' singularities but in many dimensions
- Get accurate phase boundaries at least in a simple test system