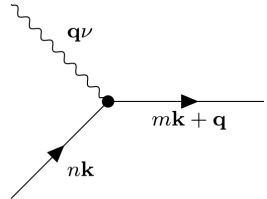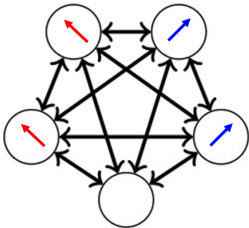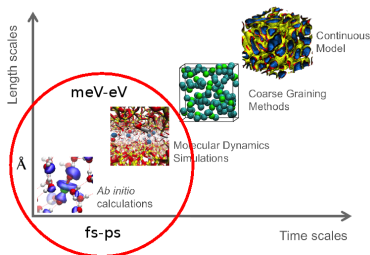# Diagrams and tensors in Computational (Materials) Physics

Cesare Franchini[1,2], Thomas Hahn[1], Dario Fiore Mosca[1]

[1]University of Vienna, [2]University of Bologna

– **Many-body or effective Hamiltonian**

– Density Functional Theory (DFT)

– Hartree-Fock Theory (HF)

– DFT+HF $\rightarrow$ Hybrid Functionals

– GW (quasiparticles)

– Bethe-Salpeter equation (BSE, electron-hole)

– Quantum Mechanical Molecular Dynamics (MD)

– **Diagrammatic Monte Carlo (Thomas)**

– **Multipolar expansions (Dario)**

Hamiltonian of a system of N electrons and M nuclei

$$
\begin{aligned}
\hat{H} &= -\frac{\hbar^2}{2m_e} \sum_{i=1}^{N} \nabla_i^2 - \sum_{n=1}^{M} \frac{\hbar^2}{2M_n} \nabla_n^2 + \frac{1}{4\pi\epsilon_0} \frac{1}{2} \sum_{i,j=1;i\neq j}^{N} \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|} \\
&\quad - \frac{1}{4\pi\epsilon_0} \sum_{n}^{M} \sum_{i}^{N} \frac{Z_n e^2}{|\mathbf{r}_i - \mathbf{R}_n|} + \frac{1}{4\pi\epsilon_0} \frac{1}{2} \sum_{n,m=1;n\neq m}^{M} \frac{Z_n Z_m e^2}{|\mathbf{R}_n - \mathbf{R}_m|}
\end{aligned}
$$

or

$$
\hat{H} = \hat{T}_e + \hat{T}_n + \hat{U}_{ee} + \hat{U}_{en} + \hat{U}_{nn}
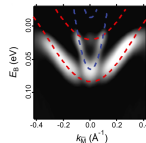$$

Hamiltonian of a system of N electrons and M nuclei

$$
\begin{aligned}
\hat{H} \;=\; & -\frac{\hbar^2}{2m_e}\sum_{i=1}^{N}\nabla_i^2 - \sum_{n=1}^{M}\frac{\hbar^2}{2M_n}\nabla_n^2 + \frac{1}{4\pi\epsilon_0}\frac{1}{2}\sum_{i,j=1;i\neq j}^{N}\frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|} \\
& -\frac{1}{4\pi\epsilon_0}\sum_{n}^{M}\sum_{i}^{N}\frac{Z_n e^2}{|\mathbf{r}_i - \mathbf{R}_n|} + \frac{1}{4\pi\epsilon_0}\frac{1}{2}\sum_{n,m=1;n\neq m}^{M}\frac{Z_n Z_m e^2}{|\mathbf{R}_n - \mathbf{R}_m|}
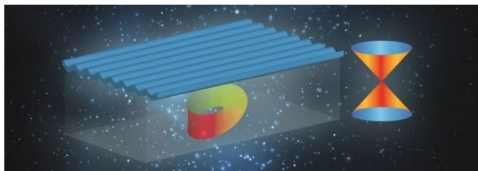\end{aligned}
$$

or

$$
\hat{H} \;=\; \hat{T}_e \;+\; \hat{T}_n \;+\; \hat{U}_{ee} \;+\; \hat{U}_{en} \;+\; \hat{U}_{nn}
$$

$\Rightarrow$

Standard model as the topological material

G E Volovik[1,2,6] **and M A Zubkov**[3,4,5]

Abstract

The study of the Weyl and Dirac topological materials (topological semimetals, insulators, superfluids and superconductors) opens the route for the investigation of the topological quantum vacua of relativistic fields. The symmetric phase of the standard model (SM), where both electroweak and chiral symmetry are not broken, represents the topological semimetal. The vacua of the SM (and its extensions) in the phases with broken electroweak symmetry represent the topological insulators of different types. We discuss in detail the topological invariants in both the symmetric and broken phases and establish their relation to the stability of vacuum.
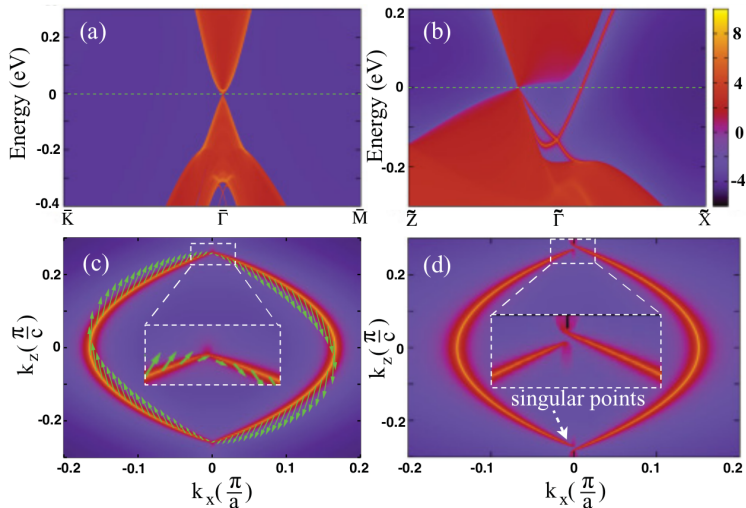
Z. Wang et al., PRB2012 (> 1000 citations)

First principles (*Ab initio*)

Solution of the many body
Schrödinger/Dirac equation

$$\hat{H}\Psi = E\Psi$$

- No empirical assumptions
- No fitting parameters
- Full electronic structure
- Different level of accuracy
- Atomistic interpretation

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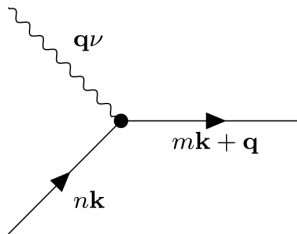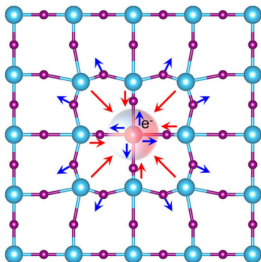- Atomistic interpretation

Model (effective) Hamiltonian

Solution of simplified lattice fermion models
(typically the Hubbard model)

$$H = -t \sum_{\langle i,j \rangle, \sigma} (c_{i,\sigma}^{\dagger} c_{j,\sigma} + c_{j,\sigma}^{\dagger} c_{i,\sigma}) + U \sum_{i=1}^{N} n_{i\uparrow} n_{i\downarrow}$$

- Restricted Hilbert space (few particles)
- Short-ranged electron interactions
- Adjustable parameters
- Accurate solution, transparent physical interpretation
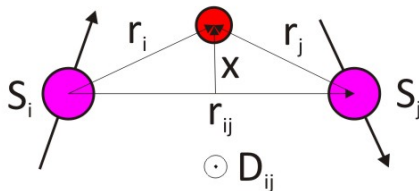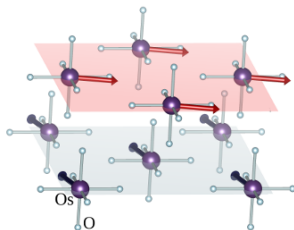
Polaron (electorn-phonon) Hamiltonians

$$H_F = \sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} \hat{c}_{\mathbf{k}}^\dagger \hat{c}_{\mathbf{k}} + \hbar\omega_0 \sum_{\mathbf{q}} \hat{a}_{\mathbf{q}}^\dagger \hat{a}_{\mathbf{q}} + \sum_{\mathbf{k},\mathbf{q}} V(\mathbf{q}) \hat{c}_{\mathbf{k}+\mathbf{q}}^\dagger \hat{c}_{\mathbf{k}} \left(\hat{a}_{\mathbf{q}} + \hat{a}_{-\mathbf{q}}^\dagger \right)$$

$\Rightarrow$ **Diagrammatic Quantum Monte Carlo**

Multipolar (spin) Hamiltonians

$$H_{ij} = \sum_{K,K'} \sum_{Q,Q'} I^{QQ'}_{KK'} O^K_Q(J_i) O^{K'}_{Q'}(J_j),$$

$\Rightarrow$ **Ab initio, Calssical/Quantum Monte Carlo, Exact Diagonalization**