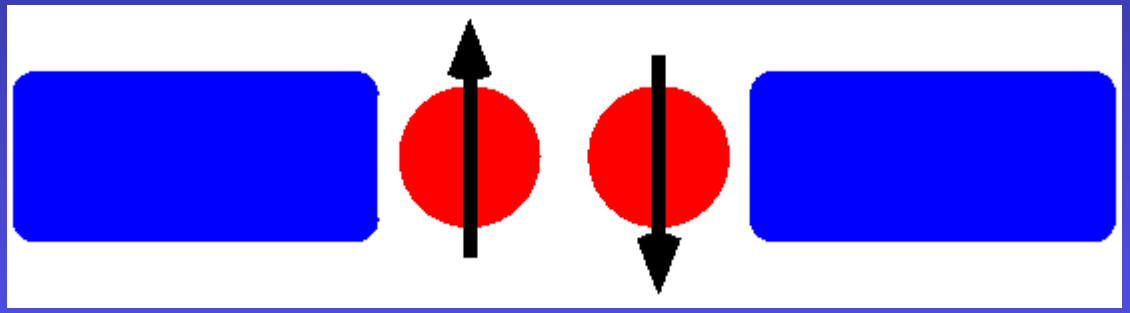
Popayan, 2012

Density Matrix Renormalization Group

DMRG



Servio Tulio Pérez M.

Departamento de Física

Facultad de Ciencias Naturales Exactas y de la Educación

Universidad del Cauca

Outline

Objetivos

Objetivo General

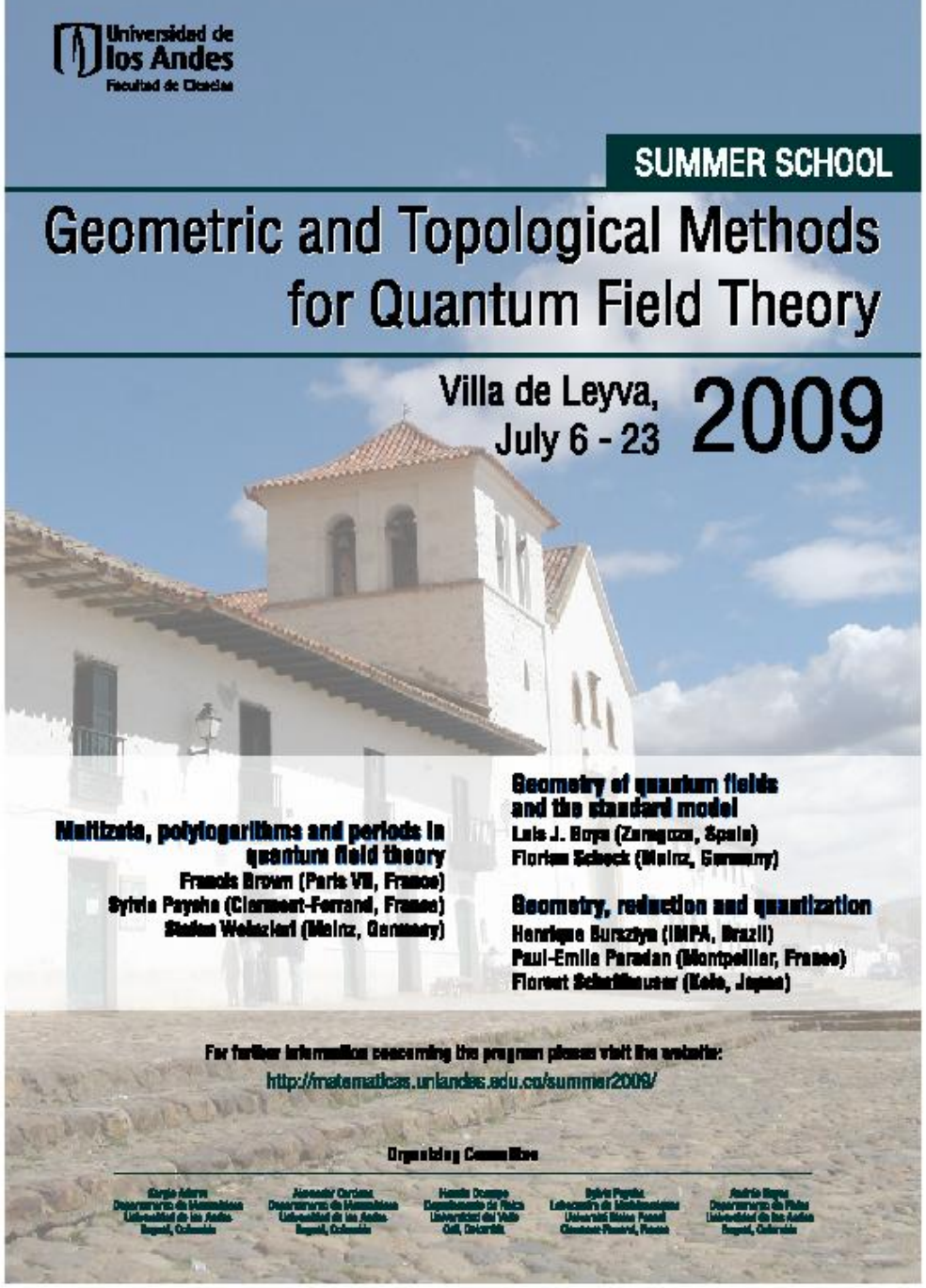
Apropiarse de las herramientas básicas que permitan el análisis del Método numérico Matriz de Renormalización (DMRG- Density Matrix Renormalization Group) a través de documentos específicos y visitas técnicas a grupos que manejen dicha herramienta.

Objetivos Específicos

- Realizar una revisión bibliográfica para describir de manera general en qué consiste la teoría de renormalización.
- Determinar específicamente la teoría de renormalización para la matriz densidad.
- Apropiarse de esta técnica para describir a través de ella el comportamiento de propiedades físicas en tópicos de materia condensada y óptica cuántica.
- Estudiar el formalismo de Green en correspondencia con el método DMRG para adaptarlo al estudio de sistemas de baja dimensionalidad correlacionados.
- Redactar un documento que muestre la potencialidad de este método de aproximación.

Abstract

The Density Matrix Renormalization Group ($DMRG$) has become a powerful numerical method that can be applied to low-dimensional strongly correlated fermionic and bosonic systems. It allows for a very precise calculation of static, dynamical and thermodynamical properties. Its field of applicability has now extended beyond Condensed Matter, and is successfully used in Statistical Mechanics and High Energy Physics as well. In this work, we briefly review the main aspects of the method. We also comment on some of the most relevant applications so as to give an overview on the scope and possibilities of DMRG and mention the most important extensions of the method such as the calculation of dynamical properties, the application to classical systems, inclusion of temperature, phonons and disorder, field theory, time-dependent properties and the ab initio calculation of electronic states in molecules.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Geometric and Topological Methods for Quantum Field Theory
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Multizeta, polylogarithms and periods in quantum field theory
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Sylvie Paycha (Clermont-Ferrand, France)
Stefan Weinzierl (Mainz, Germany)
Geometry of quantum fields and the standard model
Luis J. Boya (Zaragoza, Spain)
Florian Scheck (Mainz, Germany)
Geometry, reduction and quantization
Henrique Bursztyn (IMPA, Brazil)
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Introduction

Renormalization Group (RG)

Mathematical apparatus.

that allows systematic investigation of the changes of a physical system as viewed at different distance scales.

Particle Physics

Force Laws

QFT

Energy scale (momentum)

Resolution distance scales

Compton wavelength

Uncertainty principle

Renormalization Group (RG)

Change in Scale

Scale Transformation.

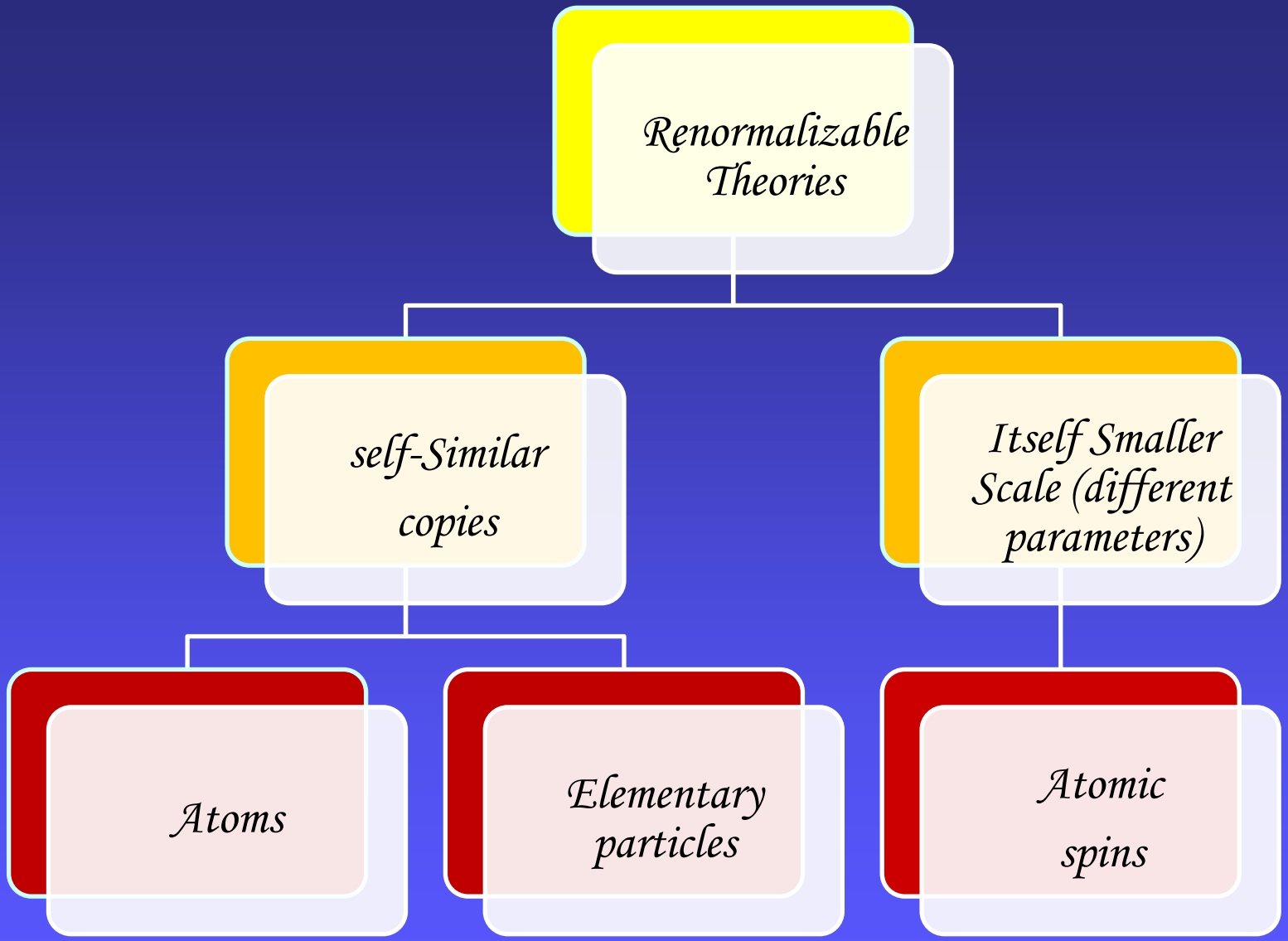
Conformal Invariance

Siymmetries

Self-Sililarity

Symmetry of generators

Conformal Transformations


Renormalizable Theories
self-Similar copies
Itself Smaller Scale (different parameters)
Atoms
Elementary particles
Atomic spins

The history Renormalization Group

The idea of scale transformations and scale invariance is old in physics. Scaling arguments were commonplace for the Pythagorean school, Euclid and up to Galileo. They became popular again at the end of the 19th century, perhaps the first example being the idea of enhanced viscosity of Osborne Reynolds, as a way to explain turbulence.

The renormalization group was initially devised in particle physics, but nowadays its applications extend to solid-state physics, fluid mechanics, cosmology and even nanotechnology. An early article [1] by Ernst Stueckelberg and Andre Petermann in 1953 anticipates the idea in quantum field theory. Stueckelberg and Petermann opened the field conceptually. They noted that renormalization exhibits a group of transformations which transfer quantities from the bare terms to the counterterms. They introduced a function h(e) in QED, which is now called the beta function (see below).

1. *Stueckelberg, E.C.G. and Petermann, A. (1953). Helv. Phys. Acta, 26, 499.*

Murray Gell-Mann and Francis E. Low in 1954 restricted the idea to scale transformations in QED,[2] which are the most physically significant, and focused on asymptotic forms of the photon propagator at high energies. They determined the variation of the electromagnetic coupling in QED, by appreciating the simplicity of the scaling structure of that theory.

The renormalization group prediction (cf Stueckelberg-Petermann and Gell-Mann-Low works) was confirmed 40 years later at the LEP accelerator experiments: the fine structure "constant" of QED was measured to be about 1/127 at energies close to 200 GeV, as opposed to the standard low-energy physics value of 1/137. (Early applications to quantum electrodynamics are discussed in the influential book of Nikolay Bogolyubov and Dmitry Shirkov in 1959.[3])

2. *Gell-Mann, M.; Low, F.E. (1954). "Quantum Electrodynamics at Small Distances". Physical Review 95 (5): 1300–1312.*
3. *N.N. Bogoliubov, D.V. Shirkov (1959): The Theory of Quantized Fields. New York, Interscience.*

A deeper understanding of the physical meaning and generalization of the renormalization process, which goes beyond the dilatation group of conventional renormalizable theories, came from condensed matter physics. Leo P. Kadanoff's paper in 1966 proposed the "block-spin" renormalization group.[4] The blocking idea is a way to define the components of the theory at large distances as aggregates of components at shorter distances.

This approach covered the conceptual point and was given full computational substance[5] in the extensive important contributions of Kenneth Wilson. The power of Wilson's ideas was demonstrated by a constructive iterative renormalization solution of a long-standing problem, the Kondo problem, in 1974, as well as the preceding seminal developments of his new method in the theory of second-order phase transitions and critical phenomena in 1971. He was awarded the Nobel prize for these decisive contributions in 1982.

4. L.P. Kadanoff (1966): "Scaling laws for Ising models near ", Physics (Long Island City, N.Y.) 2, 263.

5. K.G. Wilson(1975): The renormalization group: critical phenomena and the Kondo problem, Rev. Mod. Phys. 47, 4, 773.

Theoretical Aspects of the renormalization group

Quantum Field Theory

Ultra-violet divergences

Quantum fluctuations

Complication & opportunity to find interesting physics

Perturbatibe QCD

Factorization Theorems for strong interactions

Phenomenological consequences

The structure of a quantum field theory often simplifies when one considers processes involving

large momenta or short distances.

These simplifications are important in improving one's ability to calculate predictions from the theory

One –dimensional Ising model

These manifest themselves in Feynman graphs as divergences

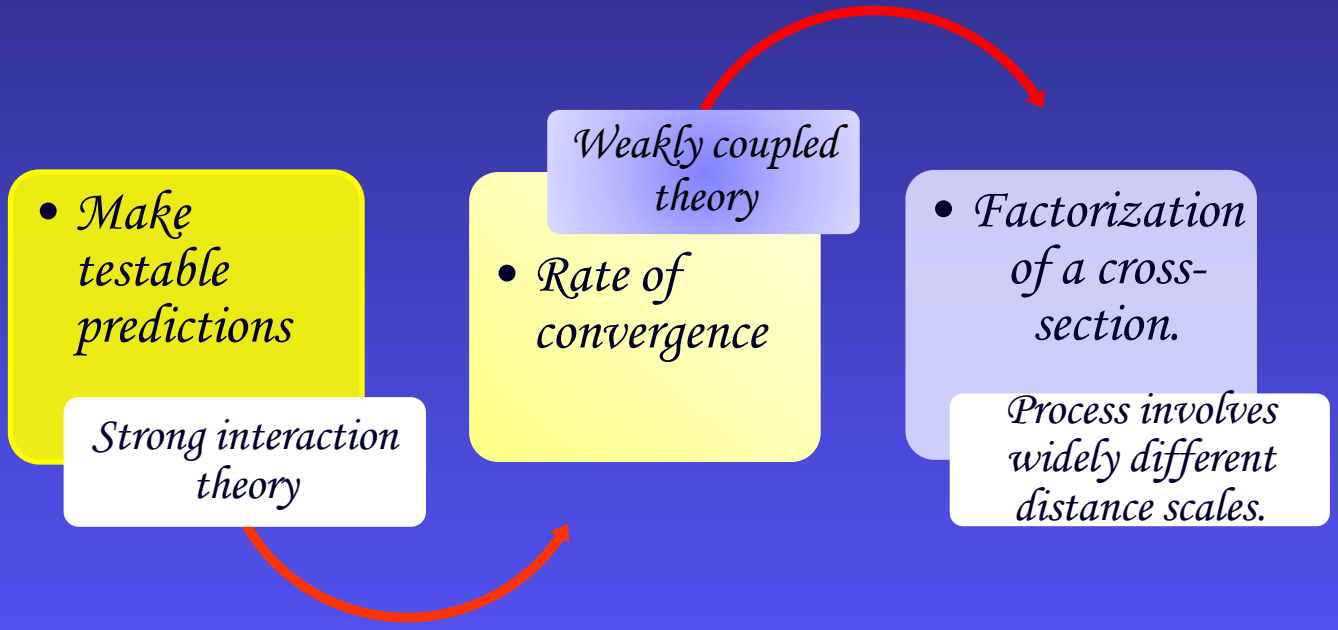
The problem is that there are usually ultra-violet divergences caused by large fluctuations of the field(s) on short distance scales.

The simplification is that the divergences can be cancelled by renormalizations of the parameters of the action

it is necessary to expose the methods to handle high-energy/short distance problems.

Consequently our first task will be to treat the ultra-violet renormalizations.

Renormalization is essential

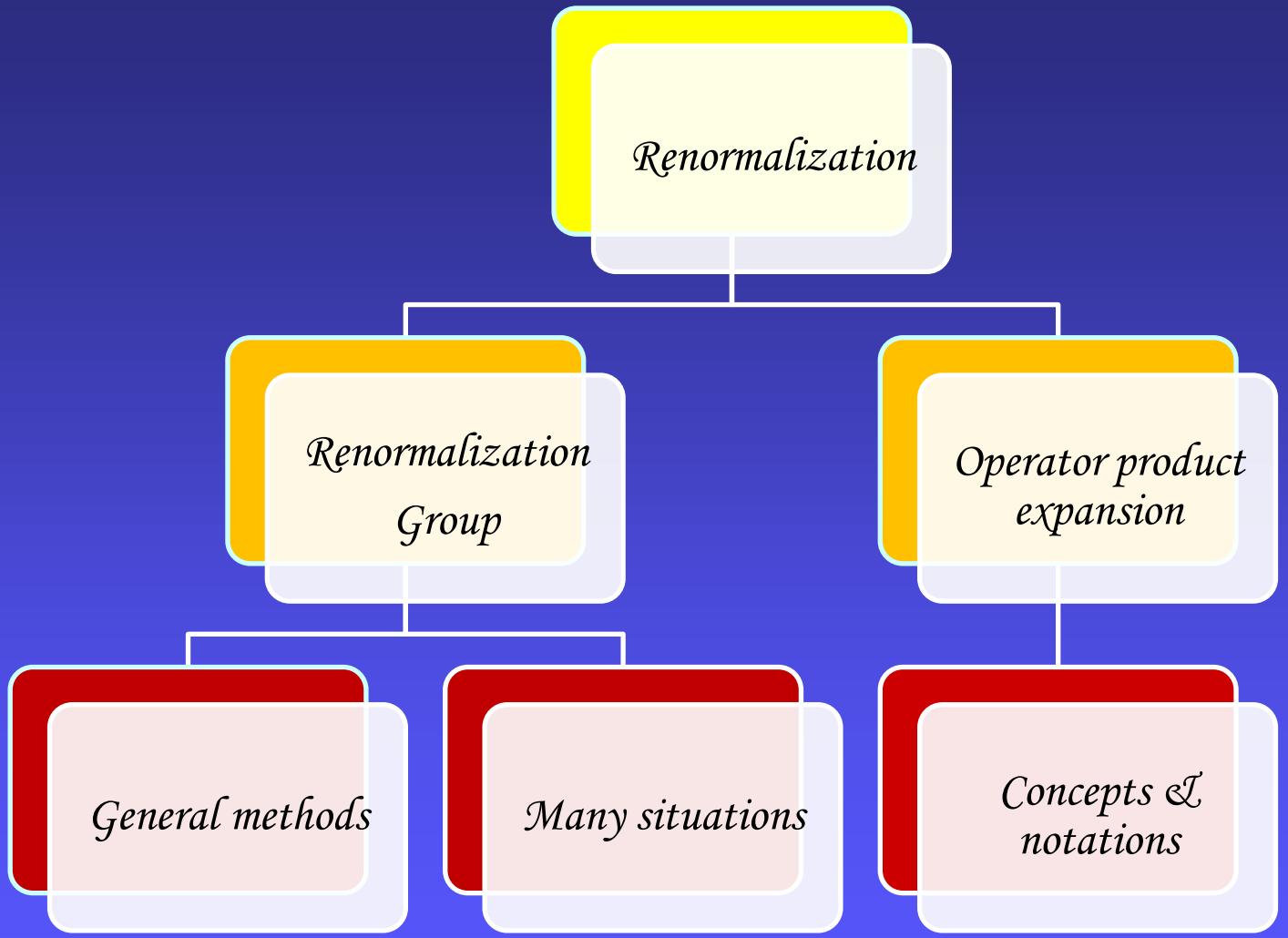

• Make testable predictions
Strong interaction theory
Weakly coupled theory
• Rate of convergence
• Factorization of a cross-section.
Process involves widely different distance scales.

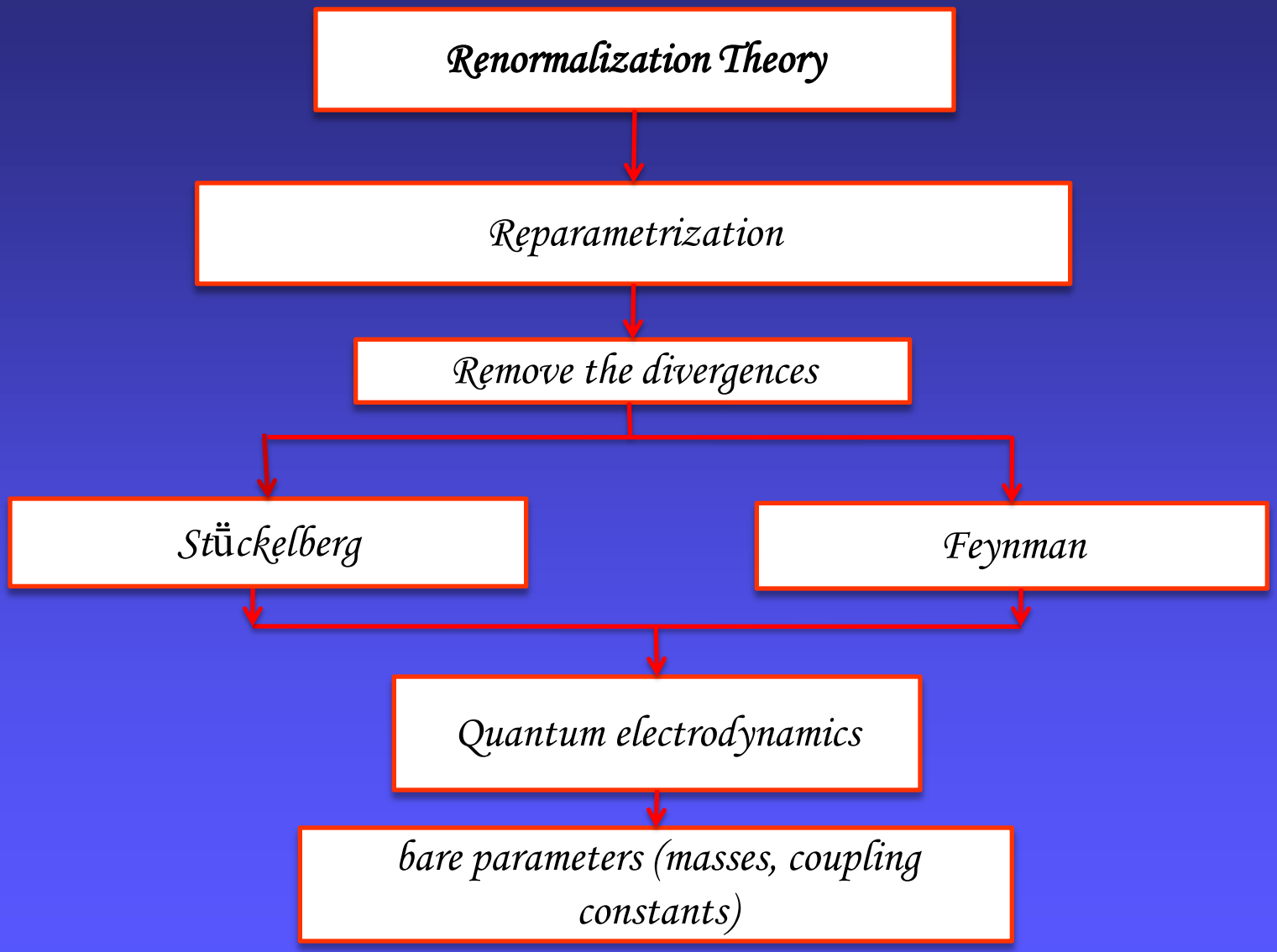
Ultra-violet divergences

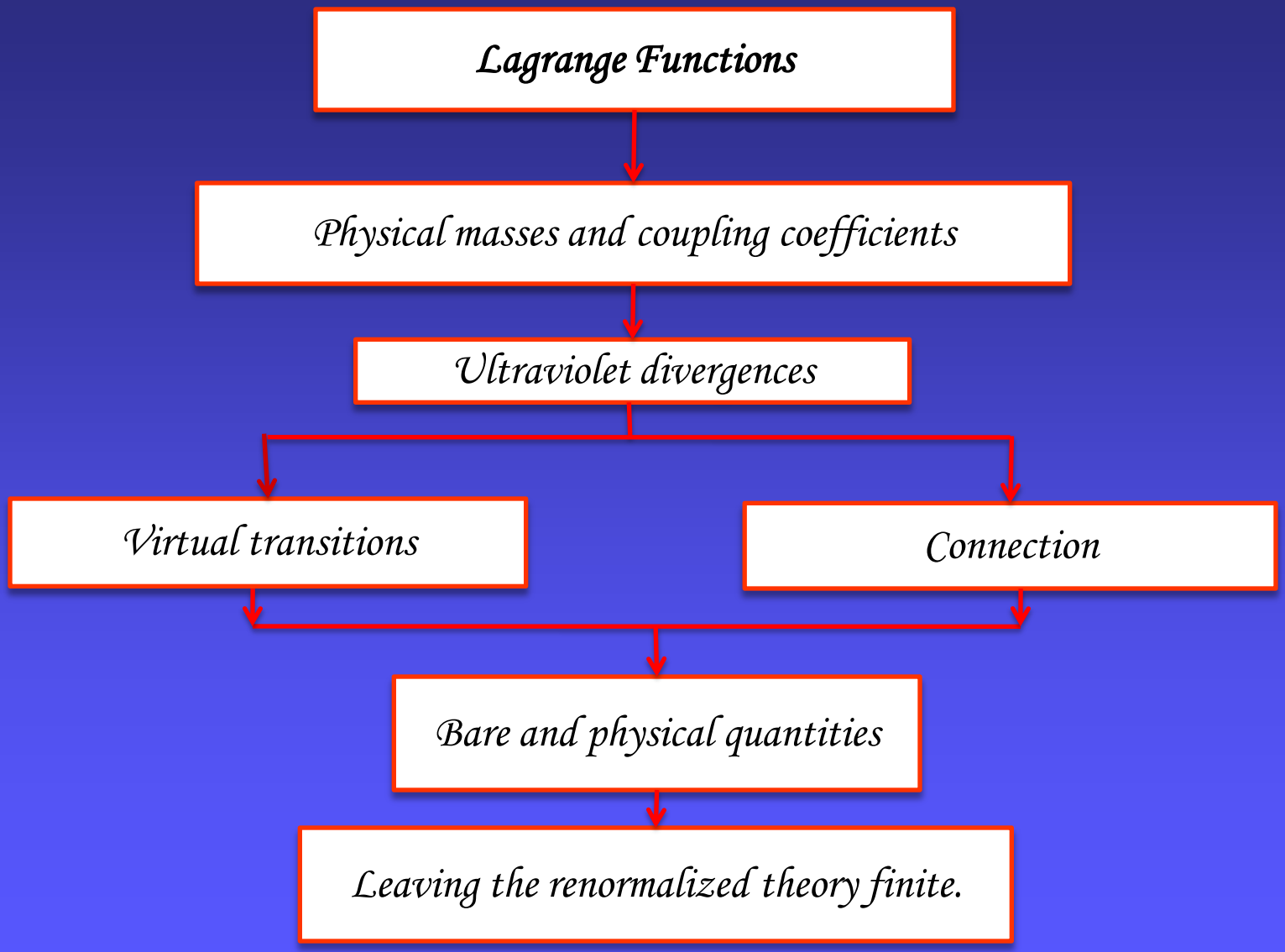
These manifest themselves in Feynman graphs as divergences when loop momenta go to infinity with the external momenta fixed

The simplification is that the divergences can be cancelled by renormalizations of the parameters of the action.

Renormalization is essential, for otherwise most field theories do not exist


Renormalization
Renormalization Group
Operator product expansion
General methods
Many situations
Concepts & notations


Renormalization Theory
Reparametrization
Remove the divergences
Stückelberg
Feynman
Quantum electrodynamics
bare parameters (masses, coupling constants)


Lagrange Functions
Physical masses and coupling coefficients
Ultraviolet divergences
Virtual transitions
Connection
Bare and physical quantities
Leaving the renormalized theory finite.

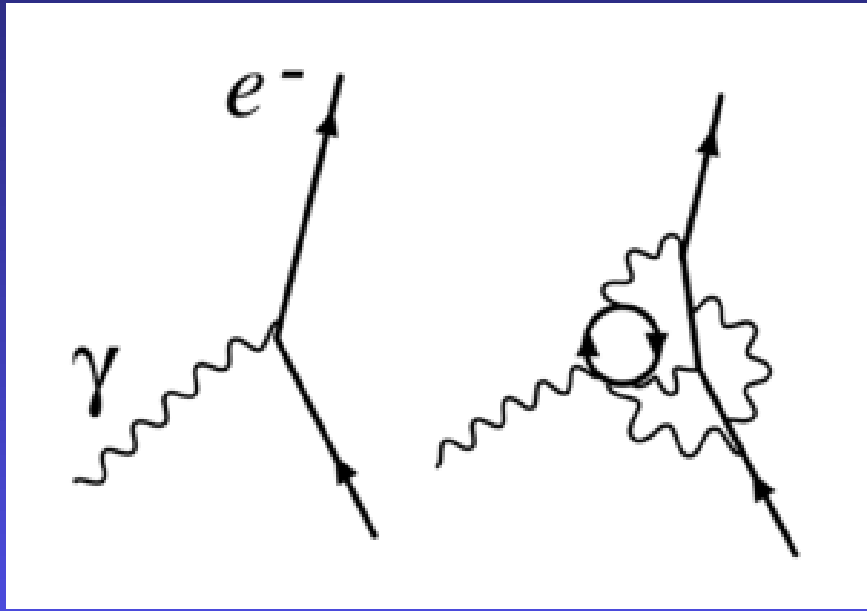


Figure 1. Renormalization in quantum electrodynamics: The simple electron-photon interaction that determines the electron's charge at one renormalization point is revealed to consist of more complicated interactions at another.

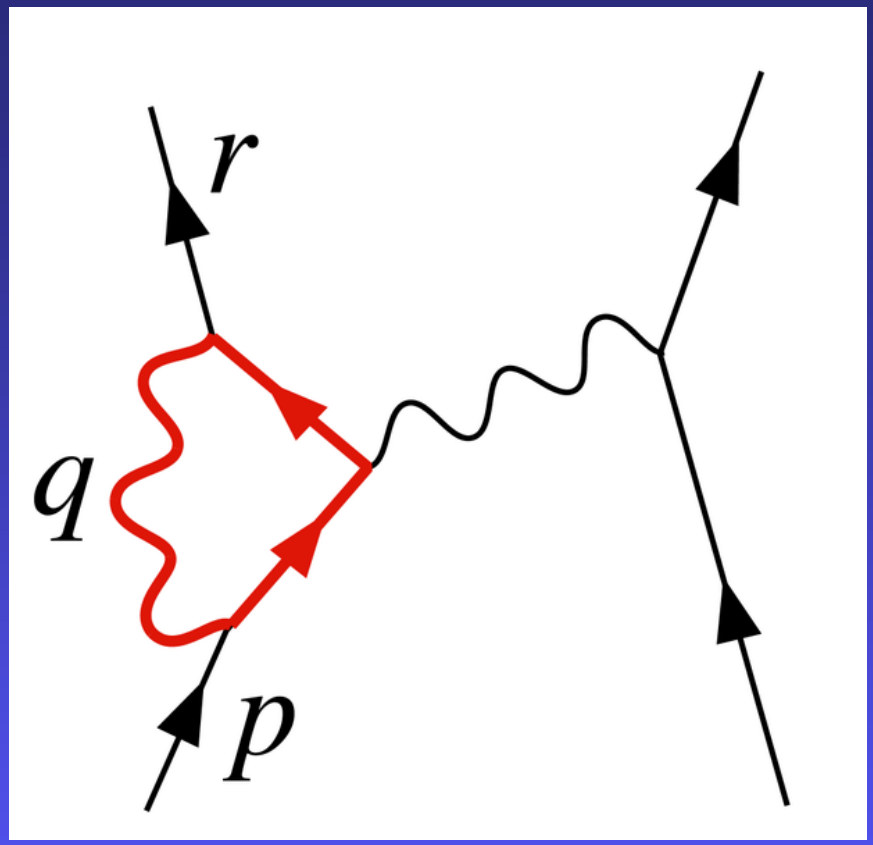


Figure 2. A diagram contributing to electron-electron scattering in QED. The loop has an ultraviolet divergence.

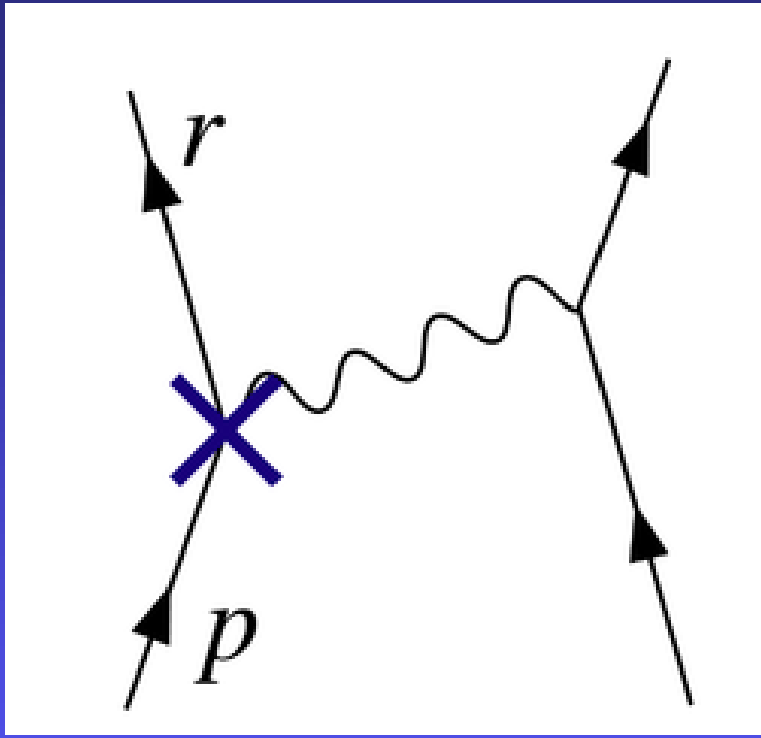


Figure 3. The vertex corresponding to the Z1 counterterm cancels the divergence in Figure 2.

Advantages

The new coupling constants could be smaller.

By repeated applications of the renormalization procedure, one could thus finally obtain

Free theory without interactions

One –dimensional Ising model

The successively interacted coupling coefficients "parameter flow" fixed point

Elimination of degrees of freedom is accompanied by a change of the underlying lattice spacing o length scale , one can anticipate that the fixed points are under certain circumstances related to Critical point.

Flow in the vicinity of these fixed point can yield information about the universal quantities in the neighborhood of the critical points..

Two –dimensional Ising model

Renormalization Group

Finally, the general structure of such transformations will be discussed with the derivation of scaling laws. A brief schematic treatment of continuous field-theoretical formulations will be undertaken following the Ginzburg–Landau theory.

The Method

What is it?

Density matrix renormalization group (DMRG) is a numerical technique for finding accurate approximations of the ground state and the low-energy excited states of strongly interacting quantum systems. Its accuracy is remarkable for one-dimensional systems with very little amount of computational effort. It is however limited by the dimensionality or range of interactions.

The method is kind of "iterative method" and is based on the truncation of the Hilbert space used to represent the Hamiltonian in a controlled way, keeping the most probable eigenstates!

The physical understanding of quantum many-body systems is hindered by the fact that the number of parameters describing the physical states grows exponentially with the number of particles, or size of the system.

More formally in a nutshell: DMRG method

- For large systems
- Accuracy comparable to exact results
- Variational and non-Perturbative
- No problems with frustration or fermions

It can calculate:

- ✓ All ground state properties (energies, correlation functions, gaps, moments)
- ✓ Finite temperature properties
- ✓ Classical systems at finite temperature
- ✓ Dynamical quantities (frequency dependent)
- ✓ Time evolution

Limitations:

Convergence depends on details of the system (dimensionality, boundary conditions, range of interactions) and efficient programming is very complicated.

Quantum Many-Body Problem

System of N quantum mechanical subsystems

Examples:

Hubbard Model: *an effective model for electrons in narrow band (eg, d or f electron metal ions). It is applicable for atoms, clusters, molecules, solids,…..*

One-tight binding band, local Coulomb interactions 4^N *degrees of freedom – states:* $|0\rangle$, $|\uparrow\rangle$, $|\downarrow\rangle$ *and* $|\uparrow\downarrow\rangle$

$$H = -t\sum_{<ij>}(a_i^+ a_j + a_j^+ a_i) + U\sum_i n_{i\uparrow} n_{i\downarrow}$$

Interesting ground state properties: (AFM at half-band filling, n=1), 1D: Luttinger liquid; 2D: d-wave superconductivity (n <1?) Dynamical properties like conductivity and temperature dependence are also quite interesting.

Heisenberg model:

$$H = -J \sum_{<ij>} S_i \cdot S_j$$

Strong coupling limit of the Hubbard model at n=1 Antiferromagnetic exchange $J=4t^2/U$

Localized QM spin degrees of freedom: $(2S+1)^N$ for N spin-S objects.

A model to describe quantum magnetism in most of the oxide materials or any system with localized spin orbitals.

Bethe-ansatz (closed form exact) solution exist only in 1D.

A good model for describing the parent phase of high-T_c cuprates

Ground state, dynamics and low-temperature properties quite interesting.

How does one study many-body interactions?

Analytic:

- ✓ Mean-field theories
- ✓ Strong and weak coupling expansions (perturbative methods)
- ✓ Field theoretical methods

Mostly uncontrolled

Numerical:

- ✓ Exact diagonalization
- ✓ Configuration Interactions and Coupled Cluster
- ✓ Quantum Monte Carlo
- ✓ Dynamical mean-field theory (DMFT)
- ✓ DMRG

Extremely involved, each method has its own difficulties

Microscopic understanding of systems for applications in magnetic, optical, electrical, mechanical, transport…..phenomena

What is RG Method?

What is RG Method?

The basic idea behind a renormalization group method is to apply a transformation to the Hamiltonian which eliminates unimportant degrees of freedom for the description of the system within a given energy range.

$$E - \delta E \leq \omega \leq E$$

dE is a small energy interval

For example, if we are interested in the low-energy states of a system with a energy cut-off E, one integrates out energy modes with energy

Then we rescale the parameters of the new system so that it reproduces the previous one.

Given a H of a system with N variables, a RG transformation R_a is a mapping in the Hamiltonian space which maps H to H' : H'=Ra(H). H' now has N' variables where N'=N/a which is less than N.

RG transformation must be unitary; i.e., it has to preserve Z=Tr exp(-H/kT) so that $Z_{N'}[H'] = Z_N[H]$.

However, an exact transformation is not possible.

Wilson and others:

Work in Fourier space and use a perturbative scheme in order to analytically solve this problem.

Extremely successful method for solving

Kondo problem and Anderson Impurity problem

- *K. G. Wilson and F. Kogut, J. Phys. Rep C **12**, 75 (1974).*
- *K. G. Wilson, Rev. Mod. Phys. **43**, 773 (1975).*
- *H. R. Krishnamurthy, J. W. Wilkins and K. G. Wilson, Phys. Rev. B **21**, 1044 (1980).*

Numerical Importance

Numerical Renormalization Group (K. G. Wilson, 1974).

Can it be applied for Correlated Lattice problem?

Idea behind all lattice renormalization group methods is to enlarge the system iteratively but keeping only a constant number of basis states.

Integrate out the degrees of freedom numerically for obtaining low-energy properties.

Let H be a Hamiltonian describing an interacting electronic systems on a lattice with L sites. Each site has four states: |0>, |down>, |up> & |2>.

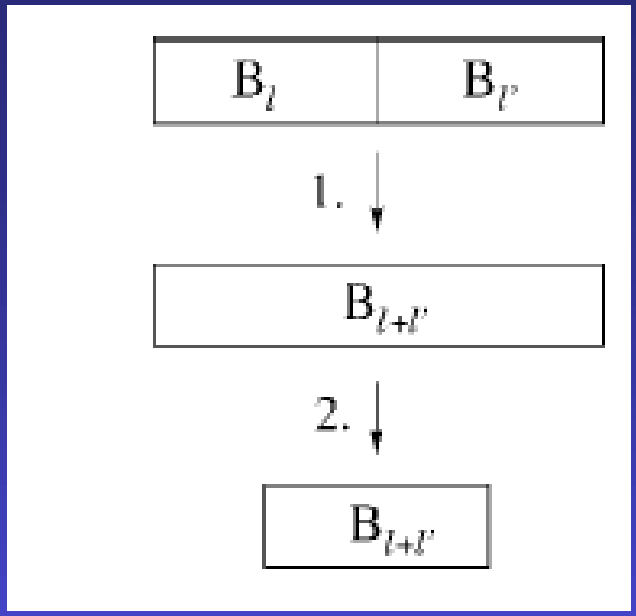
The dimension of the Hilbert space for L=100 with $N_{up}=N_{down}=50$ is 10^{58}, which is not intractable numerically. The idea is to obtain the Low-energy eigen-states of this system keeping only a small number ofstates, say 100.

REAL Space algorithm

Let B_l be a block describing the first l sites for which we only keep m states to describe the H.
The same goes for $B_{l'}$ block also with m' states.

When we put these two blocks together, the H of the new block $B_{l+l'}$ has dimensions mm'.

$$H_{l+l'} = H_l + H_{l'} + \sum C^s A^s \otimes B^s$$



Solve $H_{l+l'}$ and keep only lowest m energy eigenstates

- Isolate a finite system (N)
- Diagonalize numerically
- Keep **m** lowest energy eigenstates
- Add another finite system (N)
- Solve ($2N$) system and iterate the process.

By iterating this procedure, one obtains recursion relations on the set of coupling constants which define the Hamiltonian and the properties in the thermodynamic limit.

The message:

Low-energy states are most important for low-energy behavior of larger system

However, only for Kondo lattice or Anderson impurity models

Very bad for other quantum lattice models:

- ✓ *Hubbard (Bray, Chui, 1979)*
- ✓ *Heisenberg (White, 1992, Xiang and Gehring, 1992)*
- ✓ *Anderson localization (Lee, 1979)*

Kondo impurity problem: *Hierarchy in the matrix elements; Boundary conditions seem not important.*

Just have a look for a tight-binding model: $2t_{ii} - t_{i,\,i+1} - t_{\,i,\,i-1}$

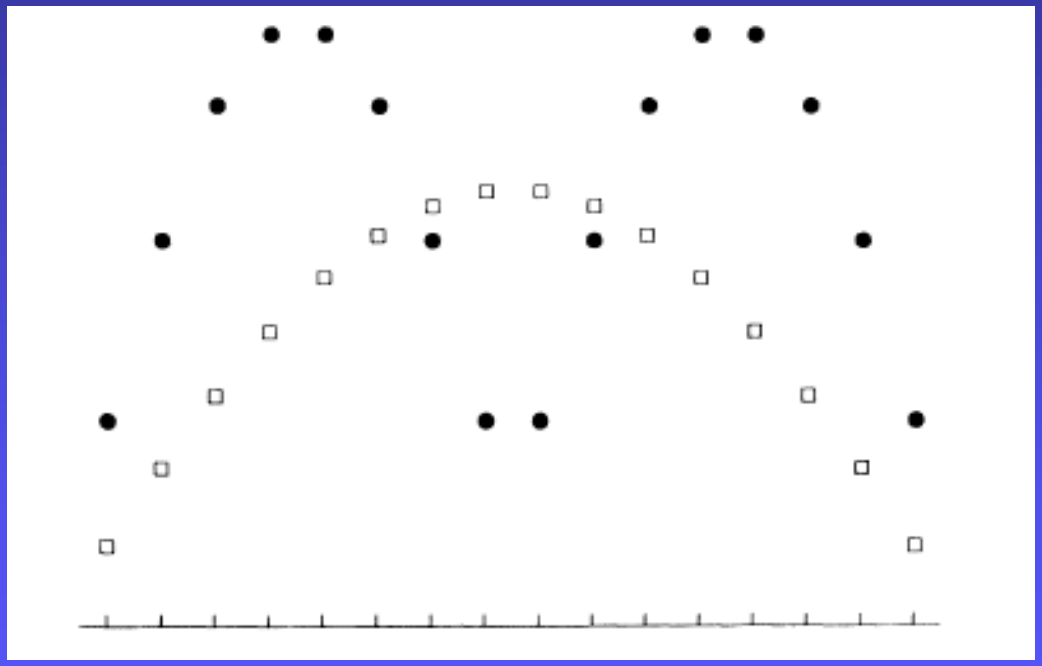
$$H = \left(\begin{array}{cc|cc} 2 & -1 & 0 & 0 \\ -1 & 2 & -1 & 0 \\ \hline 0 & -1 & 2 & -1 \\ 0 & 0 & -1 & 2 \end{array}\right)$$

If one puts two blocks together: does not represent the full system

Another way….

Two same size boxes (of length L, 1D, 1-electron problem)

Will putting together the ground states of L-length box give rise to the ground state of box of size 2L? NO



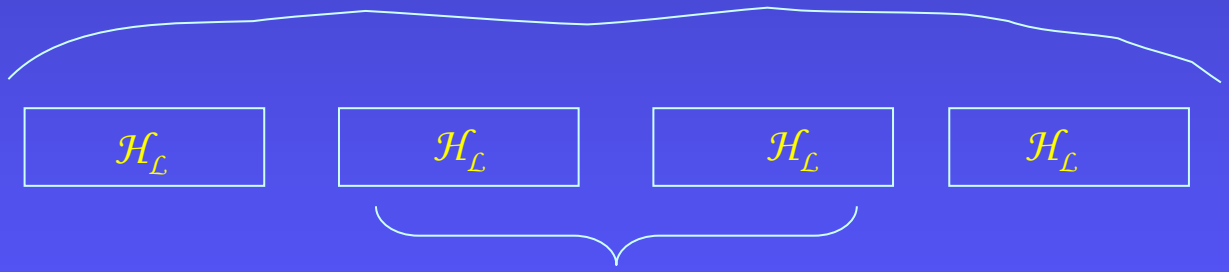
Treatment of boundary becomes critical:

Gr states of a chain of 16 atoms (open) and two 8 atoms chains (filled)

When boundary becomes critical: (White and Noack, 1992)

Use combinations of boundary conditions (BCs):

- Diagonalize a block, $\mathcal{H}_L$ with different combinations of BCs.
- Use orthogonalized set of states as new basis.
- Fluctuations in additional blocks allow general behavior at boundaries.



- ✓ Diagonalize superblock composed of **n** blocks (each block size L).
- ✓ Project wavefunctions onto size 2L block, orthogonalize.
- ✓ Exact results as **n** becomes large

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Density Matrix Formulation for Quantum Renormalization Groups

Steven R. White

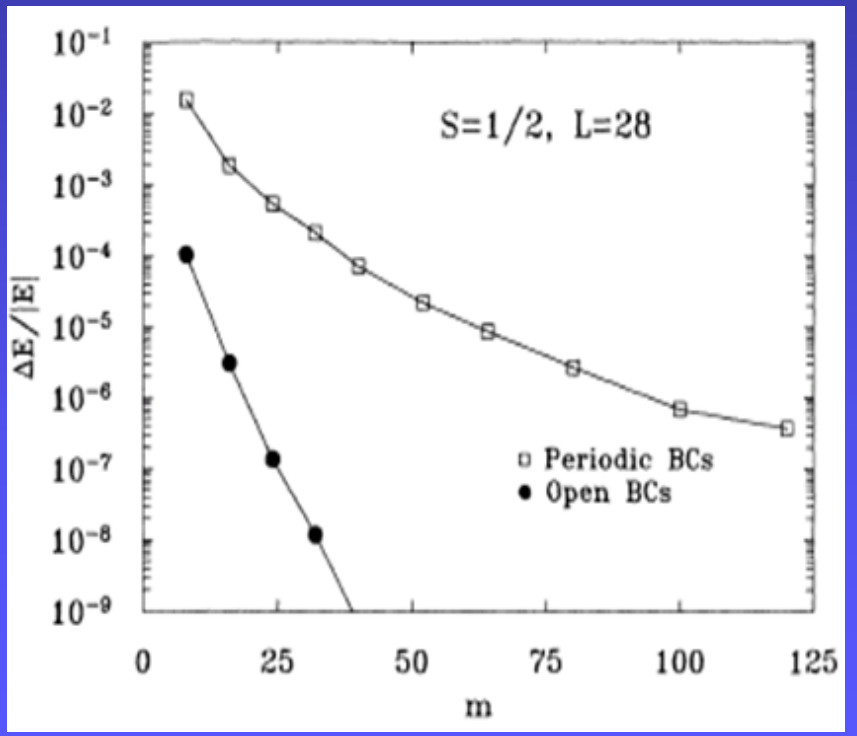
Department of Physics, University of California, Irvine, California 92717

(Received 22 May 1992)

A generalization of the numerical renormalization-group procedure used first by Wilson for the Kondo problem is presented. It is shown that this formulation is optimal in a certain sense. As a demonstration of the effectiveness of this approach, results from numerical real-space renormalization-group calculations for Heisenberg chains are presented.

The total number of states is 2^{28}

This amazing accuracy is achieved by just keeping only ~100 states!



Relative error vs no of states kept

[1] S. White, Phys. Rev. Lett. 69, 2863 (1992)
[2] Density Matrix Renormalization, edited by I. Peschel, X. Wang, M. Kaulke and K. Hallberg
(Series: Lecture Notes in Physics, Springer, Berlin, 1999)
[3] S. White, Phys. Rev. B 48, 10345 (1993)
[4] J. Bray and S. Chui, Phys. Rev. B 19, 4876 (1979)
[5] C. Pan and X. Chen, Phys. Rev. B 36, 8600 (1987); M. Kovarik, Phys. Rev. B 41, 6889 (1990)
[6] T. Xiang and G. Gehring, Phys. Rev. B 48, 303 (1993)
[7] K. Wilson, Rev. Mod. Phys. 47, 773 (1975)
[8] S. White and R. Noack, Phys. Rev. Lett. 68, 3487, (1992); R. Noack and S. White, Phys. Rev.
B 47, 9243 (1993)
[9] J. Gaite, Mod. Phys. Lett. A16, 1109 (2001)
[10] R. Noack and S. White in Ref. [2], Chap. 2(I)
[11] M. Mart´in-Delgado, G. Sierra and R. Noack, J. Phys. A: Math. Gen. 32, 6079 (1999)

Use of density matrix

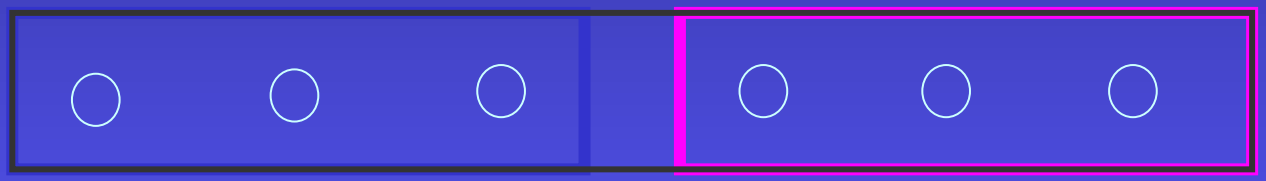
Use of density matrix

Steven White, 1992

Divide the many-body system: how?

Density matrix projection

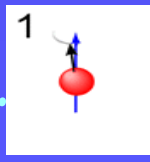
Divide the whole system into a subsystem and an environment



We know the eigenfunction for the whole system: how to describe the subsystem block best?

Reduced density matrix for the subsystem block:

Trace over states of the environment block, all many-body states.



Applications

Applications:

- Strongly correlated electronic systems
- Nuclear Physics
- Quantum information theory
- Quantum Chemistry
- Classical Statistical Physics
- Soft condensed matter Physics

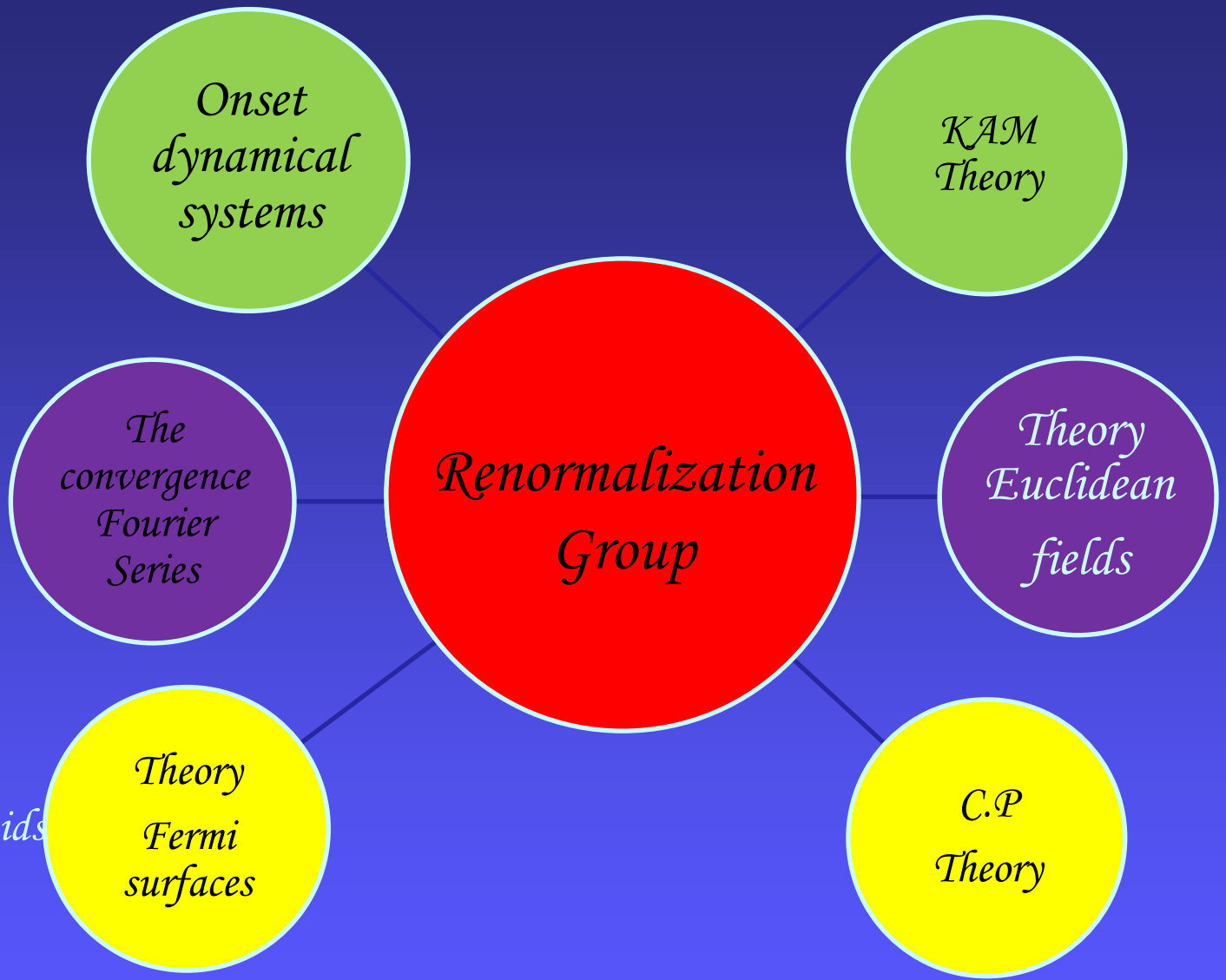
Total number of papers published with the string "density matrix renormalization" in their title or abstract from 1993 to 2005 is more than **5,000** (obtained from ISI database) and 2006-2012 aprox. 3000 more.

Distributed Multimedia Research Group
Design Methodology Research Group
Direct Marketing Resource Group
Data Management Resource Group

All are DMRG indeed !

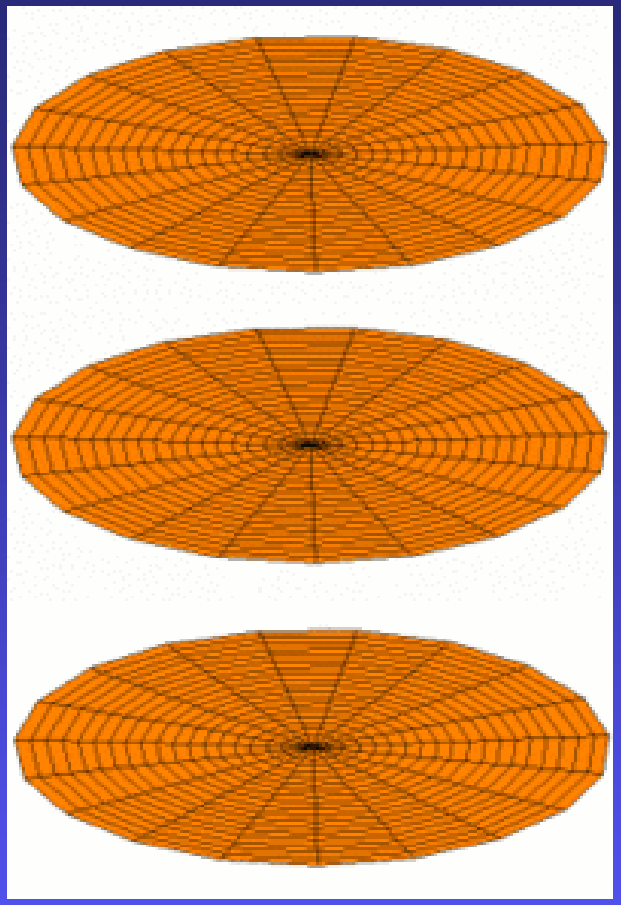
Groupe de Renormalisation de la Matrice Densite (GRMD) !!!

Solid State Physics

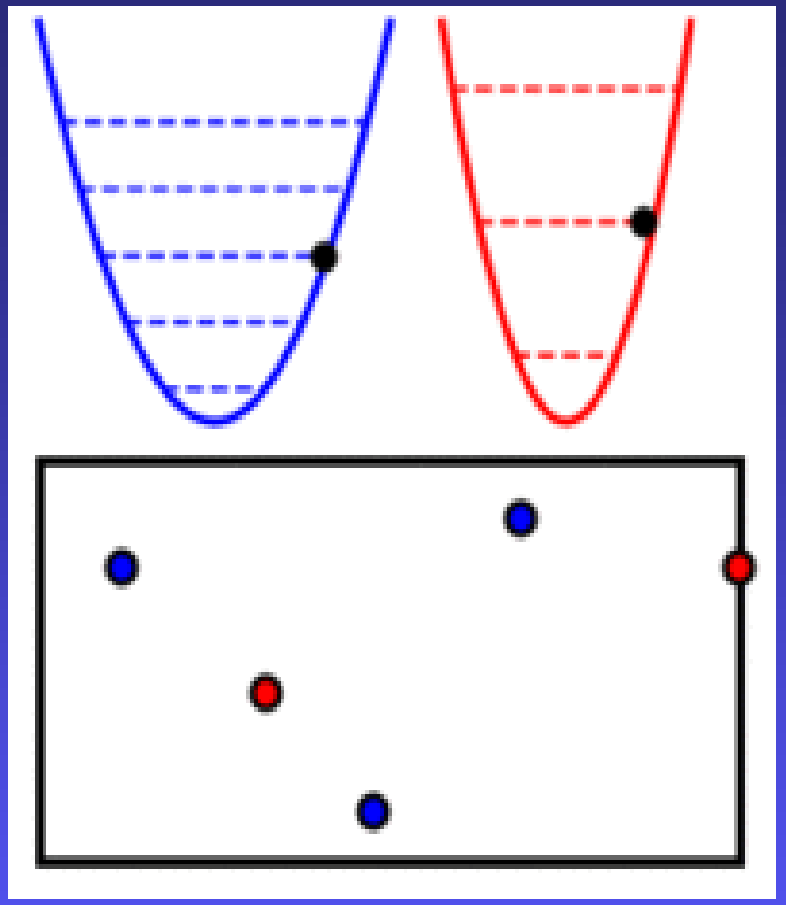


- Fermi Liquids

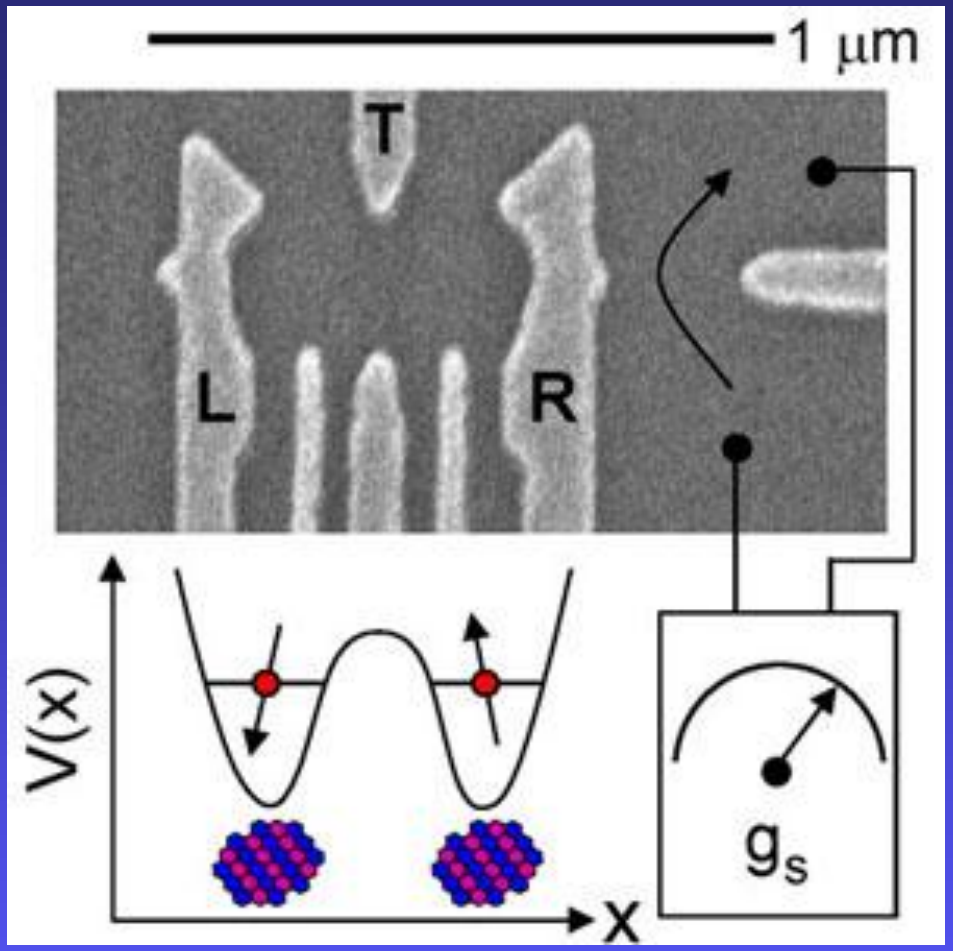
La renormalización, también es una herramienta habitual en el campo de la física de la materia condensada, donde se utiliza para describir las excitaciones colectivas de sistemas de muchas partículas, y explicar fenómenos como la superconductividad, la superfluidez o el efecto Hall cuántico



Modos normales. Los modos normales de un sistema físico son sus vibraciones colectivas más simples, como las de esta membrana elástica.

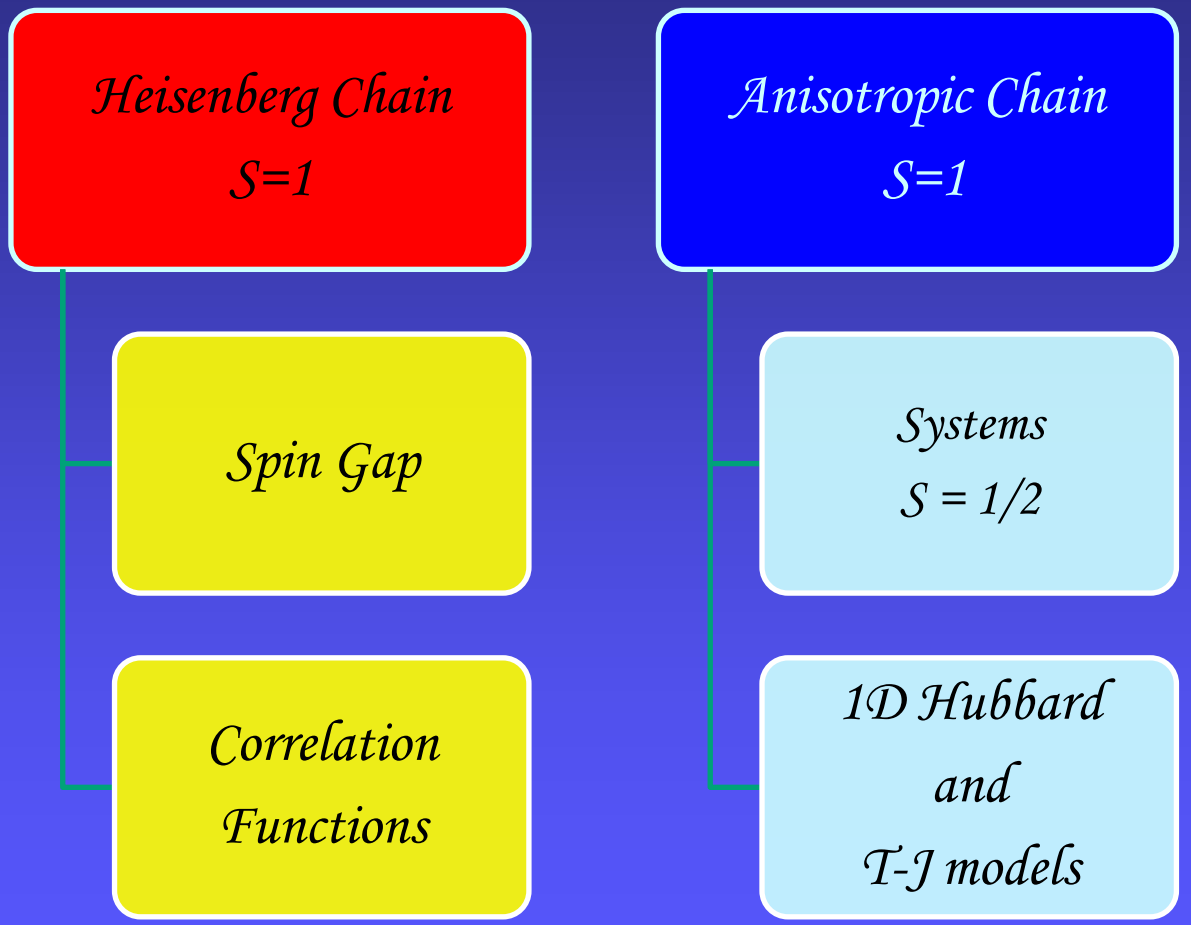


Segunda cuantización. Un sistema de dos osciladores cuánticos es equivalente a un sistema con un número variable de partículas de «dos clases».



Gate defined double quantum dot fabricated from a GaAs/AlGaAs 2-dimensional electron gas wafer. The number of electrons in the double quantum dot is determined by measuring the quantum point contact charge sensor conductance, gS. Trapped electrons are coupled to ~106 lattice nuclei through the contact hyperfine interation.

Spin Wave Theory



Renormalization group approach to the spin-1 Bose gas

Gergely Szirmai

Research Group for Statistical Physics of the Hungarian Academy of Sciences, Pázmány Péter Sétány 1/A, Budapest, H-1117

June 13, 2010

Abstract. A field theoretical renormalization group approach at two loop level is applied to the homogeneous spin-1 Bose gas in order to investigate the order of the phase transition. The beta function of the system with $d = 4 - \epsilon$ dimensions is determined up to the third power of the coupling constants and the system's free energy on the border of the classical stability is given in next to leading order. It is found that the phase transition of the interacting spin-1 Bose gases with weak spin-dependent coupling constant values is of first order.

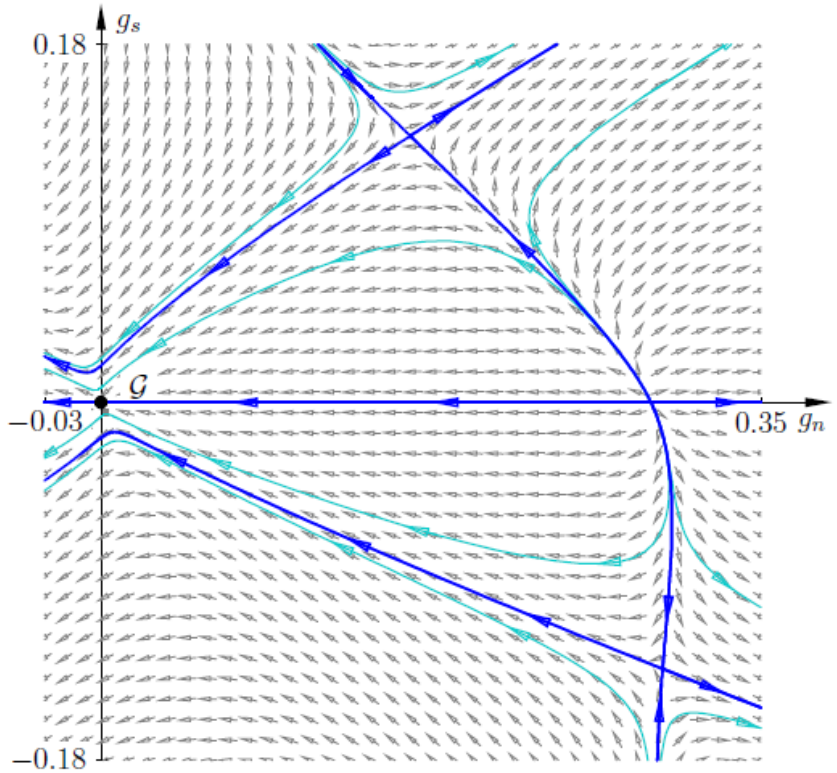


Fig. 4. The flow diagram and fixed point structure at $d = 4$ ($\epsilon = 0$).

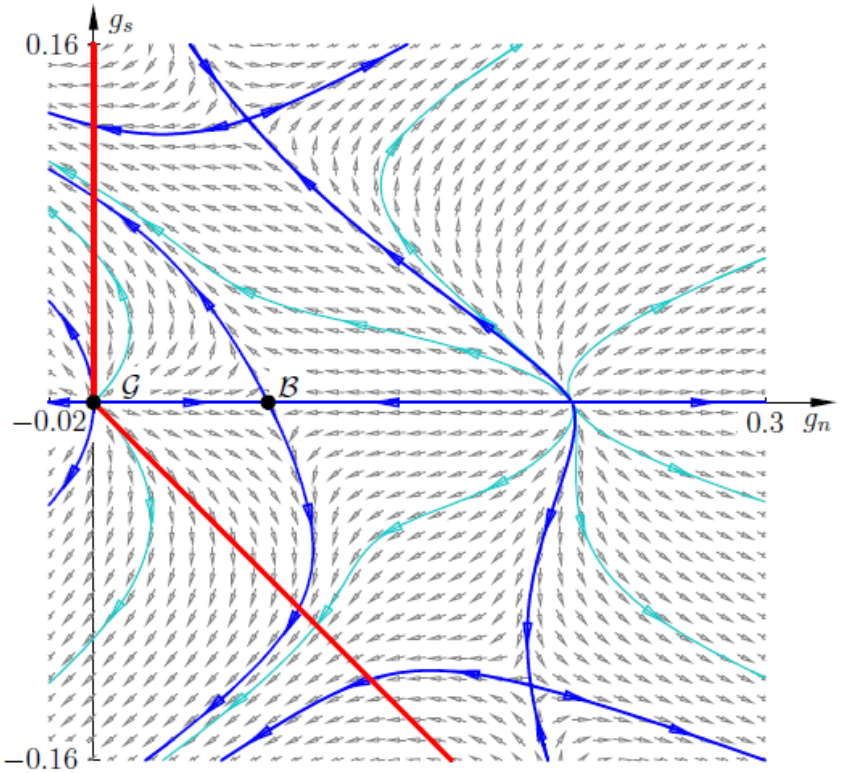
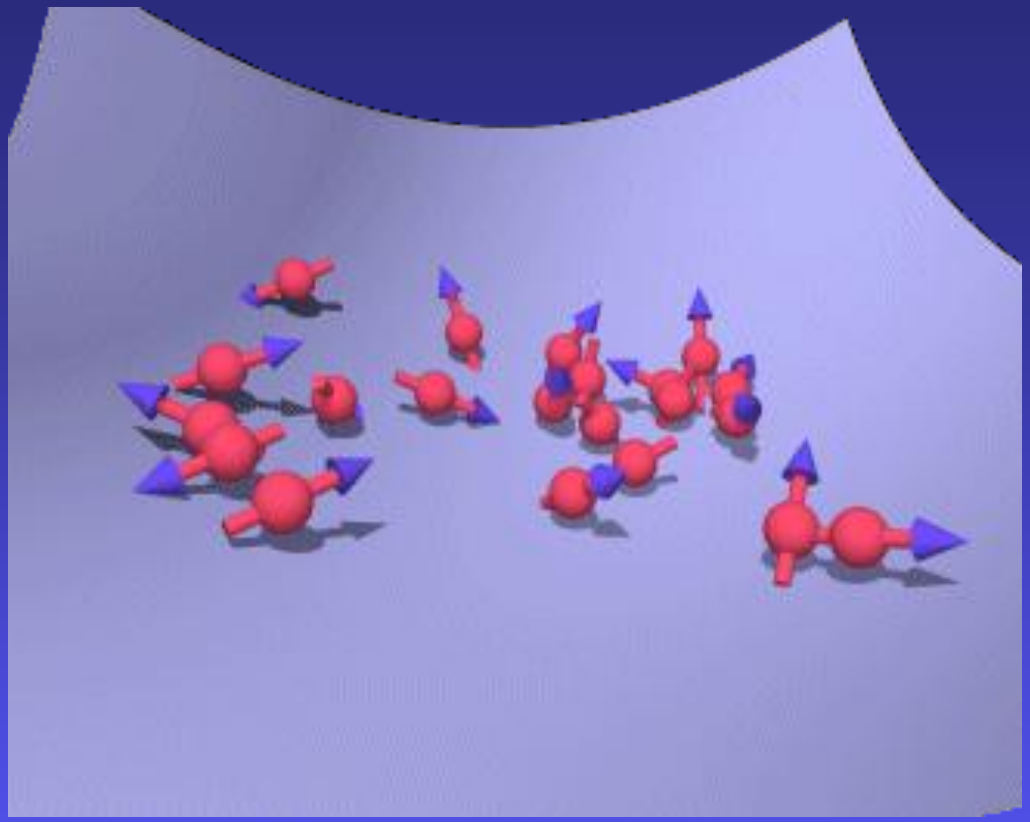
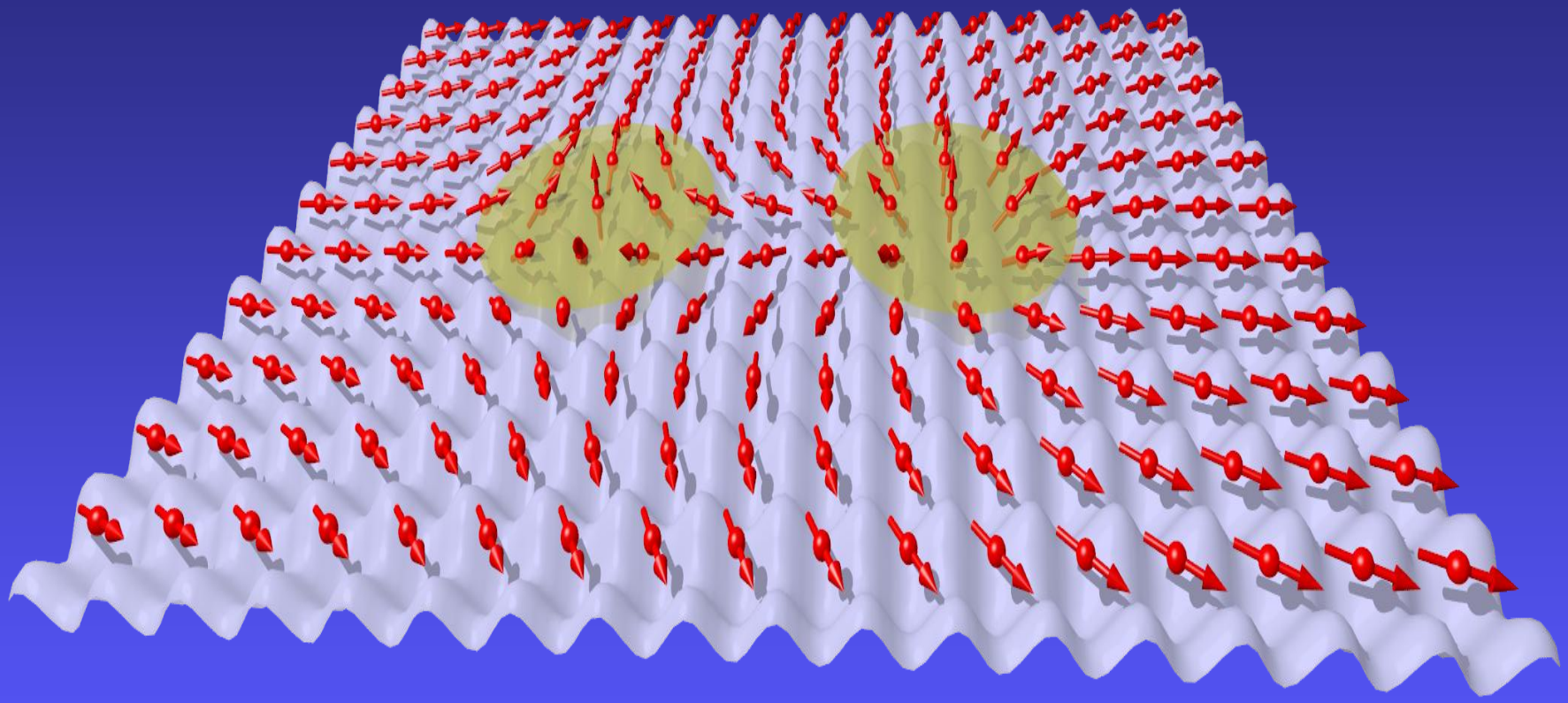


Fig. 5. The flow diagram and fixed point structure at $d < 4$ (for $\epsilon = 0.4$). The red lines indicate the boundary of the stability wedge of the zeroth order contribution of the free energy (see below).





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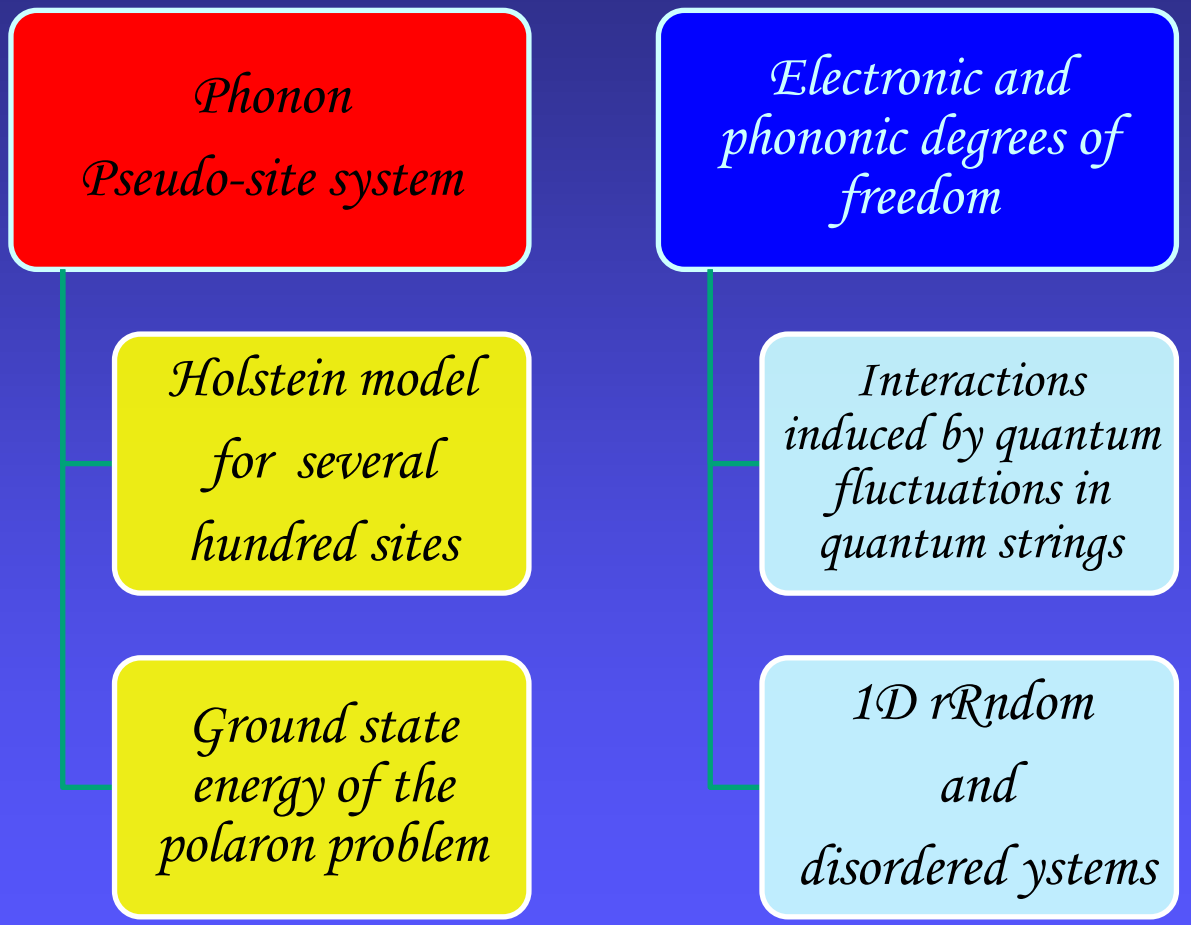
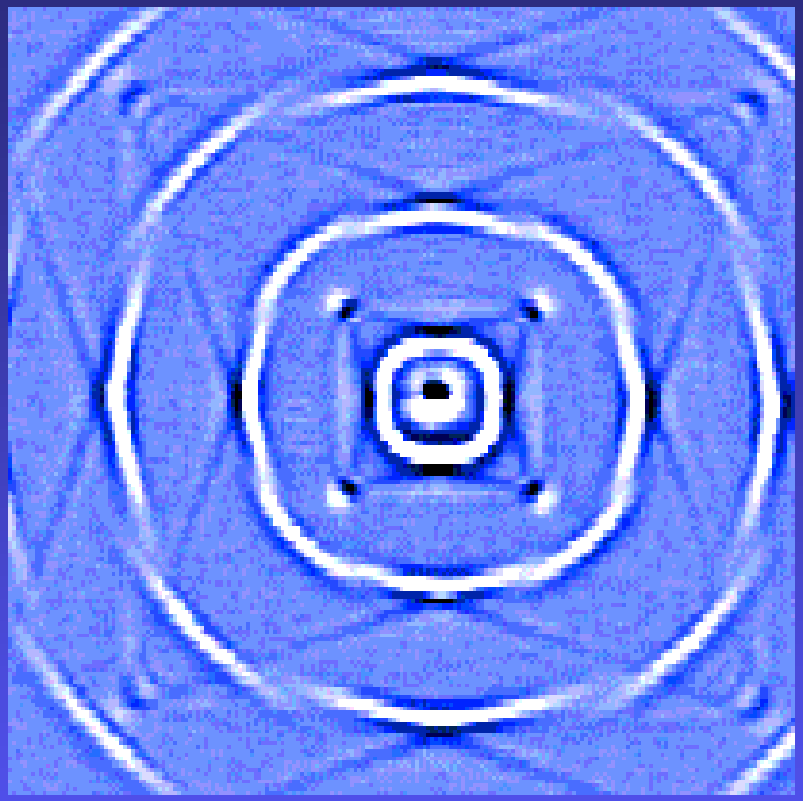
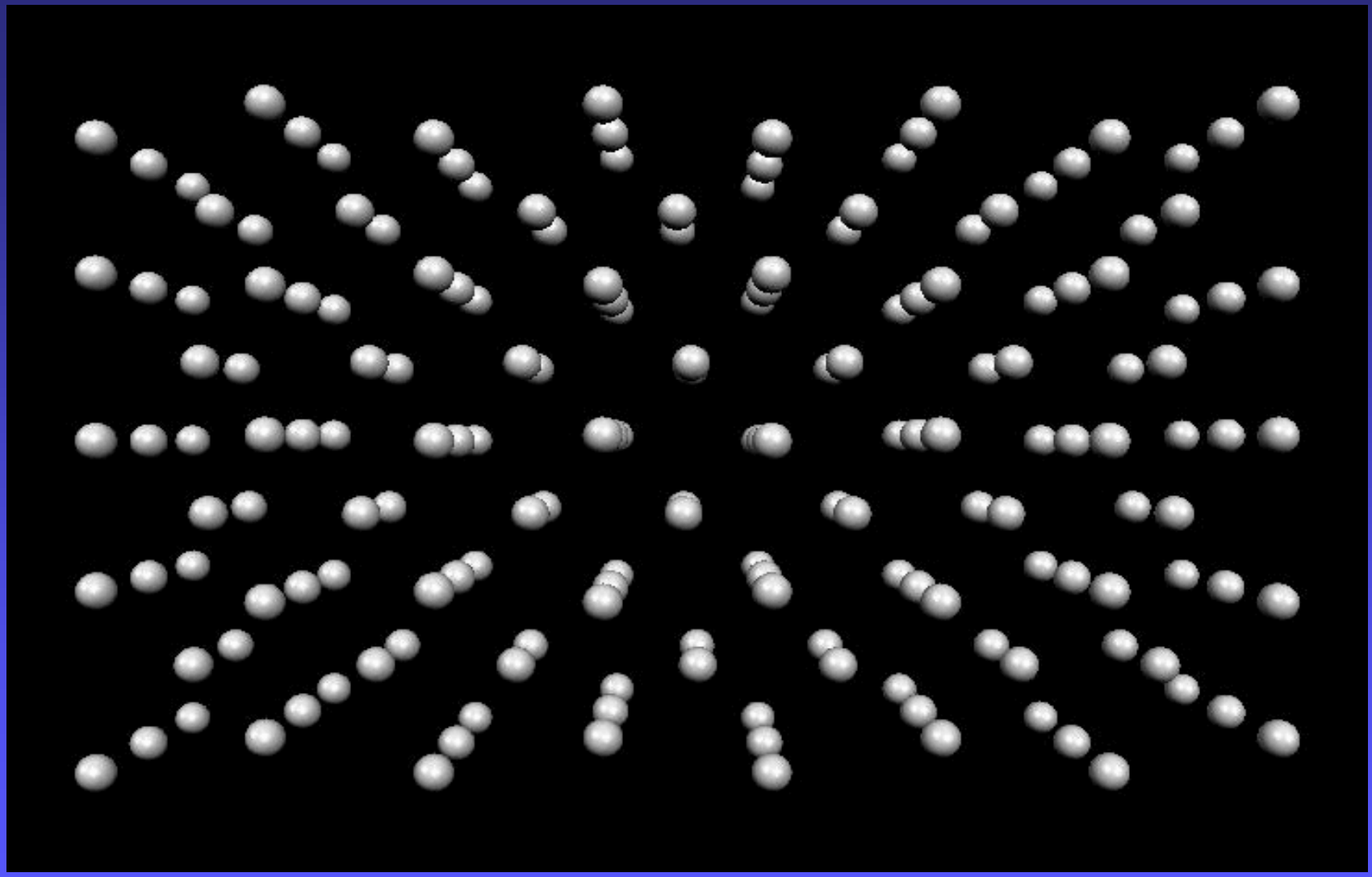
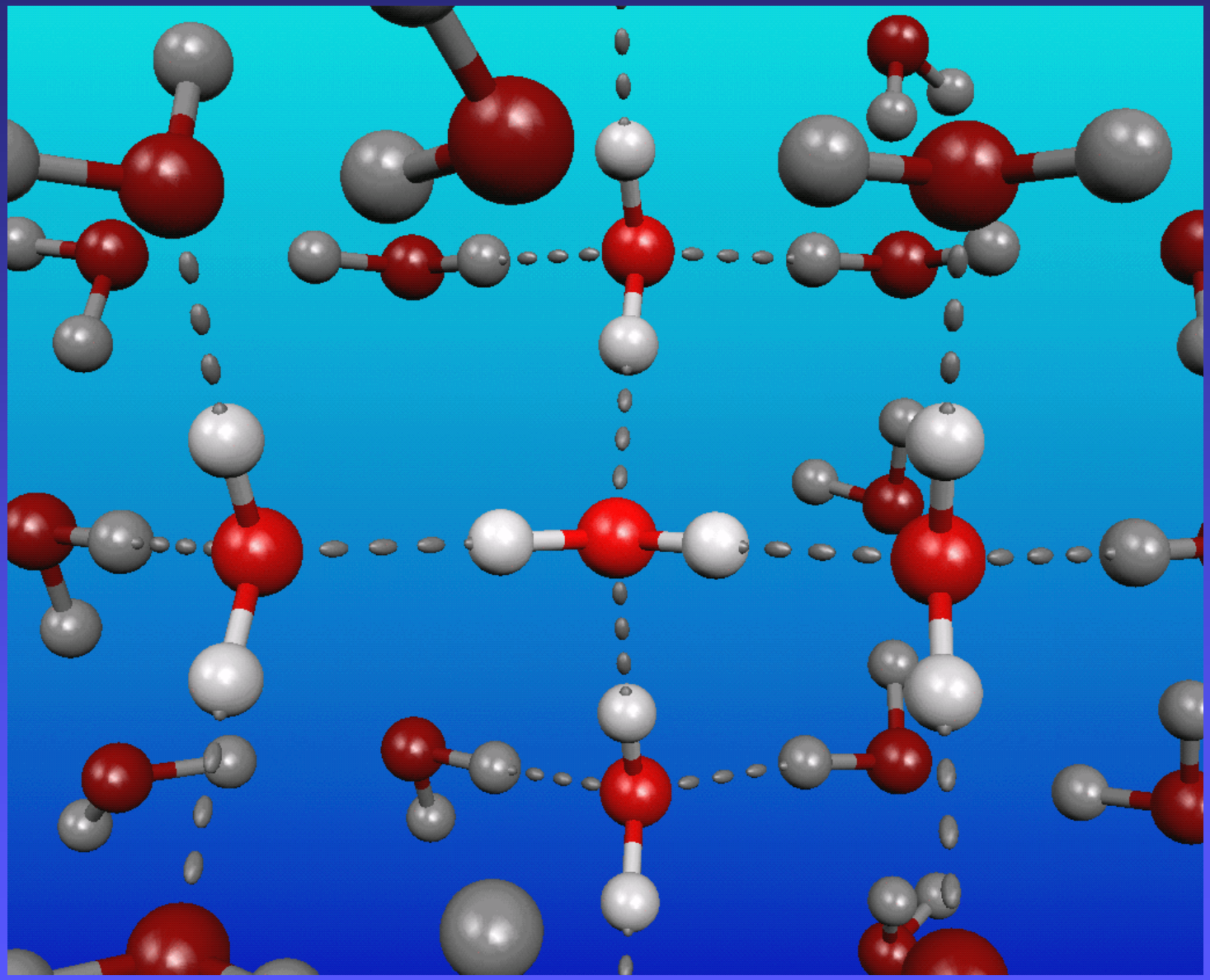
Phonons, bosons and disorder









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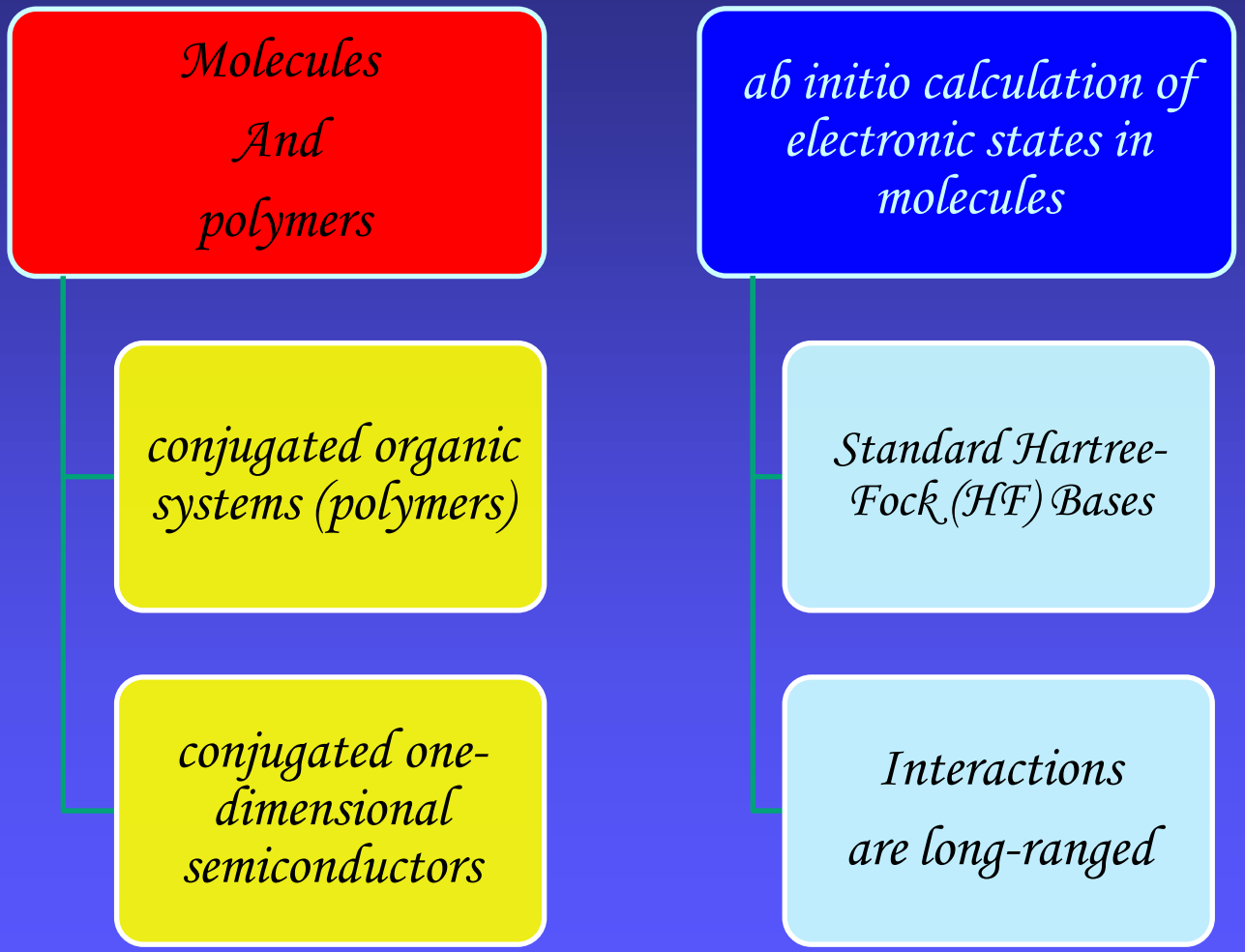
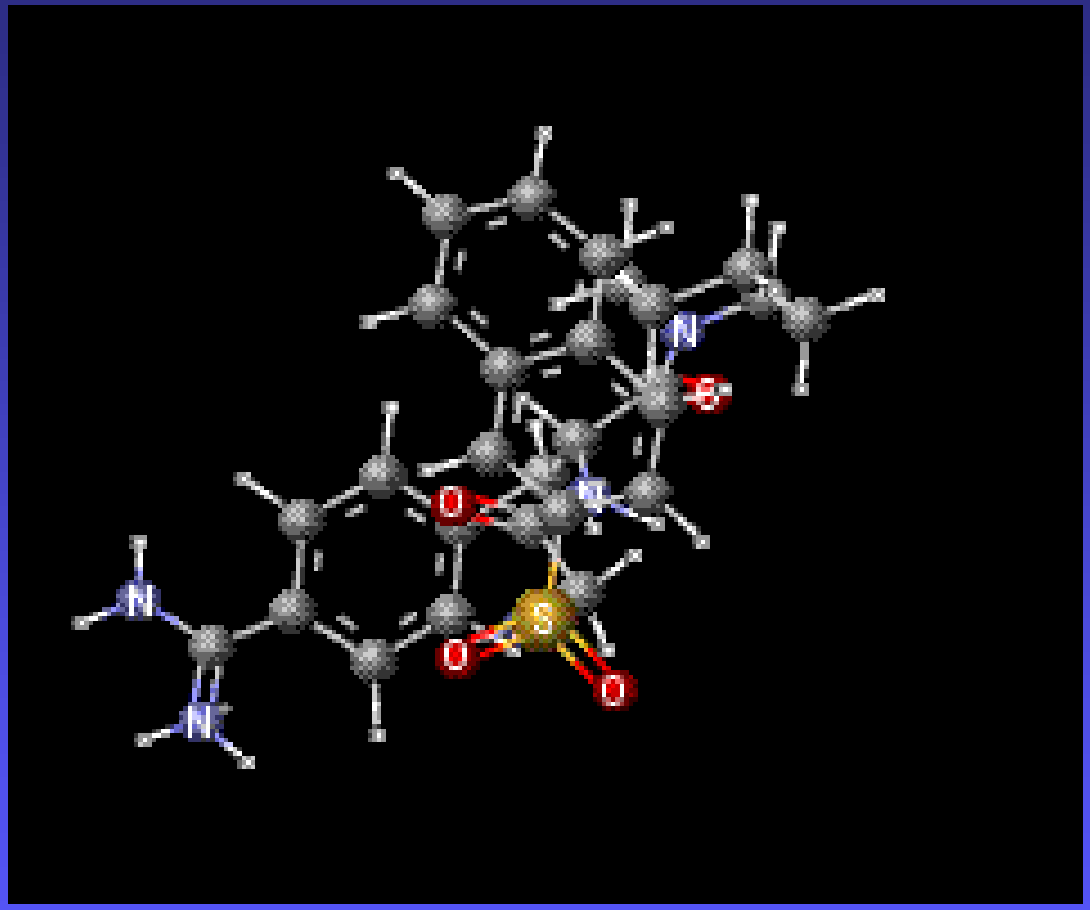
Molecules and Quantum Chemistry

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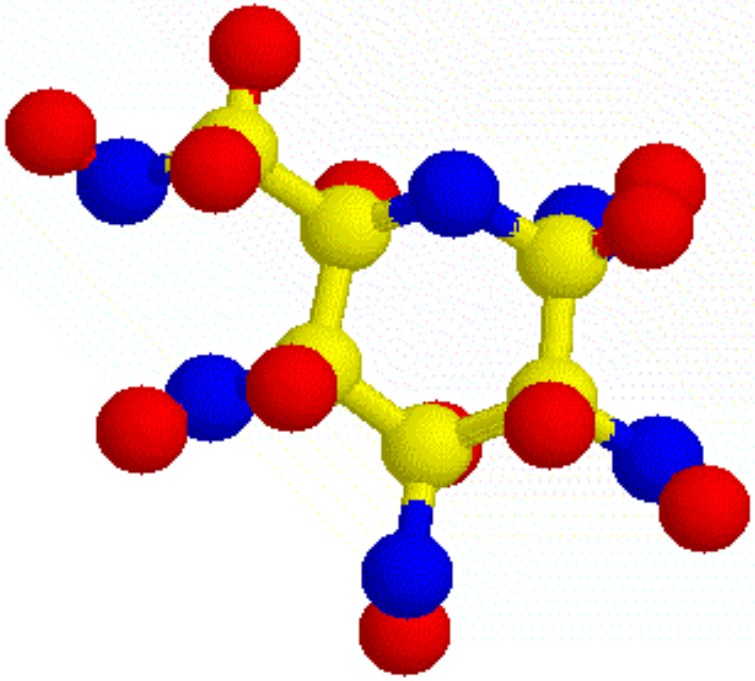

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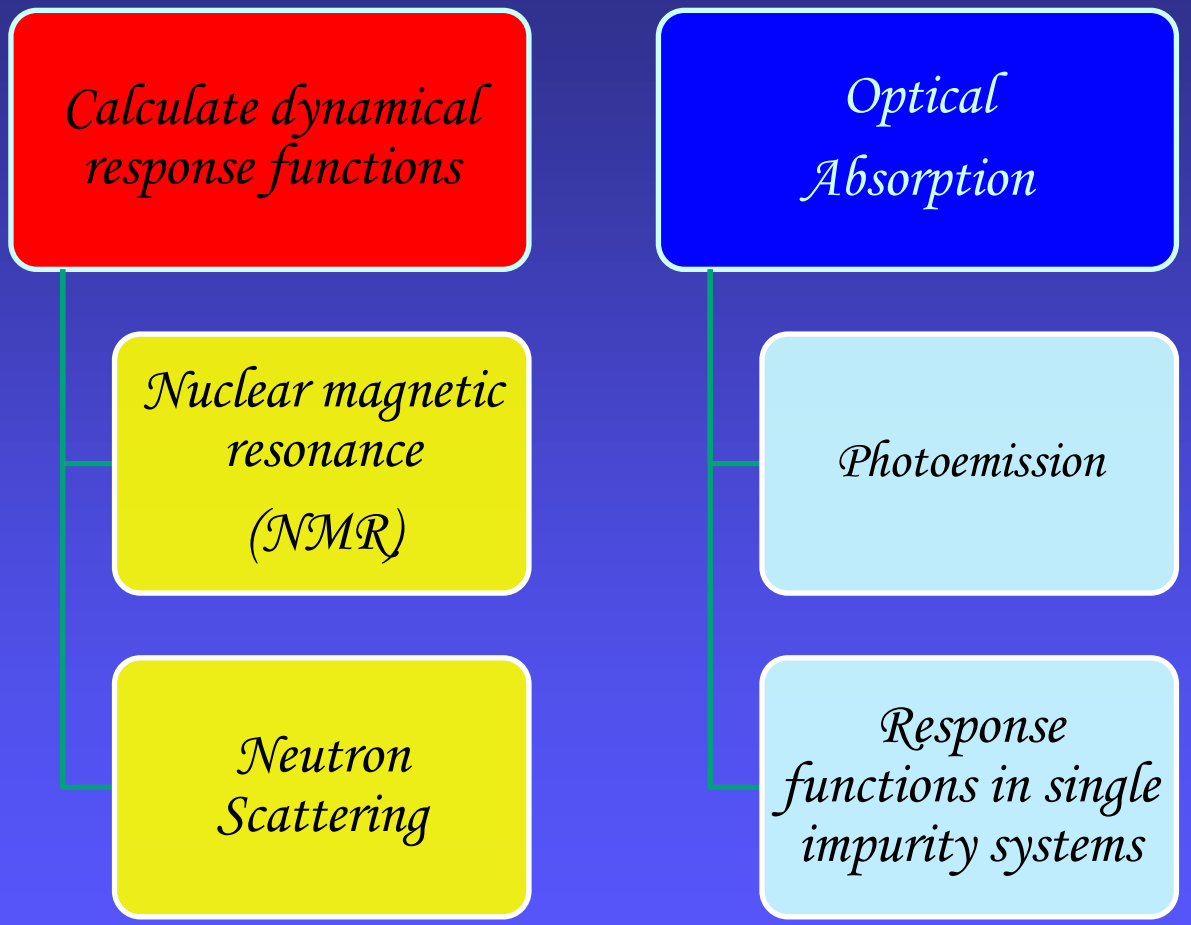
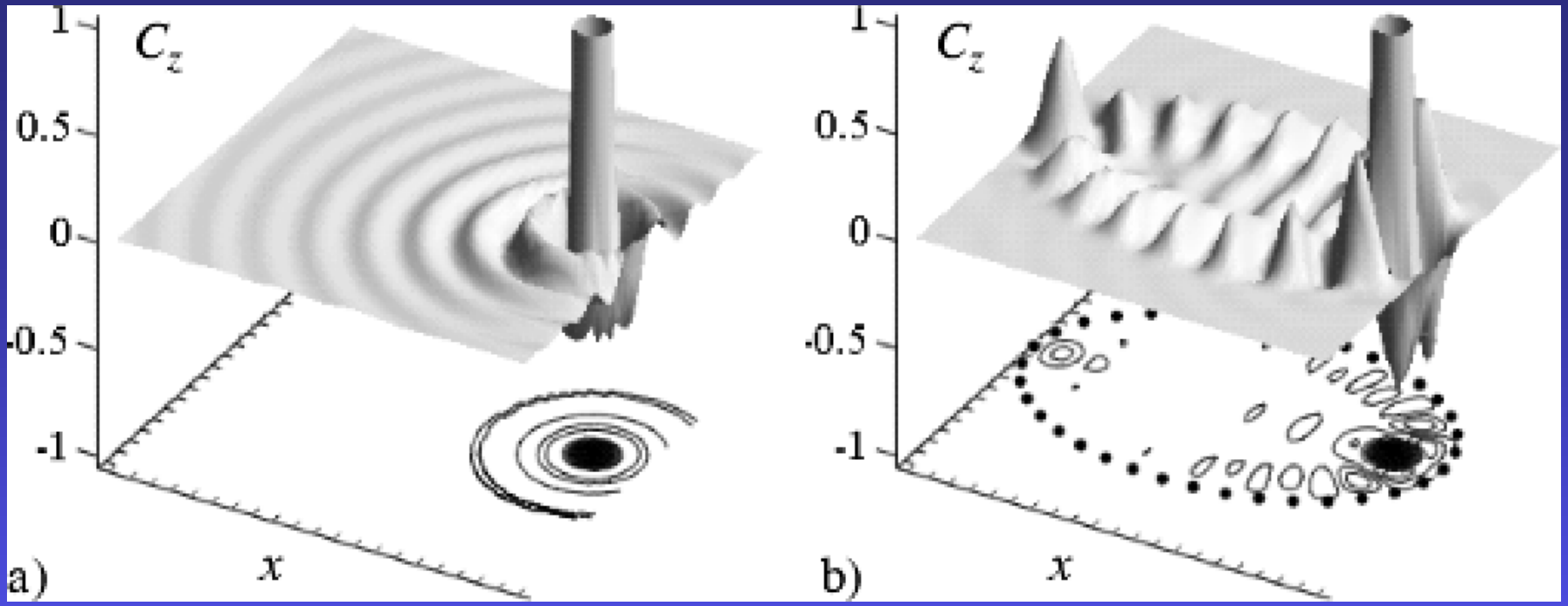
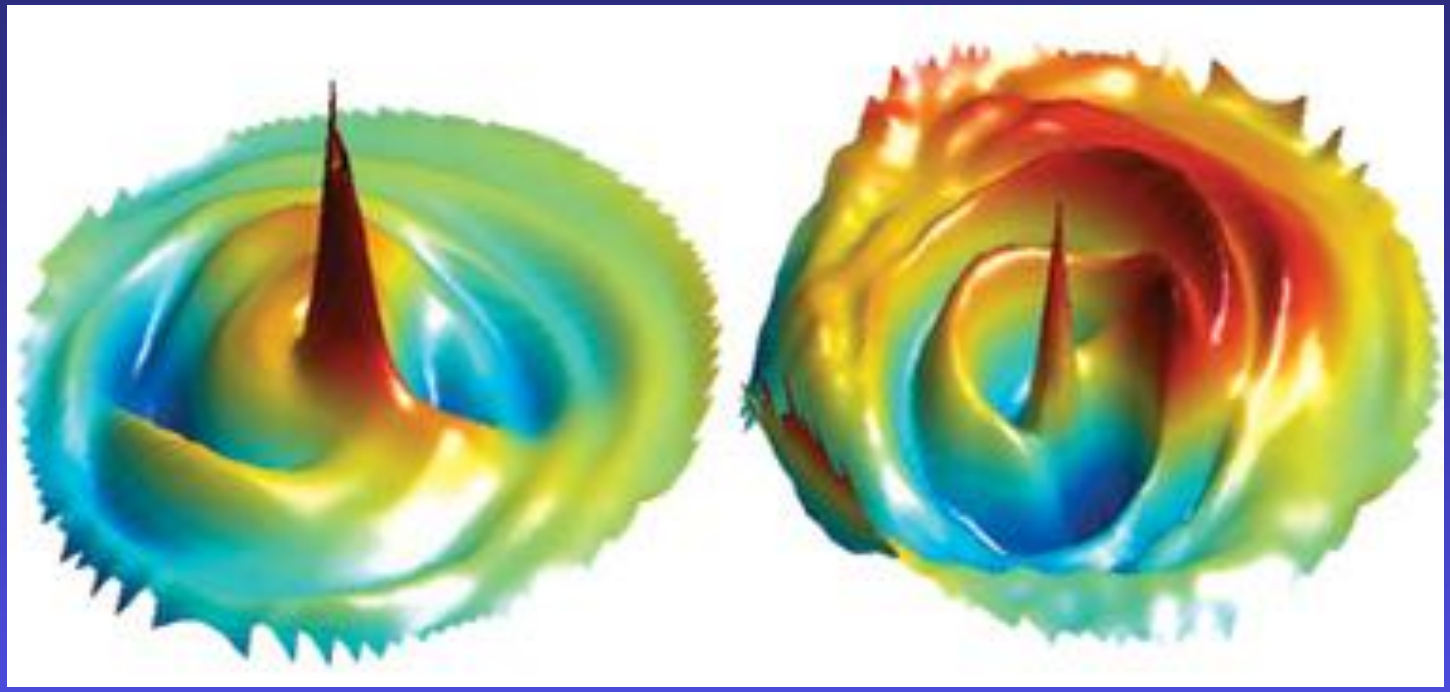
Dynamical correlation functions





Spin correlation functions Cz between the impurity and conduction band



Spin correlation functions Cz between the impurity and conduction band

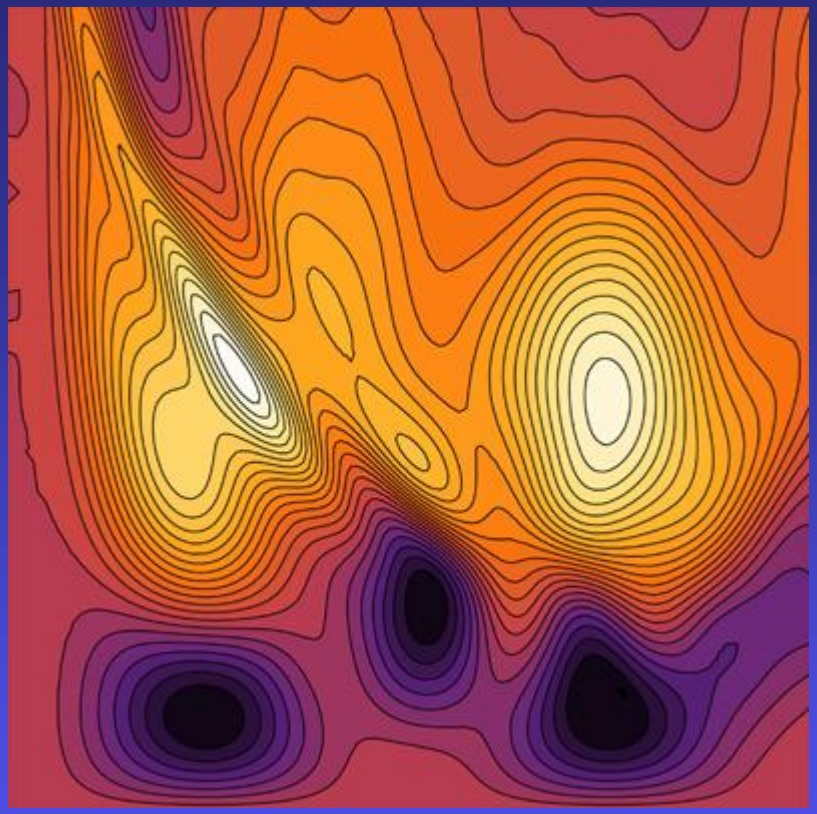


Image from "Passing quantum correlations to qubits using any two-mode state" [Mauro Paternostro, Gerardo Adesso, and Steve Campbell, Phys. Rev. A 80, 062318 (2009)]

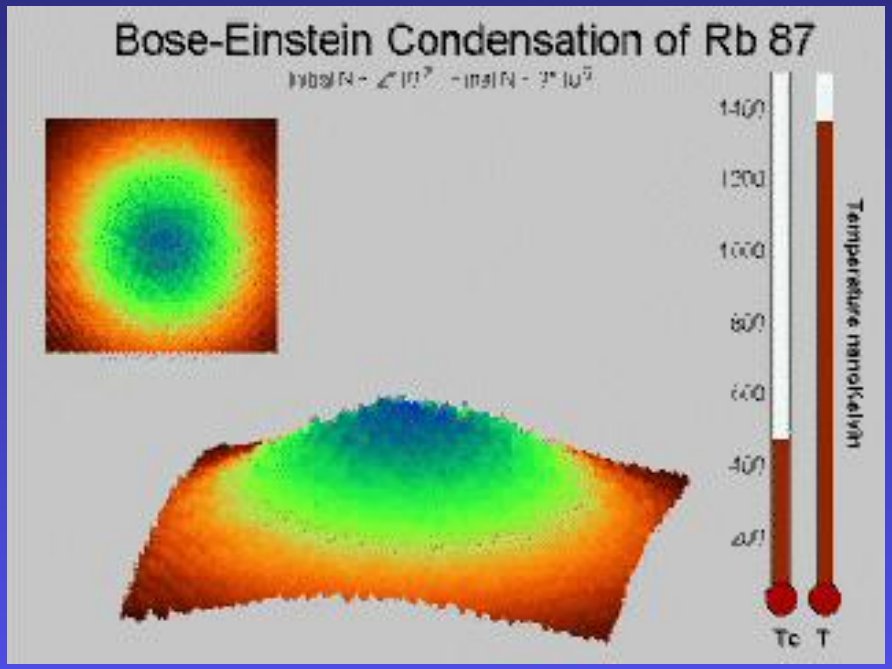
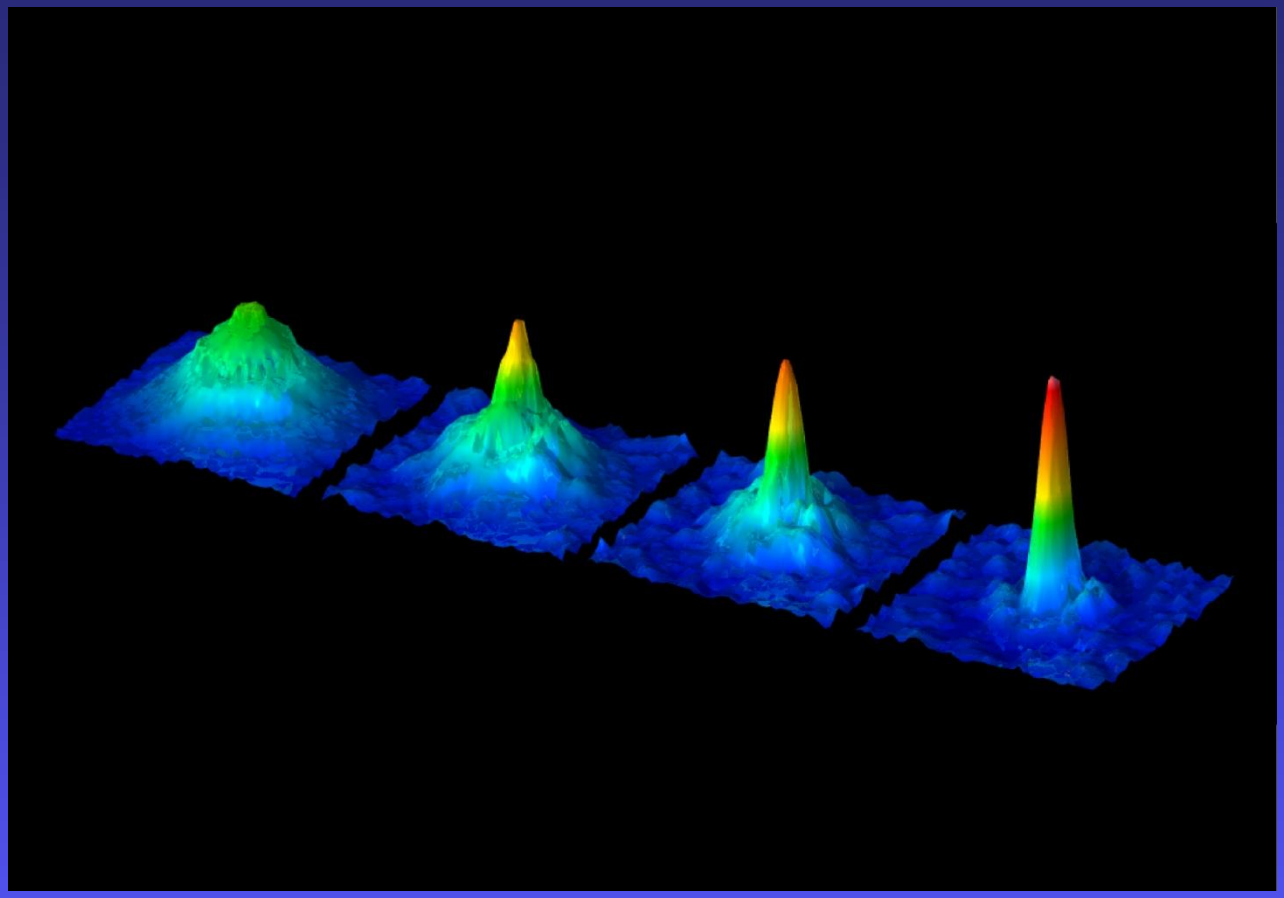
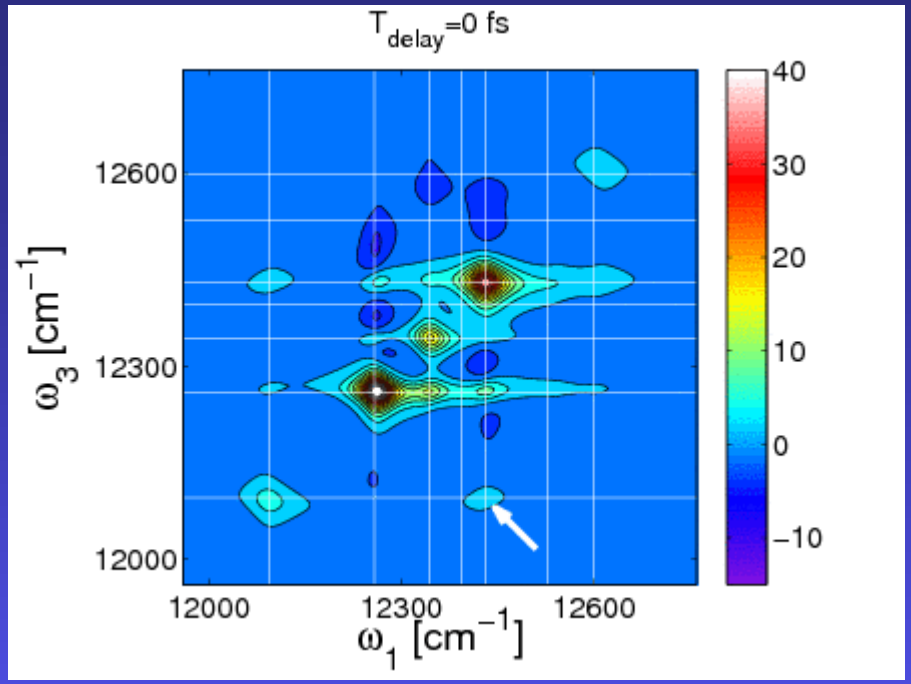


Image from "Passing quantum correlations to qubits using any two-mode state" [Mauro Paternostro, Gerardo Adesso, and Steve Campbell, Phys. Rev. A 80, 062318 (2009)]



BEC in a dilute atomic gas, extremely low temperatures are required. Our experimental setup employs a combination of laser cooling and evaporative cooling to produce cold and dense atomic clouds in a vacuum system. A double magneto-optical trap system captures and cools up to 6x 109 87Rb atoms using laser light.



he animation shows how peaks in the 2d echo-spectra are oscillation and changing for various delay times. For a full explanation, see Modelling of Oscillations in Two-Dimensional Echo-Spectra of the Fenna-Matthews-Olson Complex by B.Hein, C. Kreisbeck, T. Kramer, M. Rodríguez, New J. of Phys., 14, 023018 (2012), open access.

Density matrix renormalization group approach of the spin-boson model

Hang Wong* and Zhi-De Chen†
Department of Physics, Jinan University, Guangzhou 510632, China

We propose a density matrix renormalization group approach to tackle a two-state system coupled to a bosonic bath with continuous spectrum. In this approach, the optimized phonon scheme is applied to several hundred phonon modes which are divided linearly among the spectra. Although DMRG cannot resolve very small energy scales, the delocalized-localized transition points of the two-state system are extracted by the extrapolation of the flow diagram results. The phase diagram is compared with the numerical renormalization group results and shows good agreement in both Ohmic and sub-Ohmic cases.

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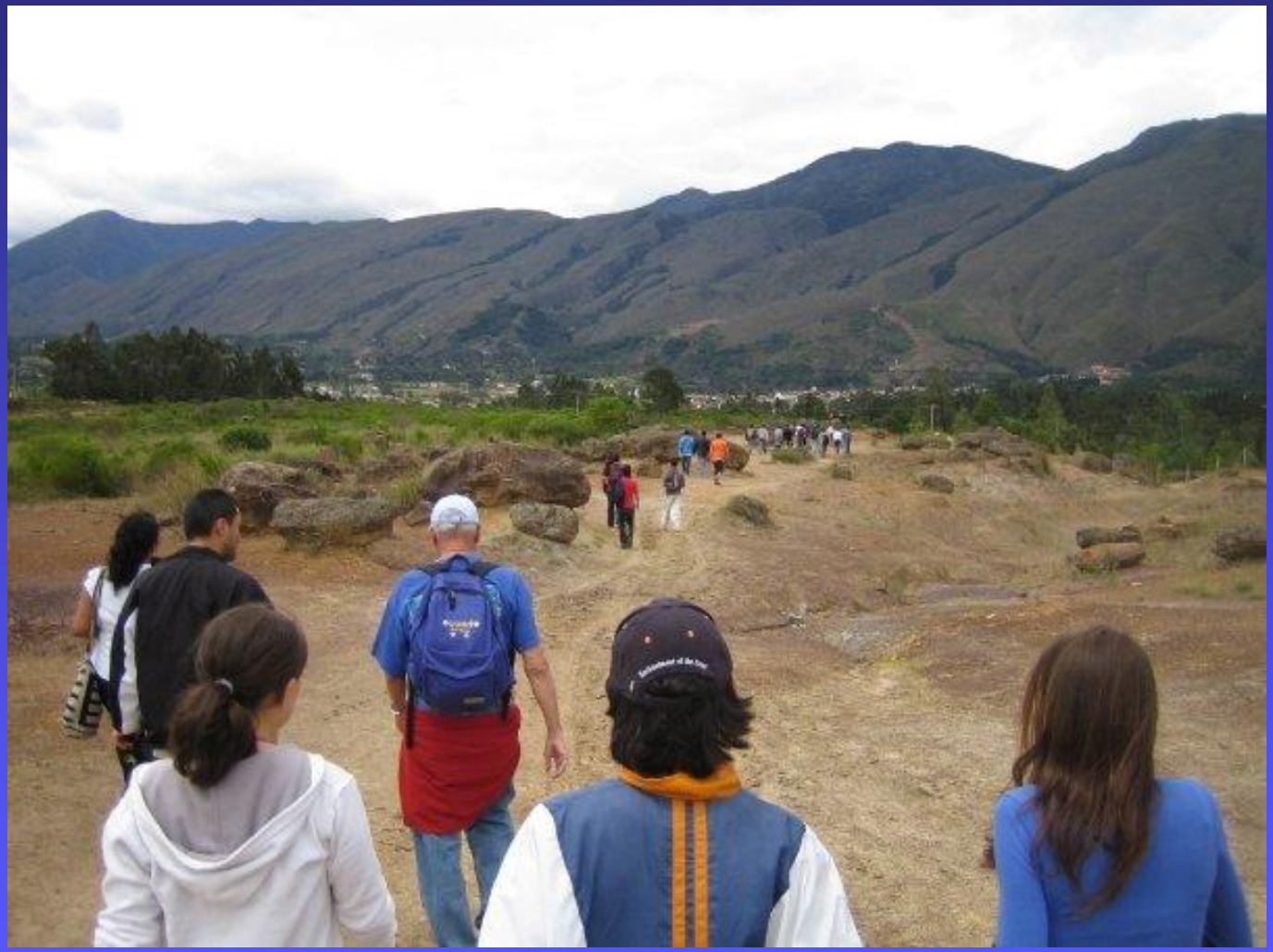

Conclusions

I have presented here a very brief description of the Density Matrix Renormalization Group technique, its applications and extensions. The aim of this work is to give the unexperienced reader an idea of the possibilities and scope of this powerful, though relatively simple method. The experienced reader can find here an extensive (however incomplete) list of references covering most applications to date using DMRG in a great variety of fields such as Condensed Matter, Statistical Mechanics and High .Energy Physics.

Thank you

Appendix The Method

Density Matrix

"When we solve a quantum-mechanical problem, what we really do is divide the universe into two parts – the system in which we are interested and the rest of the universe."

- Richard P. Feynman

(Statistical Mechanics : A set of lectures; Westview press, 1972)

When we include the part of the universe outside the system, the motivation of using the density matrices become clear.

So what does this mean ?

Let $|\phi_i\rangle$ be a complete set of vectors in the vector space describing the system, and let $|\theta_i\rangle$ be a complete set for the rest of the universe.

The most general way to write the wavefunction for the total system is

$$|\psi\rangle = \sum_{ij} C_{ij} |\phi_i\rangle |\theta_j\rangle$$

Now let A be an operator that acts only on the system, ie A does not act on $|\theta_i\rangle$

$$A|\phi_i>|\theta_j>=\sum_{ii'j} A_{ii'} |\phi_i\rangle |\theta_j\rangle\langle\theta_j| \langle\phi_{i'}|$$

Now we have,

$$\langle\psi|A|\psi\rangle = \sum_{iji'} C_{ij}^* C_{i'j} \langle\phi_i|A|\phi_{i'}\rangle$$

$$= \sum_{ii'} \langle\phi_i|A|\phi_{i'}\rangle \rho_{i'i}$$

$$\rho_{i'i} = \sum_j C_{ij}^* C_{i'j}$$

Density Matrix

We define the operator ρ to be such that,

$$\rho_{i'i} = \langle \phi_{i'} | \rho | \phi_i \rangle$$

Note that ρ is Hermitian.

Again,

$$\langle \psi | A | \psi \rangle = \sum_{ii'} \langle \phi_i | A | \phi_{i'} \rangle \rho_{i'i}$$

$$= \sum_i \langle \phi_i | A \sum_{i'} | \phi_{i'} \rangle \langle \phi_{i'} | \rho | \phi_i \rangle$$

$$= \sum_i \langle \phi_i | A \rho | \phi_i \rangle$$

$$= Tr\, A\rho$$

Due to the Hermitian nature of ρ it can be diagonalized with a complete orthonormal set of eigenvectors $|i\rangle$ *with real eigenvalues* w_i

$$\rho = \sum_i w_i |i\rangle\langle i|$$

So, we have $\langle y|A|y\rangle = Tr\,Ar$ and $\rho = \sum_i w_i |i\rangle\langle i|$

If we let A be 1, we obtain

$$\sum_i w_i = Tr\,\rho = \langle A\rangle = \langle\psi|\psi\rangle = 1$$

If we let A be $|i'\rangle\langle i'|$ we have

$$w_i = TrA\rho = \langle A\rangle = \langle\psi|A|\psi\rangle = \sum_j (\langle\psi|i'\rangle|\theta_j\rangle)(\langle\theta_j|\langle i'|\psi\rangle)$$

$$= \sum_j |(\langle i'|\langle\theta_j|)|\psi\rangle|^2$$

Therefore, we have

$$w_i \geq 0 \qquad \text{and} \qquad \sum_i w_i = 1$$

Orthonormal set of eigenvectors and real eigenvalues.

Any system is described by a density matrix ρ, where ρ is of the form $\sum_i w_i |i\rangle\langle i|$ *and*

(a) *The set* $|i\rangle$ *is a complete orthonormal set of vectors.*

$w_i \geq 0$ (b)

$\sum_i w_i = 1$ (c)

(d) *Given an operator A, the expectation of A is given by*

$$\langle A\rangle = Tr\rho A$$

Notice that,

$$\langle A\rangle = Tr\,\rho = \sum_{i'}\langle i'|\rho A|i'\rangle = \sum_{i'i} w_i\langle i'|i\rangle\langle i|A|i'\rangle = \sum_i w_i\langle i|A|i\rangle$$

Thus, w_i *is the probability that the system is in state* $|i\rangle$ *. If all but one* w_i *are zero, we say that the system is in a* ***pure state****; otherwise it is in a* ***mixed state*** *.*

1 *Consider a pure state:* $|\psi\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle + |\downarrow\rangle\right)$

$$\rho = |\psi\rangle\langle\psi| = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix}\begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{pmatrix}$$

Notice that $\rho^2 = \rho$ *and* $Tr\,\rho = 1$

2 *Consider a mixed state: 50%* $|\uparrow\rangle$ *and 50%* $|\downarrow\rangle$

$$\rho = \frac{1}{2}\left(|\uparrow\rangle\langle\uparrow|\right) + \frac{1}{2}\left(|\downarrow\rangle\langle\downarrow|\right)$$

$$= \frac{1}{2}\begin{pmatrix} 1 \\ 0 \end{pmatrix}\begin{pmatrix} 1 & 0 \end{pmatrix} + \frac{1}{2}\begin{pmatrix} 0 \\ 1 \end{pmatrix}\begin{pmatrix} 0 & 1 \end{pmatrix}$$

$$= \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

Notice that $\rho^2 \neq \rho$ *and* $Tr\,\rho = 1$

3 *50% and 50% mixture of* $|\psi\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle + |\downarrow\rangle\right)$ & $|\varphi\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle - |\downarrow\rangle\right)$

$$\rho = \frac{1}{2}\left(|\psi\rangle\langle\psi|\right) + \frac{1}{2}\left(|\varphi\rangle\langle\varphi|\right)$$

$$= \frac{1}{2}\begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{pmatrix} + \frac{1}{2}\begin{pmatrix} \frac{1}{2} & -\frac{1}{2} \\ -\frac{1}{2} & \frac{1}{2} \end{pmatrix}$$

$$= \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

Notice that $\rho^2 \neq \rho$ *and* $Tr\,\rho = 1$

Diagonal elements = Populations
Off-diagonal elements = Coherence

It is important to note that in 2 and 3, both cases we describe a system about which we know nothing, ie, A state of total ignorance.

Density matrix:

Eigenstates of density matrix form complete basis for subsystem block
Eigenvalues give the weight of a state
Keep the m eigenstates corresponding to m highest eigenvalues
Eigenstate of the whole system thus given by:

$$|\psi_0> \approx \sum_{\alpha} \sqrt{w_\alpha}\, |\phi_\alpha> |\chi_\alpha>$$

Schmidt decomposition

The optimal approximation

Entanglement states (mutual quantum information):

$$S(\rho) = -Tr(\rho \log \rho) = -\sum_{\alpha} w_\alpha \log w_\alpha$$

DM can be defined for pure, coherent superposition or statistical averaged states

Density matrix renormalization group: Formulation

- Diagonalization of a small finite lattice
- Division of system
- Reduction of the subsystem block via density matrix
- Renormalize the matrix formulation of all the operators
- Add one or two sites (few possible degrees of freedom)
- Construct the bigger lattice
- Repeat all the steps

Environment block:

a) Exact sites only
b) Reflection of subsystem block
c) Stored block from a previous step

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Thank you