

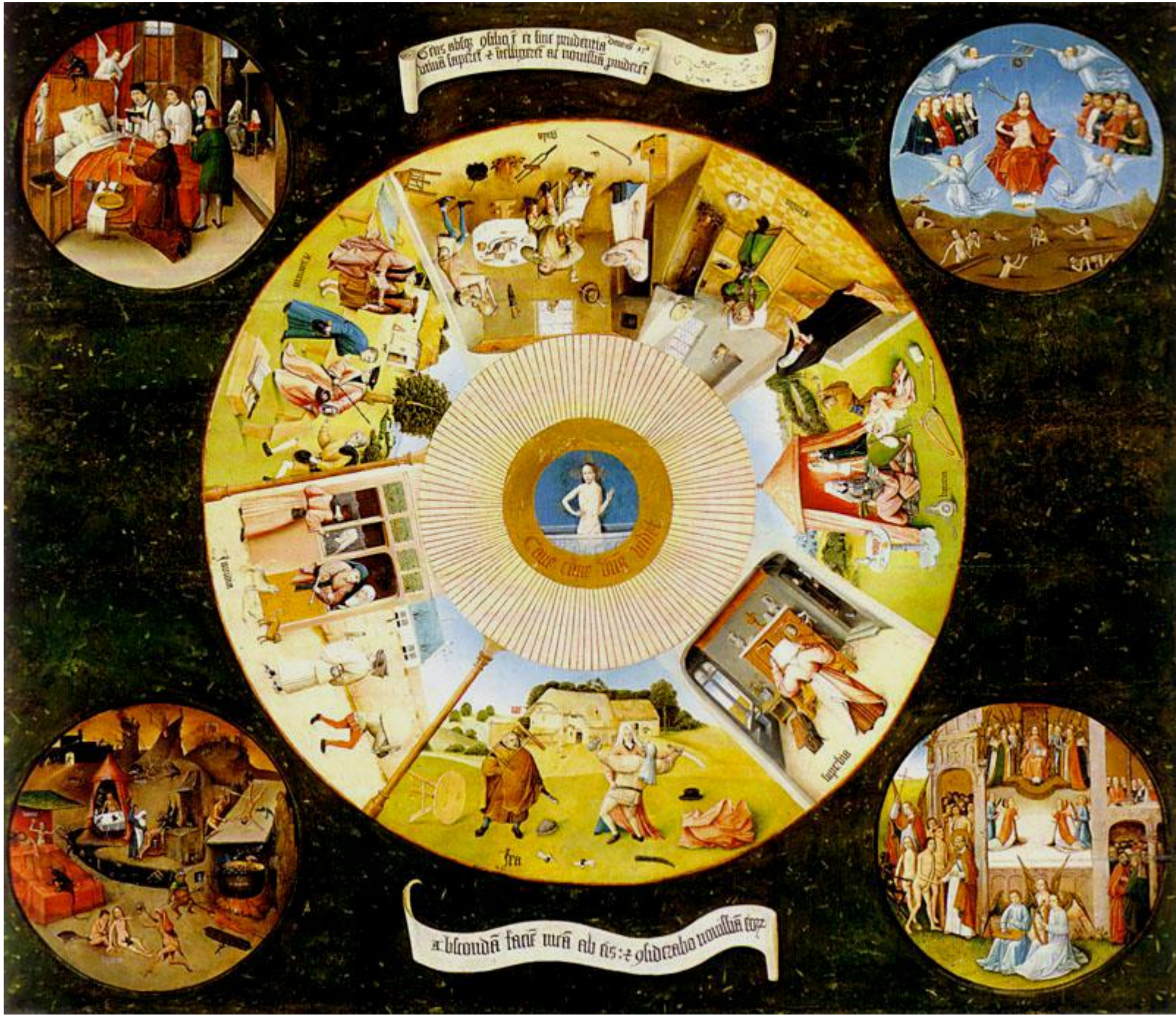
Summary of EXCITM09

With slides borrowed from Adam
Wasserman

Kieron Burke, UC Irvine

KITP Dec 18, 2009

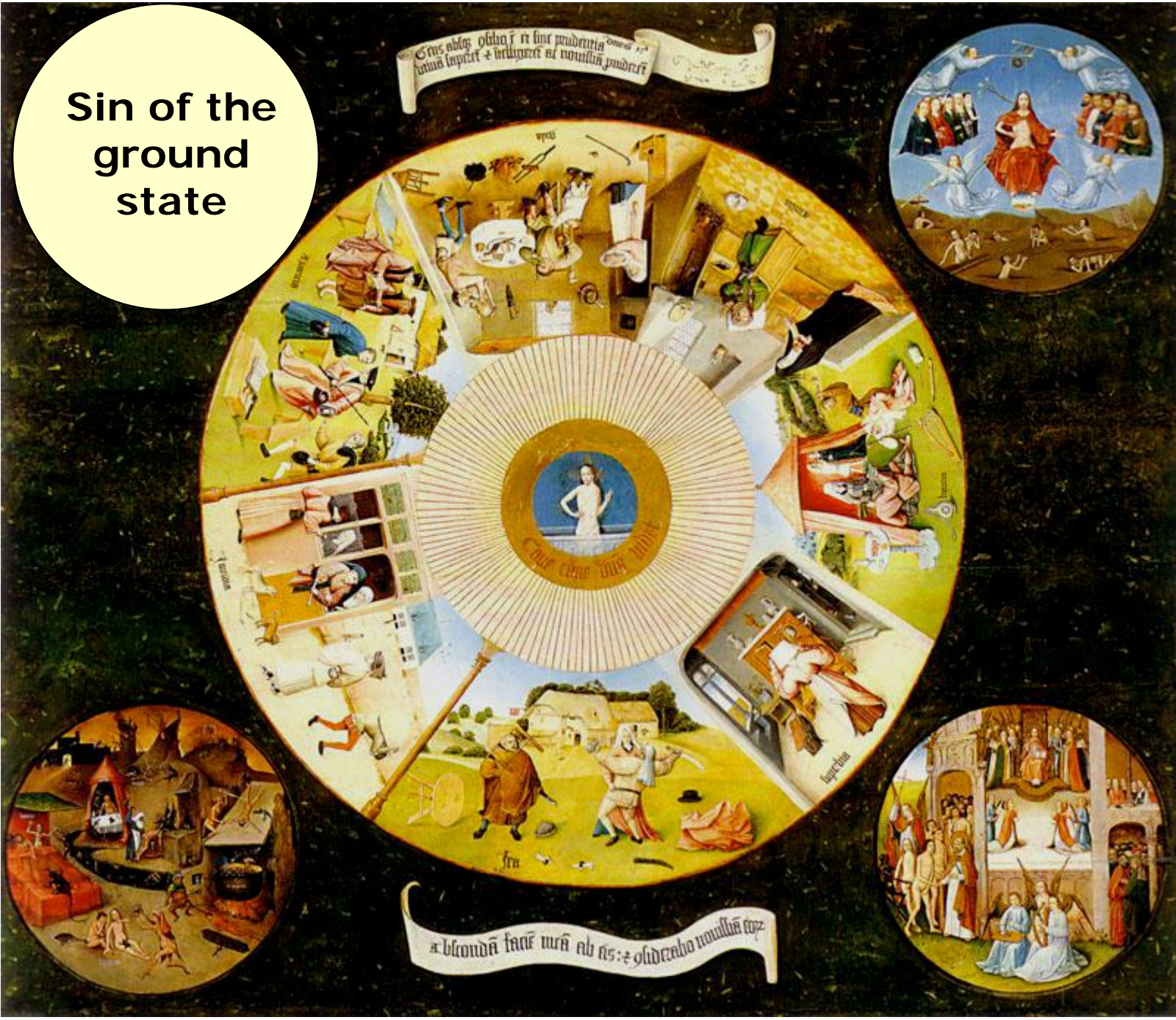
Hieronymus Bosch: The Seven Deadly Sins and the Four Last Things (1485, oil on panel)



K. Burke, J. Werschlik, and E.K.U.Gross, J.Chem.Phys.
123, 062206 (2005).

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Sin of the ground state

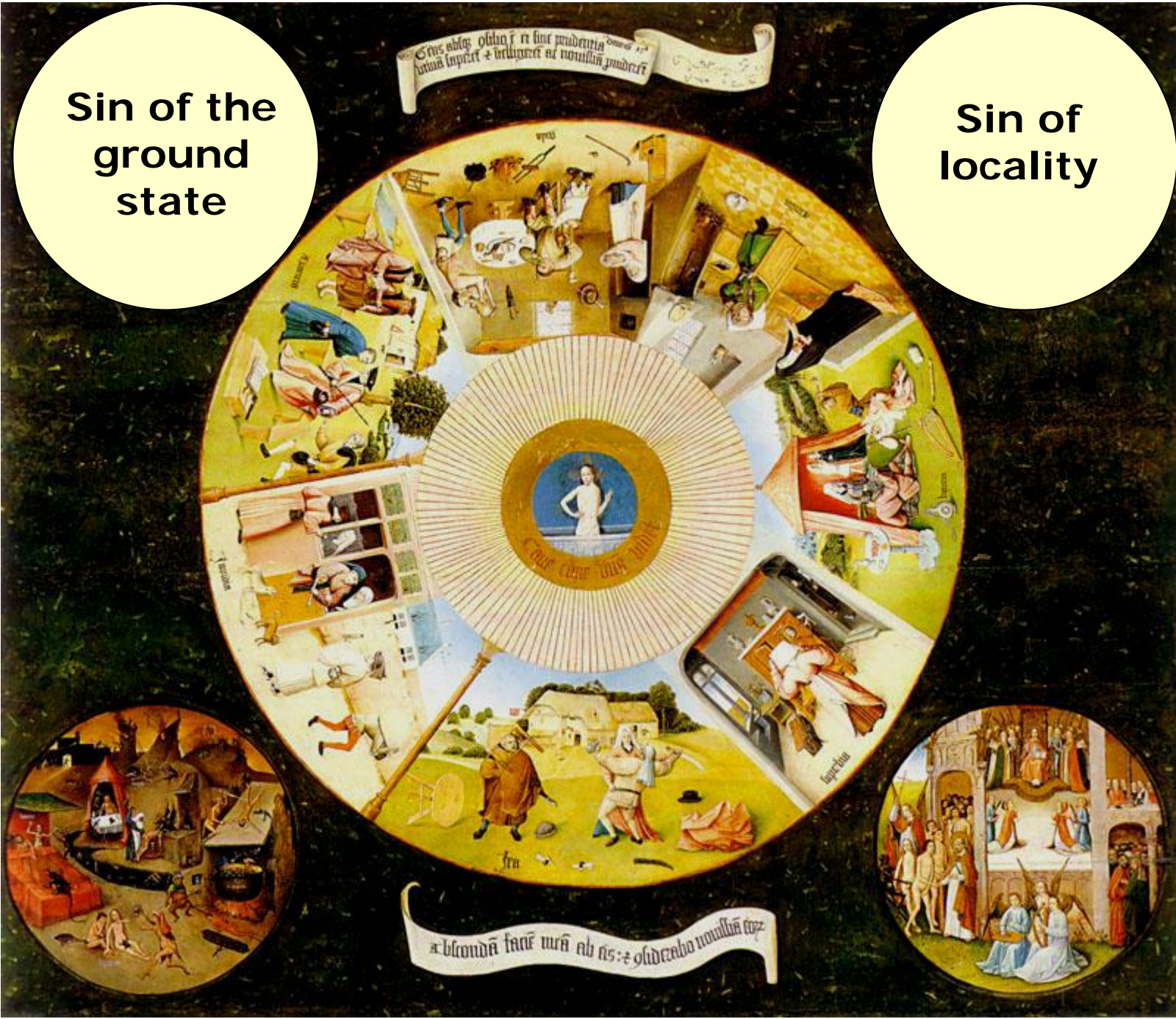


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**Sin of the
ground
state**

**Sin of
locality**



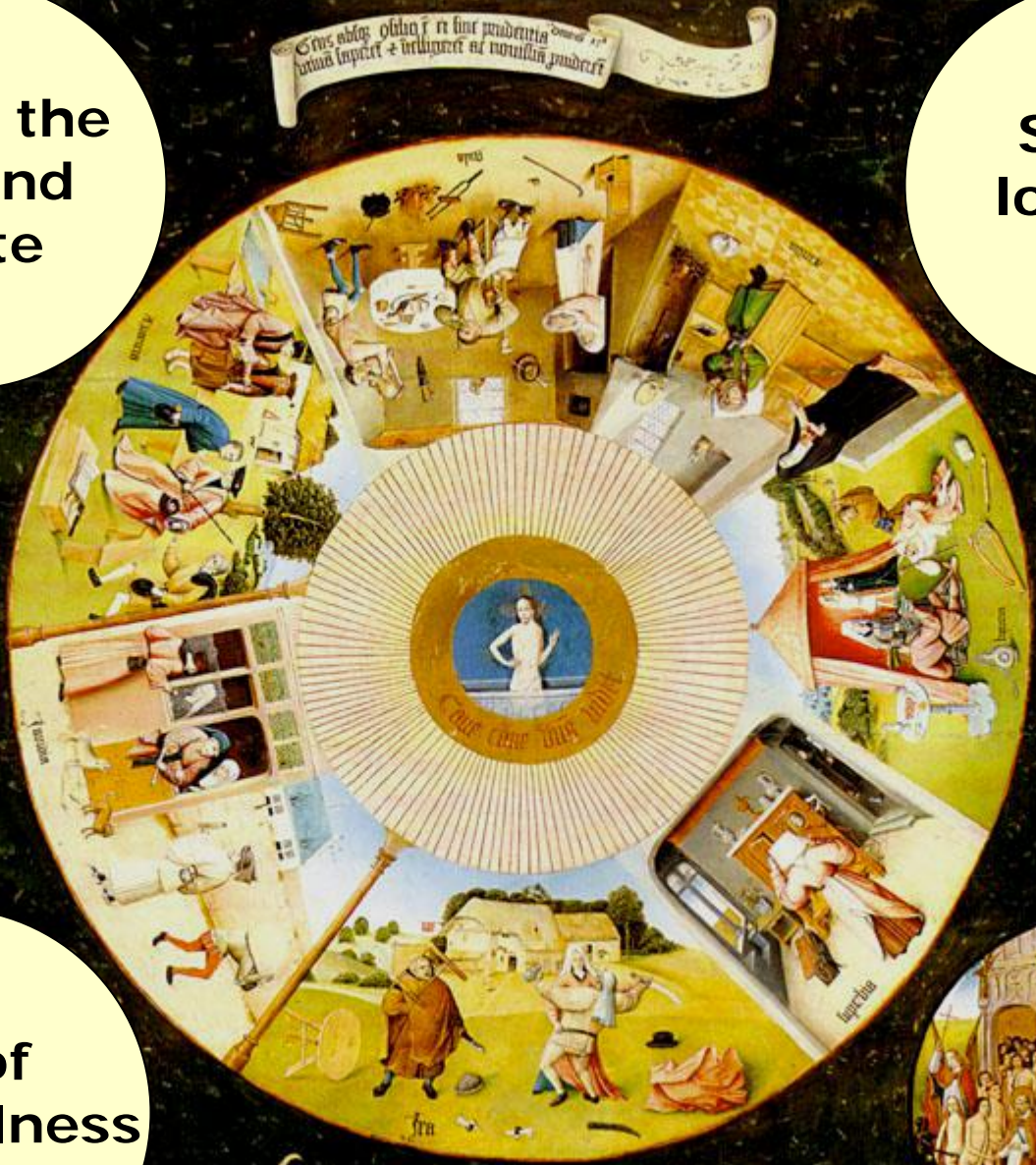
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Sin of the ground state

Sin of locality

Sin of forgetfulness



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Sin of forgetfulness

Sin of the ground state

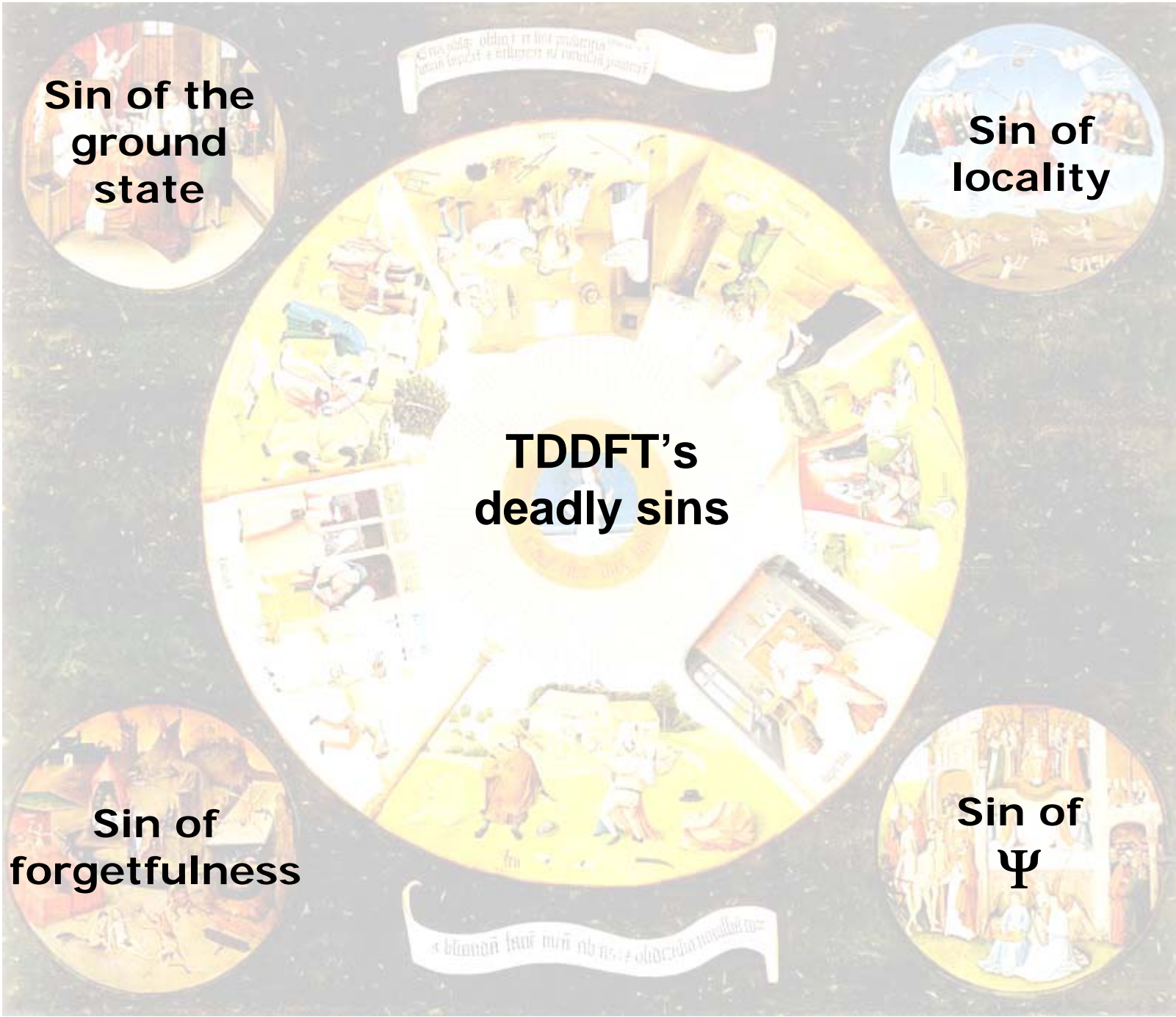


Sin of locality

Sin of Ψ

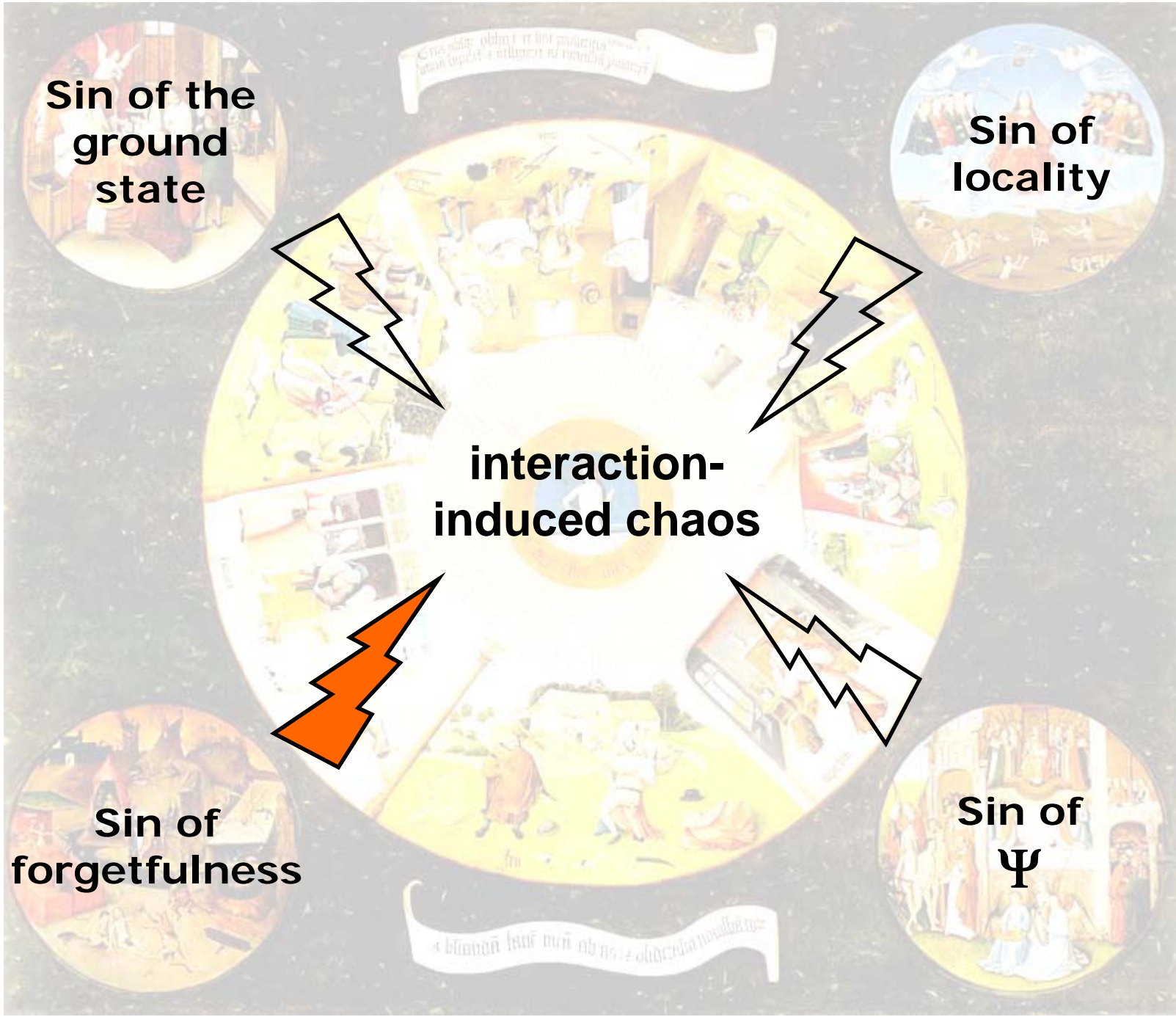
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Kieron's summary of EXCITCM

- Good things
 - Era of multiple codes running interesting materials
 - Many approximations being calculated more carefully
 - Materials trends studied
 - GW and DMFT trying to meet
 - van der Waals frontier wide open
 - Honing in on many-body effects in transport and comparison between theory/expt

Kieron's summary of EXCITCM

- Bad things
 - Many different details hidden in implementations
 - Too many functionals
 - Too many ways to do GW
 - Too much dependence on starting points
 - TDDFT with nanoquanta kernel too expensive in many situations
 - Arbitrary decisions on Wannier functions
 - Have not yet bridged gap to DMFT

Kieron's challenges

- Easy
 - Construct G2 data set of theoretical results (cf Stiles) eg LDA numbers for standard systems.
 - Construct complimentary set for accurate experiment numbers, e.g. lattice parameters

Kieron's challenges

- Harder
 - What is exact relation between G and photoemission spectrum?
 - Exact G for some finite systems, just to see it.

Kieron's challenges

- Harder still
 - Exact properties of many-body wavefunctions for periodic boundary conditions
 - Real practical connections between DFT and MBT

Kieron's challenges

- Hardest of all
 - Fix the stretched H_2 problem
 - Why does DFT work so well?
 - How can we take advantage of Coulomb nature of the problem?