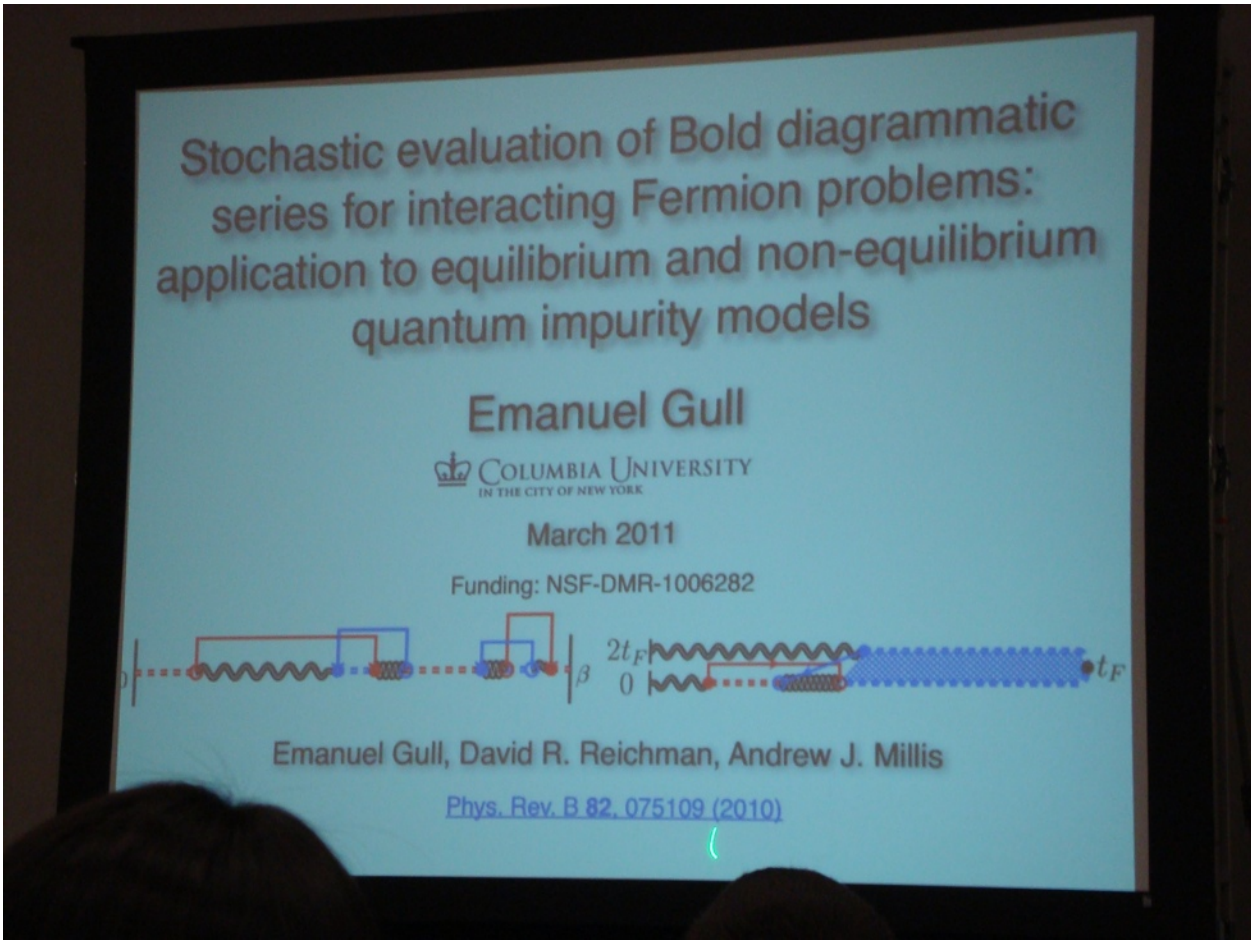
Stochastic evaluation of Bold diagrammatic series for interacting Fermion problems: application to equilibrium and non-equilibrium quantum impurity models
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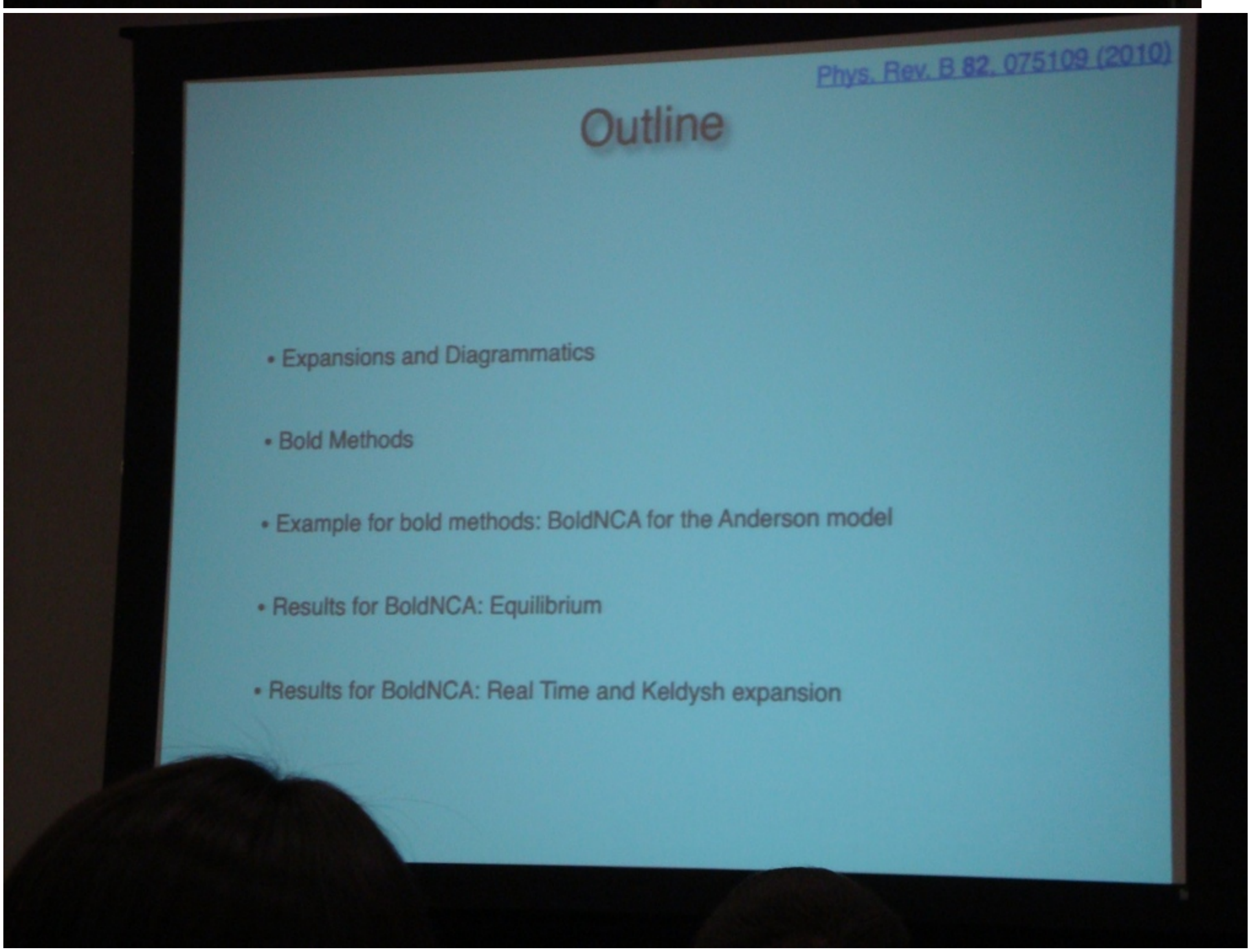
in the City of New York
March 2011
Funding: NSF-DMR-1006282
β
2t_F
0
t_F
Emanuel Gull, David R. Reichman, Andrew J. Millis
Phys. Rev. B 82, 075109 (2010)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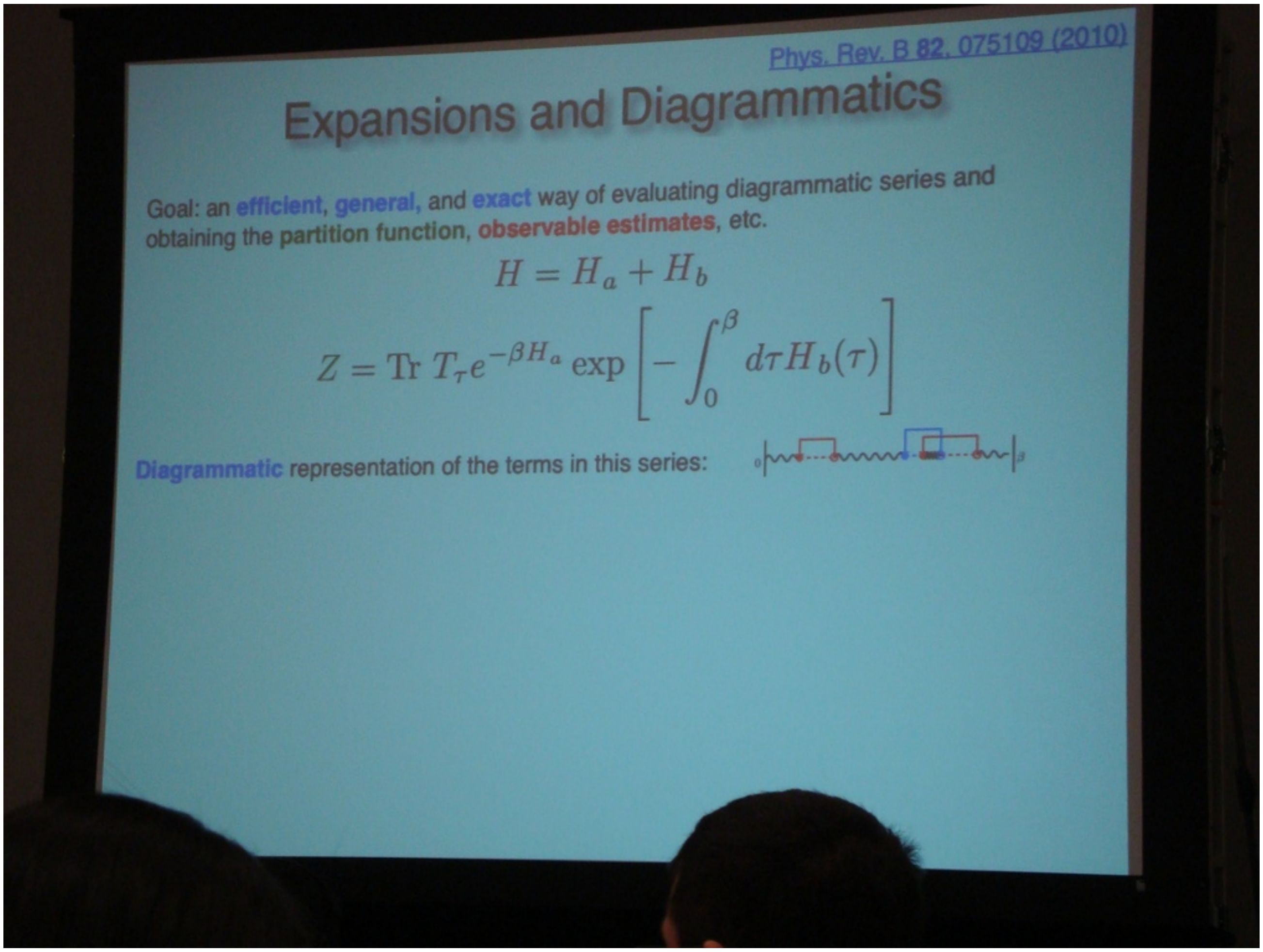
Outline
• Expansions and Diagrammatics
• Bold Methods
• Example for bold methods: BoldNCA for the Anderson model
• Results for BoldNCA: Equilibrium
• Results for BoldNCA: Real Time and Keldysh expansion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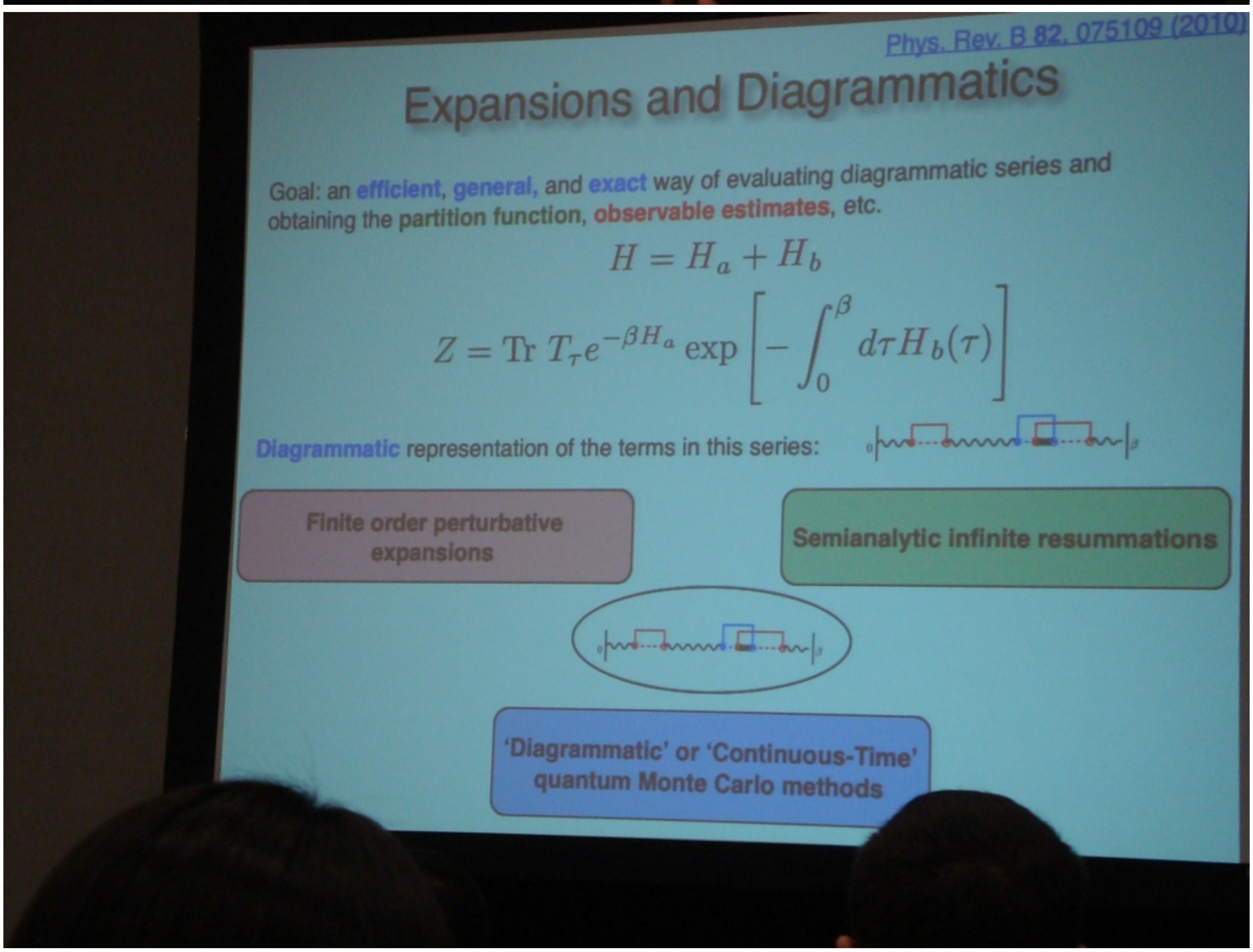
Expansions and Diagrammatics
Goal: an efficient, general, and exact way of evaluating diagrammatic series and obtaining the partition function, observable estimates, etc.
$H = H_a + H_b$
$Z = \mathrm{Tr}\, T_\tau e^{-\beta H_a} \exp\left[-\int_0^\beta d\tau H_b(\tau)\right]$
Diagrammatic representation of the terms in this series: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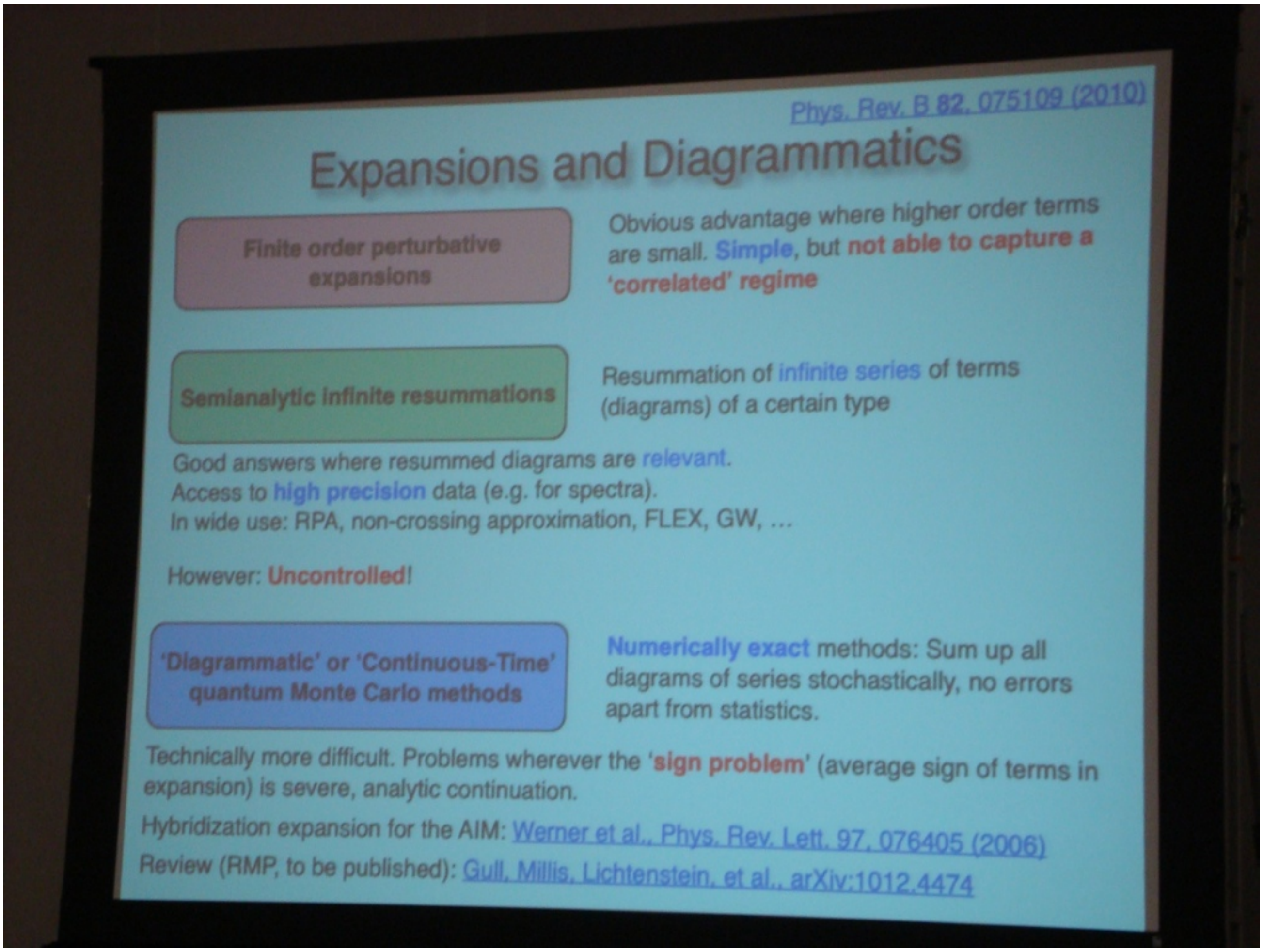
Diagrammatic representation of the terms in this series:
Finite order perturbative expansions
Semianalytic infinite resummations
'Diagrammatic' or 'Continuous-Time' quantum Monte Carlo methods



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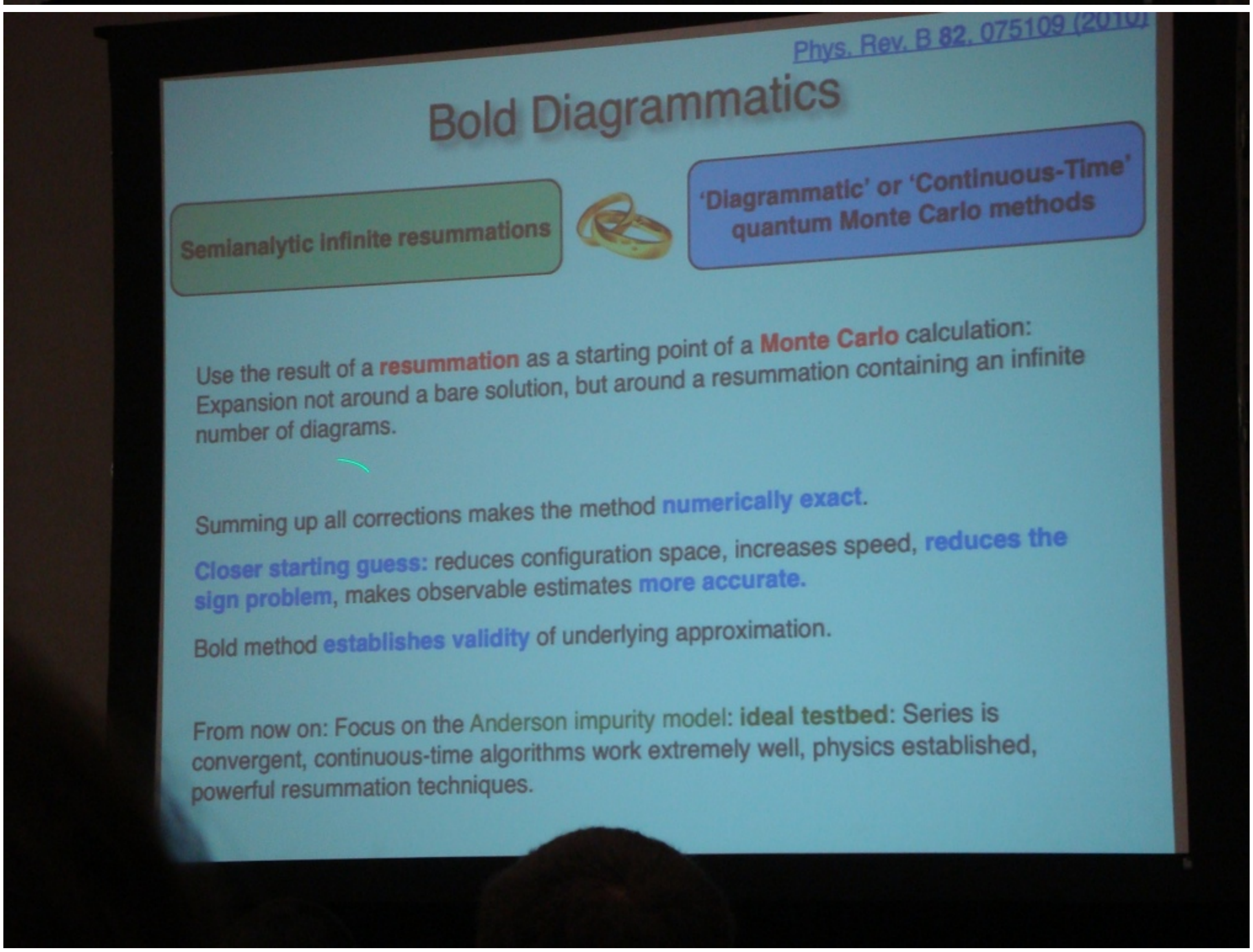
Expansions and Diagrammatics
Finite order perturbative expansions
Obvious advantage where higher order terms are small. Simple, but not able to capture a 'correlated' regime
Semianalytic infinite resummations
Resummation of infinite series of terms (diagrams) of a certain type
Good answers where resummed diagrams are relevant.
Access to high precision data (e.g. for spectra).
In wide use: RPA, non-crossing approximation, FLEX, GW, ...
However: Uncontrolled!
'Diagrammatic' or 'Continuous-Time' quantum Monte Carlo methods
Numerically exact methods: Sum up all diagrams of series stochastically, no errors apart from statistics.
Technically more difficult. Problems wherever the 'sign problem' (average sign of terms in expansion) is severe, analytic continuation.
Hybridization expansion for the AIM: Werner et al., Phys. Rev. Lett. 97, 076405 (2006)
Review (RMP, to be published): Gull, Millis, Lichtenstein, et al., arXiv:1012.4474



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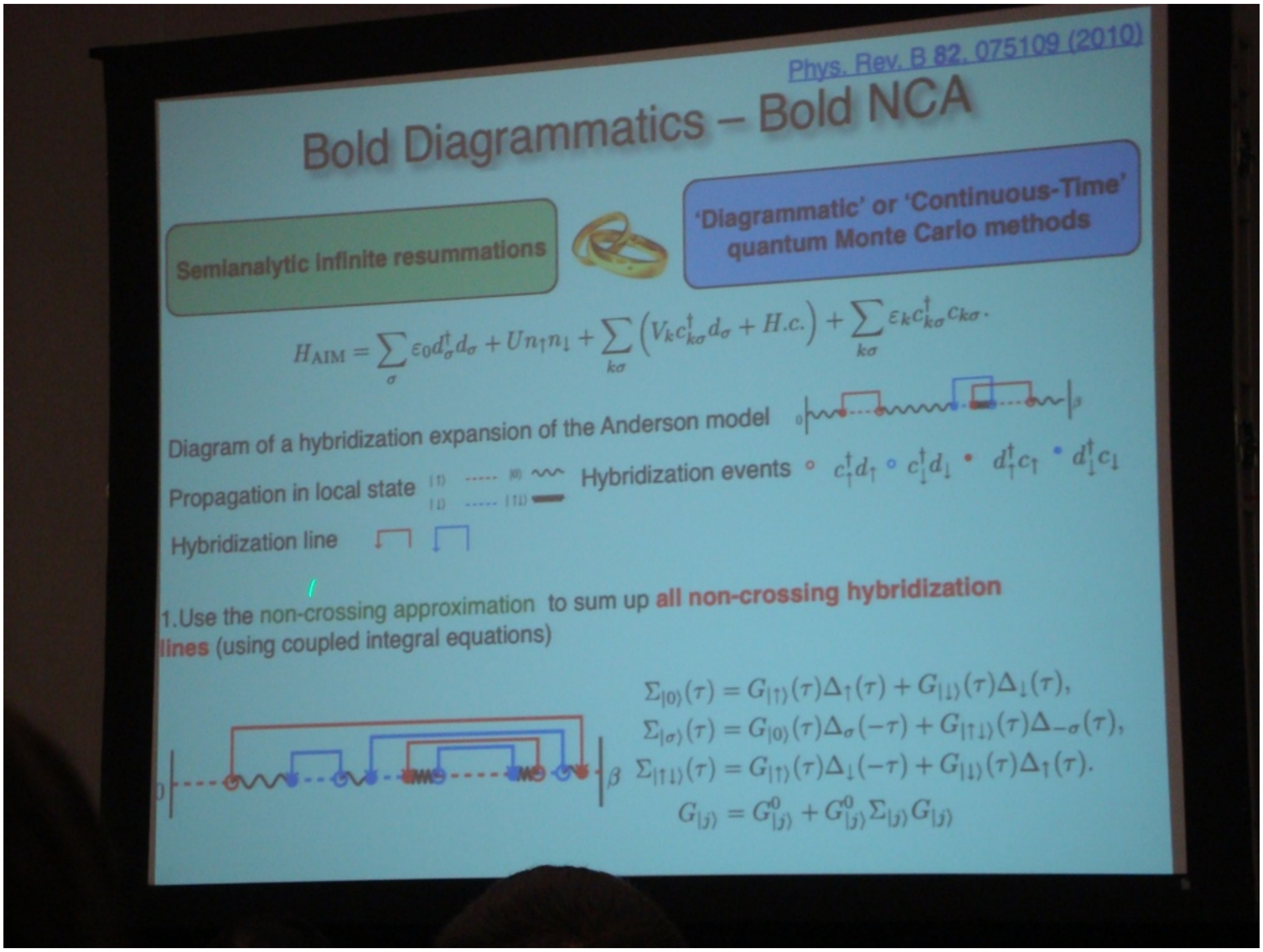
Bold Diagrammatics
Semianalytic infinite resummations
'Diagrammatic' or 'Continuous-Time' quantum Monte Carlo methods
Use the result of a resummation as a starting point of a Monte Carlo calculation:
Expansion not around a bare solution, but around a resummation containing an infinite number of diagrams.
Summing up all corrections makes the method numerically exact.
Closer starting guess: reduces configuration space, increases speed, reduces the sign problem, makes observable estimates more accurate.
Bold method establishes validity of underlying approximation.
From now on: Focus on the Anderson impurity model: ideal testbed: Series is convergent, continuous-time algorithms work extremely well, physics established, powerful resummation techniques.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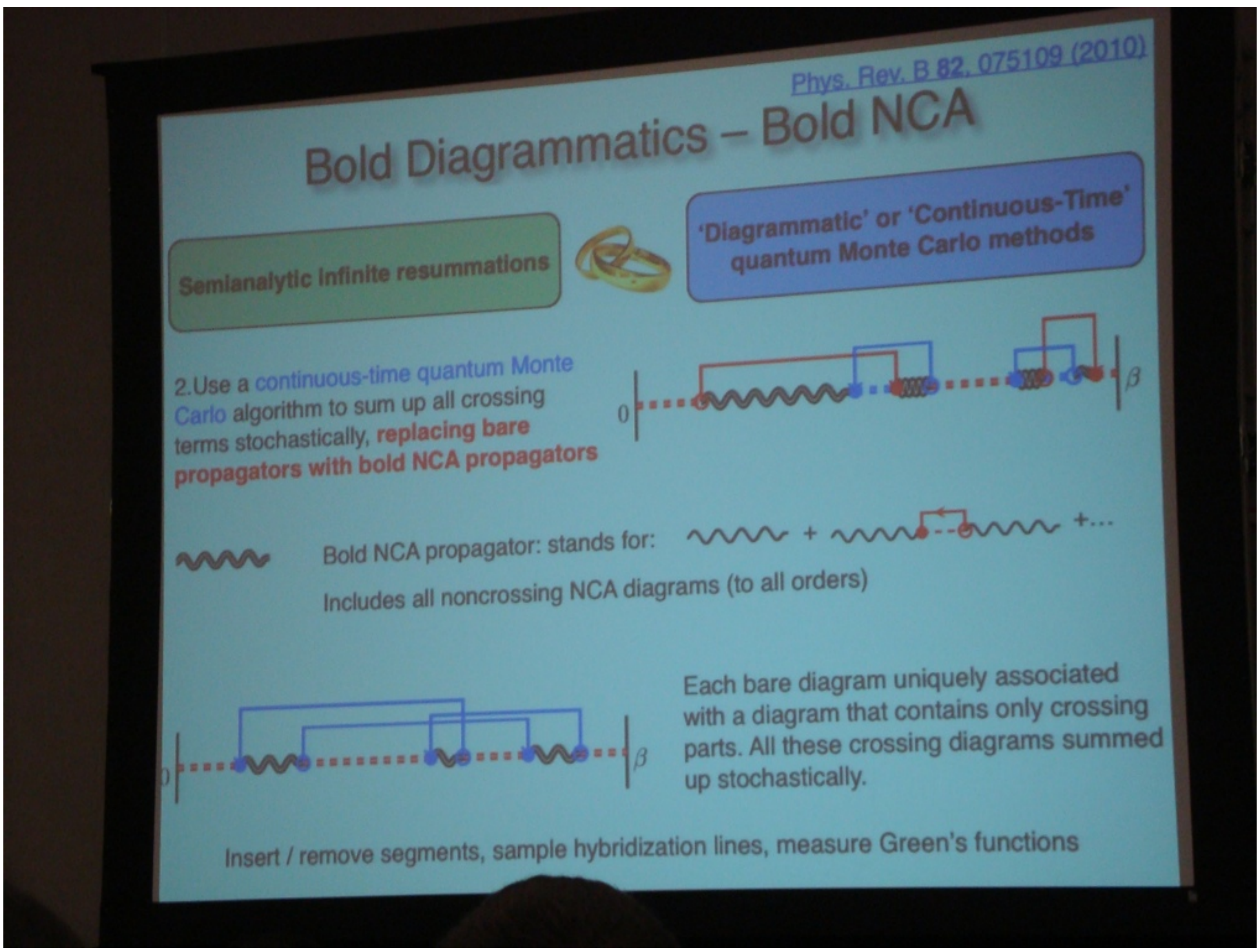
Bold Diagrammatics – Bold NCA
Semianalytic infinite resummations
'Diagrammatic' or 'Continuous-Time' quantum Monte Carlo methods
$H_{\mathrm{AIM}} = \sum_\sigma \varepsilon_0 d_\sigma^\dagger d_\sigma + U n_\uparrow n_\downarrow + \sum_{k\sigma} \left(V_k c_{k\sigma}^\dagger d_\sigma + H.c. \right) + \sum_{k\sigma} \varepsilon_k c_{k\sigma}^\dagger c_{k\sigma}.$
Diagram of a hybridization expansion of the Anderson model
Propagation in local state
Hybridization events $c_\uparrow^\dagger d_\uparrow$ $c_\downarrow^\dagger d_\downarrow$ $d_\uparrow^\dagger c_\uparrow$ $d_\downarrow^\dagger c_\downarrow$
Hybridization line
1.Use the non-crossing approximation to sum up all non-crossing hybridization lines (using coupled integral equations)
$\Sigma_{|0\rangle}(\tau) = G_{|\uparrow\rangle}(\tau)\Delta_\uparrow(\tau) + G_{|\downarrow\rangle}(\tau)\Delta_\downarrow(\tau),$
$\Sigma_{|\sigma\rangle}(\tau) = G_{|0\rangle}(\tau)\Delta_\sigma(-\tau) + G_{|\uparrow\downarrow\rangle}(\tau)\Delta_{-\sigma}(\tau),$
$\Sigma_{|\uparrow\downarrow\rangle}(\tau) = G_{|\uparrow\rangle}(\tau)\Delta_\downarrow(-\tau) + G_{|\downarrow\rangle}(\tau)\Delta_\uparrow(\tau).$
$G_{|j\rangle} = G^0_{|j\rangle} + G^0_{|j\rangle}\Sigma_{|j\rangle}G_{|j\rangle}$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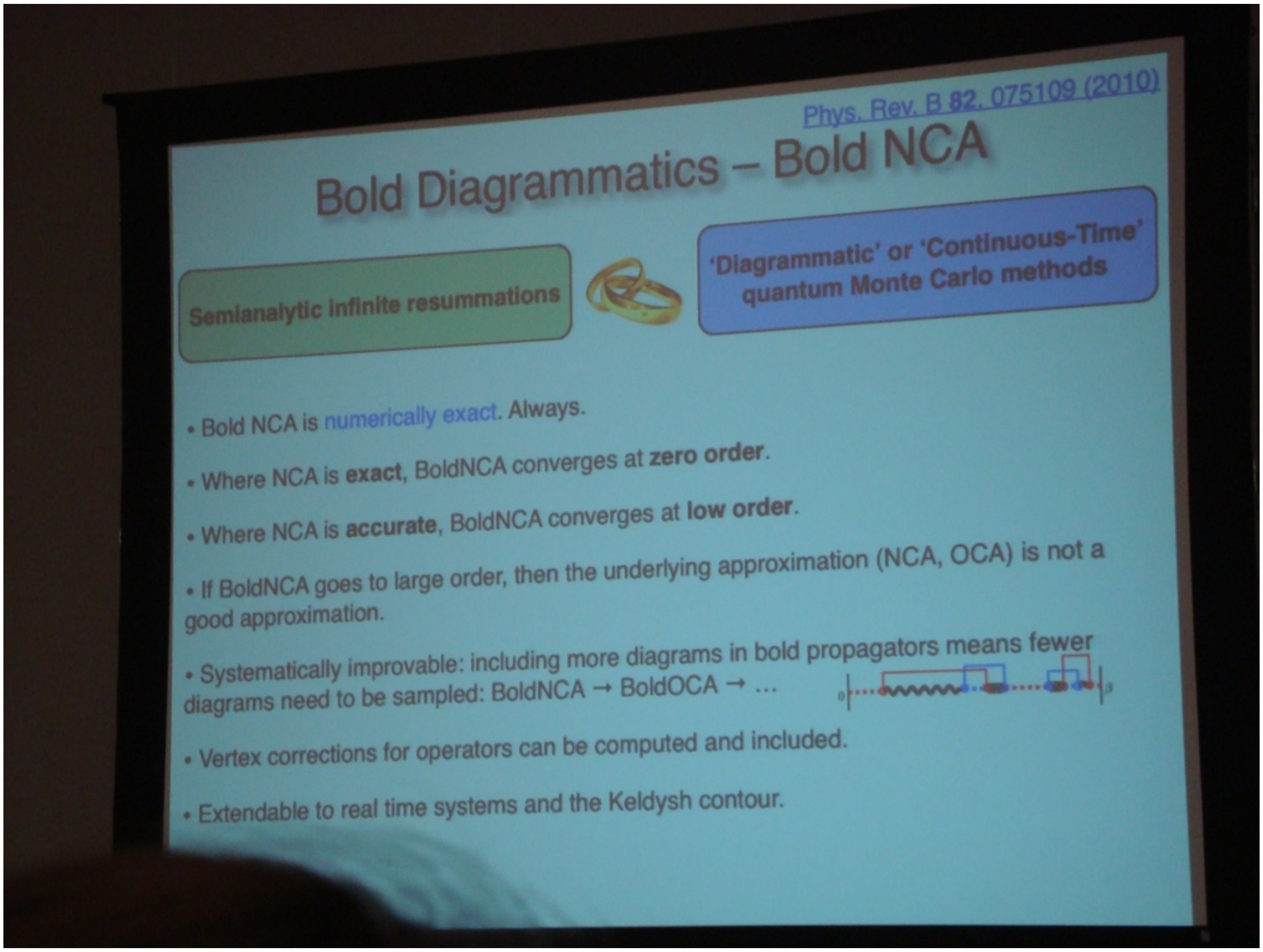
Bold Diagrammatics – Bold NCA
Semianalytic infinite resummations
'Diagrammatic' or 'Continuous-Time' quantum Monte Carlo methods
2.Use a continuous-time quantum Monte Carlo algorithm to sum up all crossing terms stochastically, replacing bare propagators with bold NCA propagators
Bold NCA propagator: stands for: + +...
Includes all noncrossing NCA diagrams (to all orders)
Each bare diagram uniquely associated with a diagram that contains only crossing parts. All these crossing diagrams summed up stochastically.
Insert / remove segments, sample hybridization lines, measure Green's functions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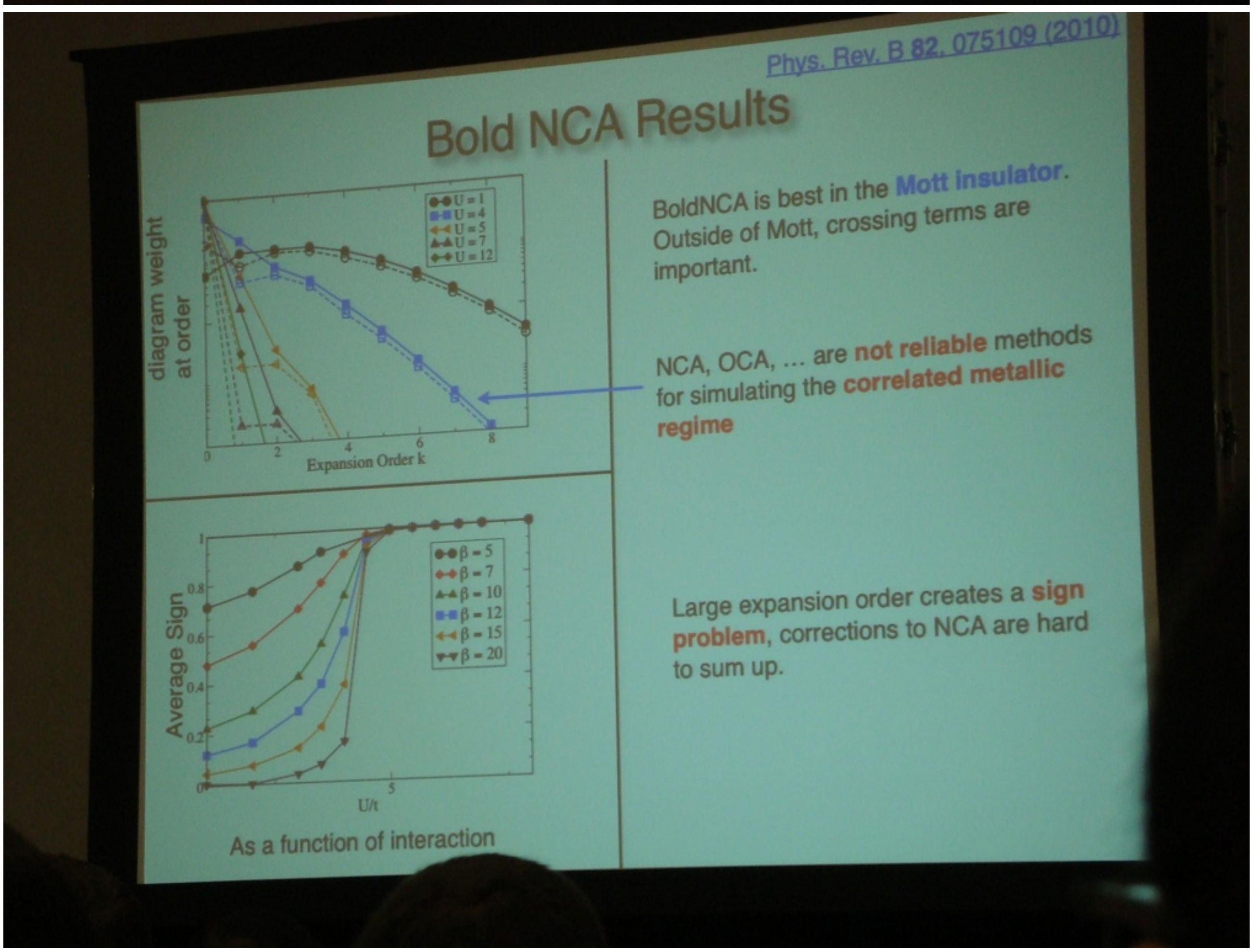
Bold Diagrammatics – Bold NCA
Semianalytic infinite resummations
'Diagrammatic' or 'Continuous-Time' quantum Monte Carlo methods
• Bold NCA is numerically exact. Always.
• Where NCA is exact, BoldNCA converges at zero order.
• Where NCA is accurate, BoldNCA converges at low order.
• If BoldNCA goes to large order, then the underlying approximation (NCA, OCA) is not a good approximation.
• Systematically improvable: including more diagrams in bold propagators means fewer diagrams need to be sampled: BoldNCA → BoldOCA → …
• Vertex corrections for operators can be computed and included.
• Extendable to real time systems and the Keldysh contour.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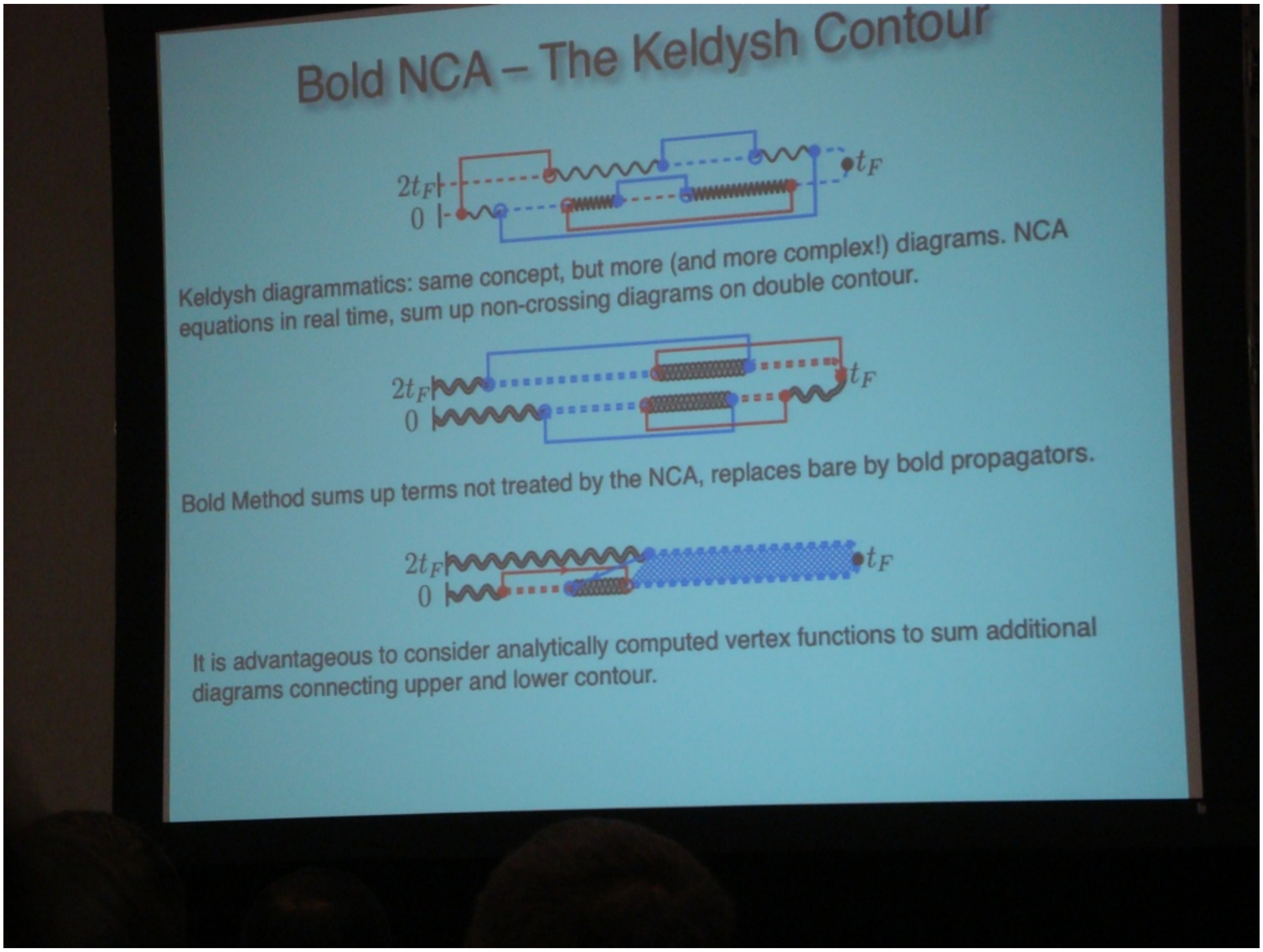
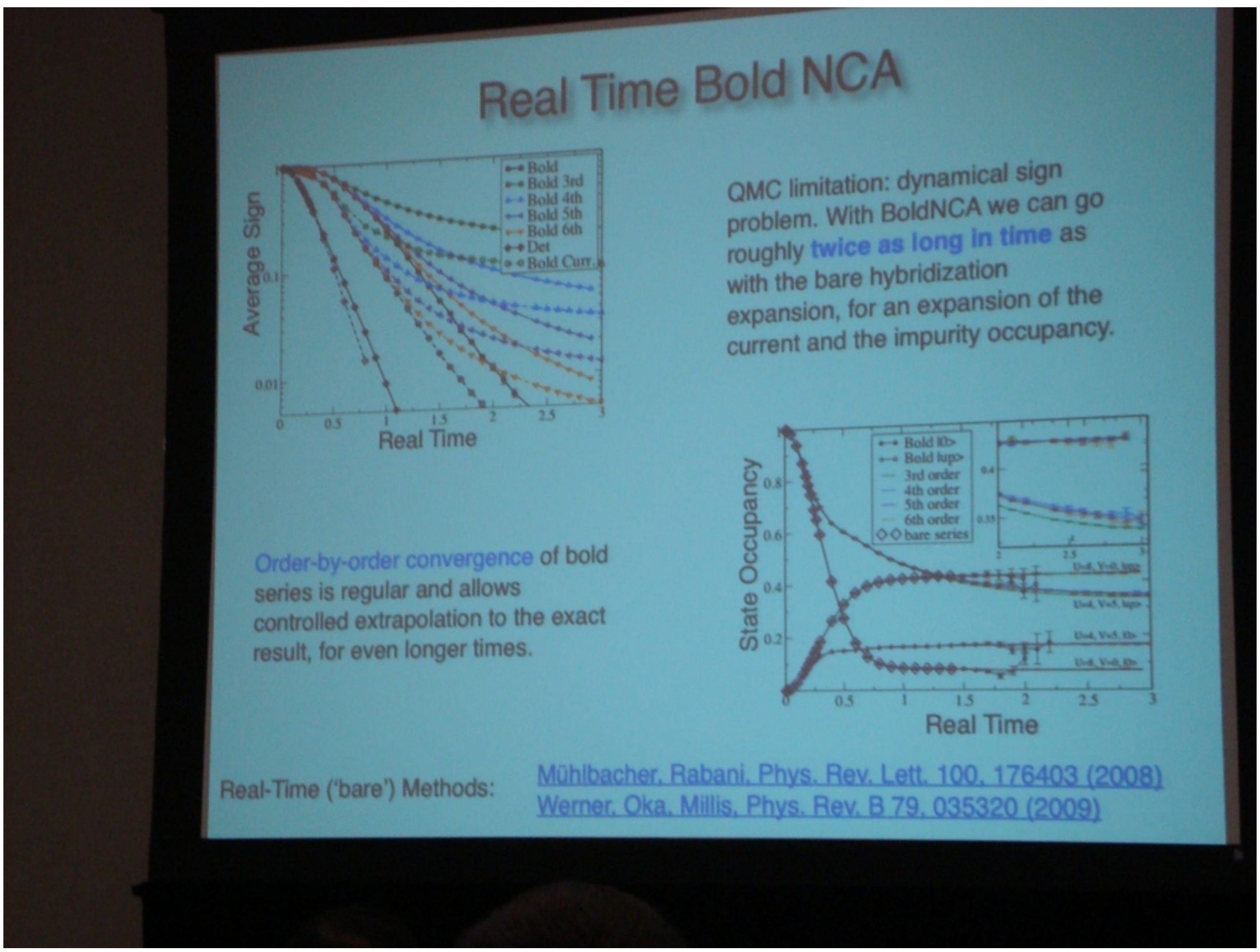
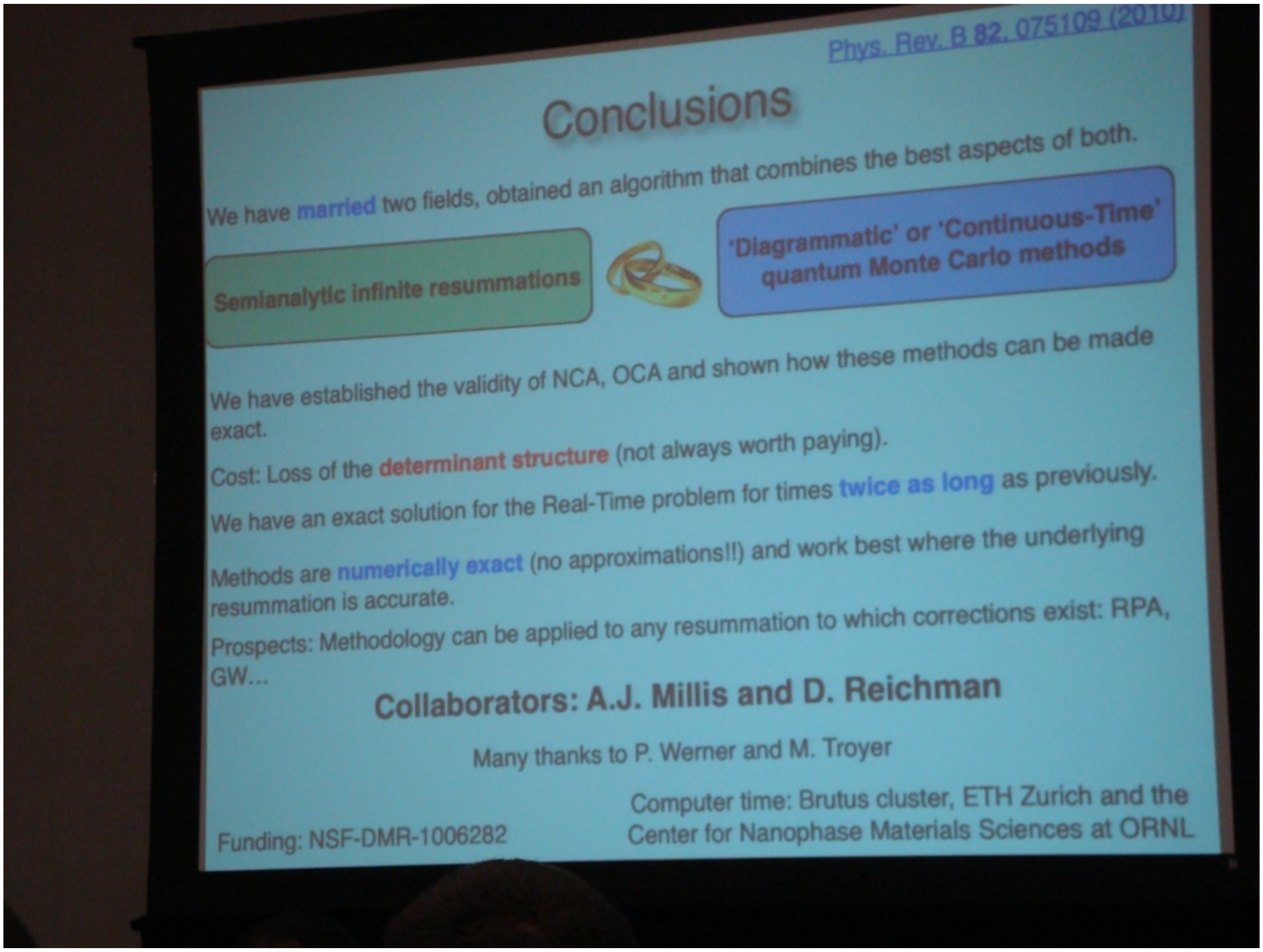
Bold NCA Results
diagram weight at order
U = 1
U = 4
U = 5
U = 7
U = 12
Expansion Order k
BoldNCA is best in the Mott insulator. Outside of Mott, crossing terms are important.
NCA, OCA, ... are not reliable methods for simulating the correlated metallic regime
Average Sign
β = 5
β = 7
β = 10
β = 12
β = 15
β = 20
U/t
As a function of interaction
Large expansion order creates a sign problem, corrections to NCA are hard to sum up.


Bold NCA – The Keldysh Contour
$2t_F$
0
t_F
Keldysh diagrammatics: same concept, but more (and more complex!) diagrams. NCA equations in real time, sum up non-crossing diagrams on double contour.
$2t_F$
0
t_F
Bold Method sums up terms not treated by the NCA, replaces bare by bold propagators.
$2t_F$
0
t_F
It is advantageous to consider analytically computed vertex functions to sum additional diagrams connecting upper and lower contour.


Real Time Bold NCA
Average Sign
Real Time
Bold
Bold 3rd
Bold 4th
Bold 5th
Bold 6th
Det
Bold Curr.
0.1
0.01
0
0.5
1
1.5
2
2.5
3
QMC limitation: dynamical sign problem. With BoldNCA we can go roughly twice as long in time as with the bare hybridization expansion, for an expansion of the current and the impurity occupancy.
Order-by-order convergence of bold series is regular and allows controlled extrapolation to the exact result, for even longer times.
State Occupancy
Real Time
Bold |0>
Bold |up>
3rd order
4th order
5th order
6th order
bare series
0.2
0.4
0.6
0.8
0
0.5
1
1.5
2
2.5
3
Real-Time ('bare') Methods:
Mühlbacher, Rabani, Phys. Rev. Lett. 100, 176403 (2008)
Werner, Oka, Millis, Phys. Rev. B 79, 035320 (2009)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Conclusions
We have married two fields, obtained an algorithm that combines the best aspects of both.
Semianalytic infinite resummations
'Diagrammatic' or 'Continuous-Time' quantum Monte Carlo methods
We have established the validity of NCA, OCA and shown how these methods can be made exact.
Cost: Loss of the determinant structure (not always worth paying).
We have an exact solution for the Real-Time problem for times twice as long as previously.
Methods are numerically exact (no approximations!!) and work best where the underlying resummation is accurate.
Prospects: Methodology can be applied to any resummation to which corrections exist: RPA, GW...
Collaborators: A.J. Millis and D. Reichman
Many thanks to P. Werner and M. Troyer
Funding: NSF-DMR-1006282
Computer time: Brutus cluster, ETH Zurich and the Center for Nanophase Materials Sciences at ORNL