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Engineering of quantum Hamiltonians by high-frequency laser fields

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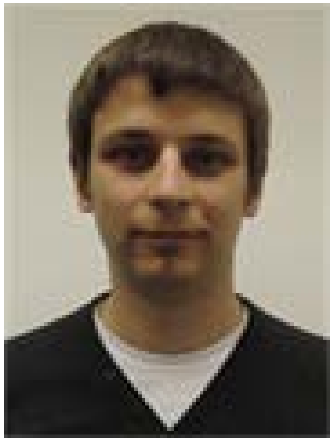
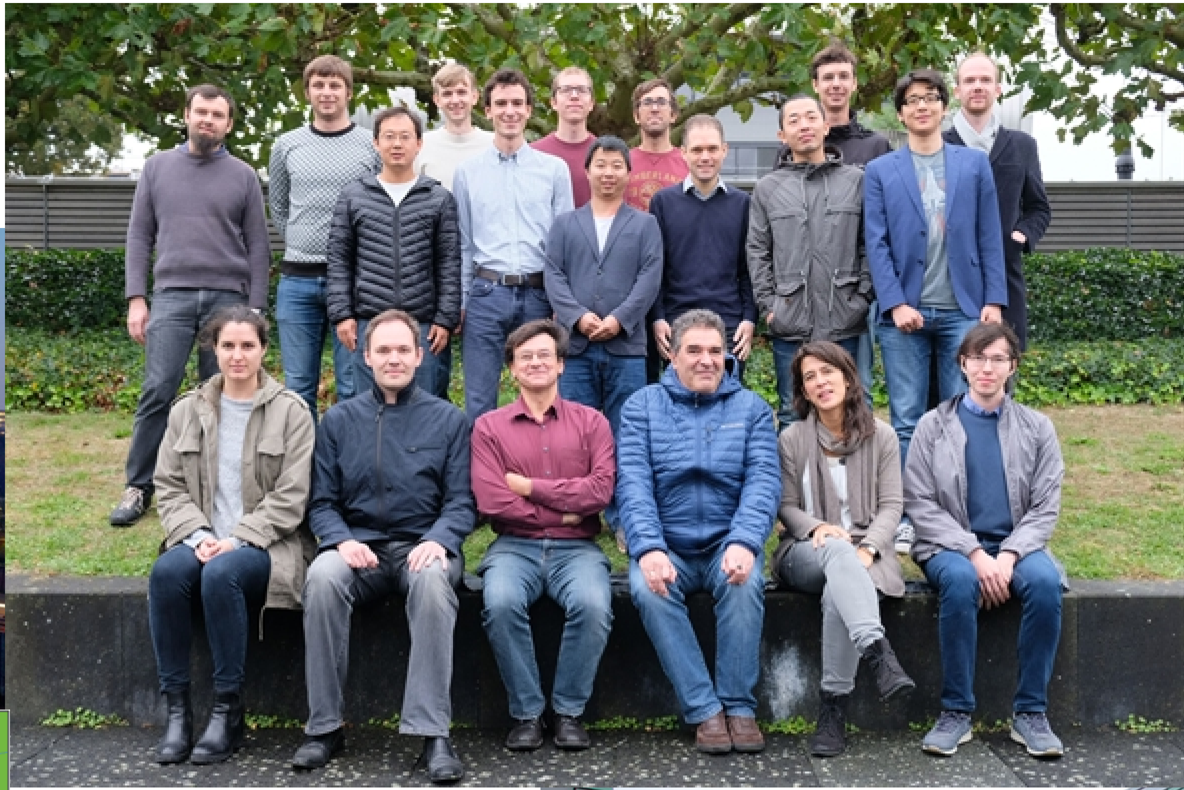
Main collaborators:

Sasha Itin	Clément Dutreix	Zhenya Stepanov
		

Theory of Condensed Matter group

http://www.ru.nl/tcm



Nijmegen,
province
Gelderland
(not Holland!)

Quantum Hamiltonians: General

In condensed matter physics we know the basic laws, it is laws of quantum mechanics

Time-dependent Schrödinger equation *(general)*

$$i\hbar\frac{\partial}{\partial t}|\Psi(\mathbf{r},t)\rangle = \hat{H}|\Psi(\mathbf{r},t)\rangle$$

In solids/liquids/molecules/clusters...

$$\hat{H} = \hat{T}_n + V_{nn}(\vec{R}_l) + \hat{H}_e(\vec{R}_l)$$

$$\hat{T}_n = \sum_l \frac{\hat{\vec{P}}_l^2}{2M_l}$$

Kinetic energy of nuclei

$$V_{nn}(\vec{R}_l) = \frac{1}{2}\sum_{l\neq l'} \frac{Z_l Z_{l'} e^2}{|\vec{R}_l - \vec{R}_{l'}|}$$

Coulomb repulsion of nuclei

$$\hat{H}_e(\vec{R}_l) = \sum_i \frac{\hat{\vec{p}}_i^2}{2m} + \frac{1}{2}\sum_{i\neq j}\frac{e^2}{|\vec{r}_i - \vec{r}_j|} - \sum_{il}\frac{Z_l e^2}{|\vec{r}_i - \vec{R}_l|}$$

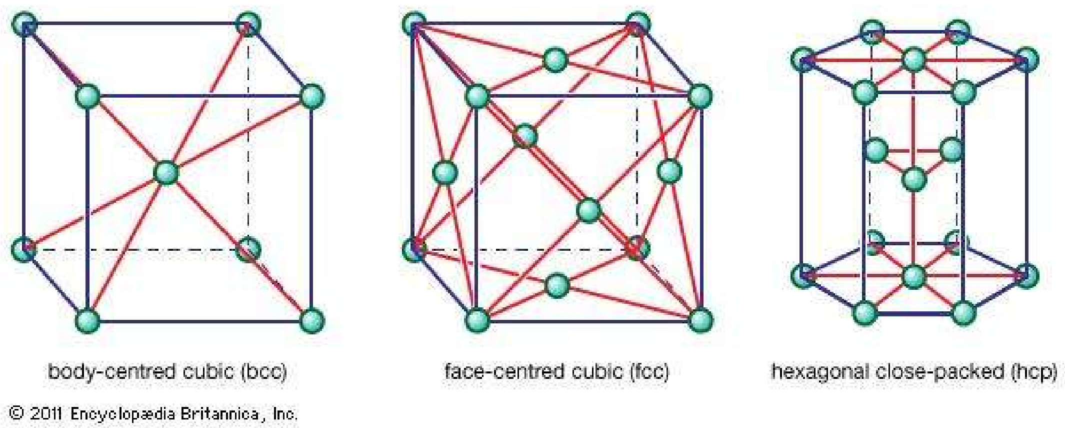
Electron Hamiltonian at a given position of nuclei

Quantum Hamiltonians: General II

Adiabatic approximation: small parameter $\kappa = \left(\frac{m}{M}\right)^{1/4}$ allows to separate lattice and electron degrees of freedom

Crystals: periodic arrange of atoms

Common metallic crystal structures

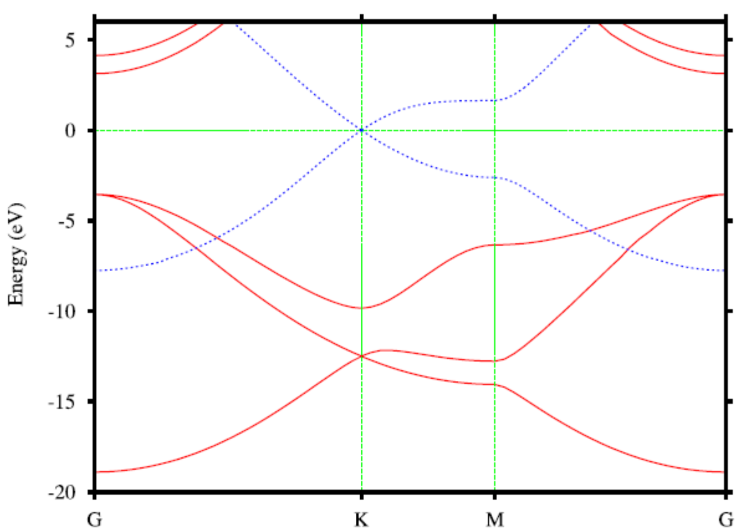


In single-electron approximation:
Bloch theorem and band structure

$$\psi_{n\vec{k}}(\vec{r}) = u_{n\vec{k}}(\vec{r})\exp\left(i\vec{k}\vec{r}\right)$$

$u_{n\vec{k}}(\vec{r})$ is periodic with the periodicity of the crystal
n is band index

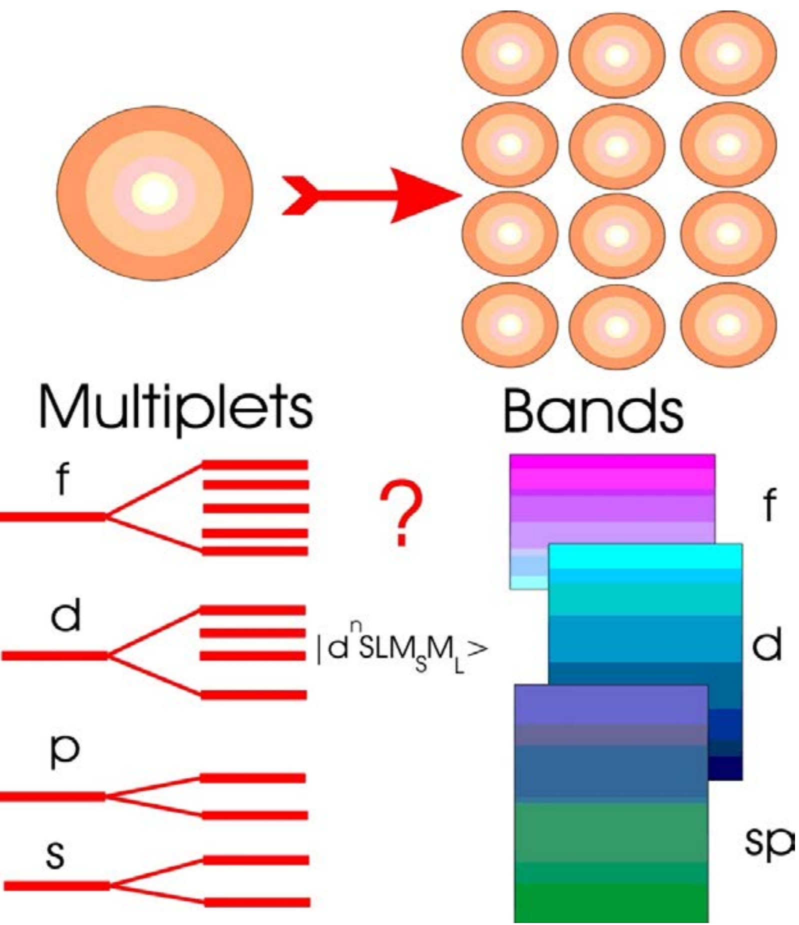
Electron energy bands in graphene



Quantum Hamiltonians: General III

The problem with this description: it neglects interelectron interaction, and the intercation is not small

Two limits: free atoms and bands of noninteracting electrons: the description is dramatically different



PRL **104,** 117601 (2010) PHYSICAL REVIEW LETTERS week ending 19 MARCH 2010

Correlated Electrons Step by Step: Itinerant-to-Localized Transition of Fe Impurities in Free-Electron Metal Hosts

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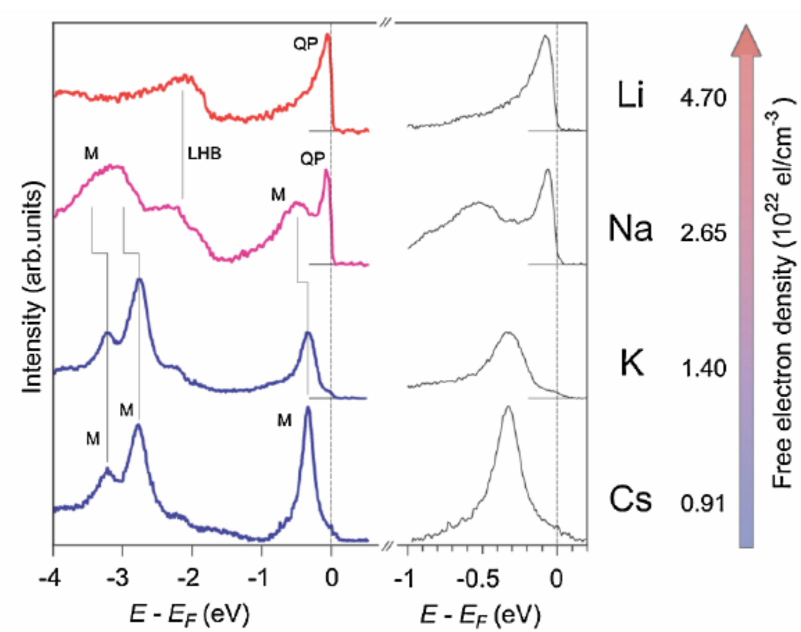


The beginning: “Polar model”

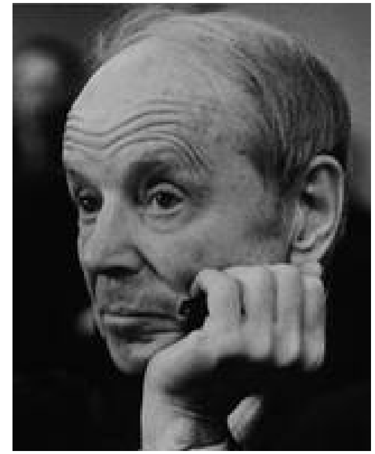
On the Electron Theory of Metals.

By S. Schubin and S. Wonsowsky.

Sverdlovsk Physical Technical Institute.

(Communicated by R. H. Fowler, F.R.S.—Received December 29, 1933.)

Proc. R. Soc. Lond. A 1934 **145**, published 2 June 1934



S. P. Shubin (1908-1938) S. V. Vonsovsky (1910-1998)

$$\int \frac{e^2}{|x - x'|} \phi_\alpha^2(x)\, \phi_\alpha^2(x')\, dx\, dx' = \mathrm{A}$$

$$\int \sum_{\gamma \neq \beta} \left[\mathrm{G}_\gamma(x)\, \phi_\alpha^2(x') + \frac{e^2}{|x - x'|} \phi_\gamma^2(x') \right] \phi_\alpha(x)\, \phi_\beta(x)\, dx\, dx' = \mathrm{L}_{\alpha\beta}$$

$$\int \frac{e^2}{|x - x'|} \phi_\alpha^2(x)\, \phi_\beta^2(x')\, dx\, dx' = \mathrm{B}_{\alpha\beta}$$

$$\int \frac{e^2}{|x - x'|} \phi_\alpha(x)\, \phi_\beta(x)\, \phi_\alpha(x')\, \phi_\beta(x')\, dx\, dx' = \mathrm{J}_{\alpha\beta}$$

Fig. 1.

Fig. 2.

The beginning: "Polar model" II

Schrödinger equation in "atomic representation" (double *f*, hole *g*, spin right *k*, spin left *h*)

$$\{\varepsilon - s(\mathrm{A}+\mathrm{D}) - [\sum_{f<f'} (\mathrm{B}_{ff'} - \mathrm{J}_{ff'}) + \sum_{g<g'} (\mathrm{B}_{gg'} - \mathrm{J}_{gg'}) - \sum_{f,g} (\mathrm{B}_{fg} + \mathrm{J}_{fg})]\}\mathrm{C}(fgh)$$
$$+ \sum_{h,k} \mathrm{J}_{hk}[\mathrm{C}(\mathrm{T}_{hk}|fgh) - \mathrm{C}(fgh)] + \sum_{f,g} \mathrm{J}_{fg}[\mathrm{C}(\mathrm{T}_{fg}|fgh) - \mathrm{C}(fgh)]$$
$$+ \sum_{f,p} \mathrm{L}_{fp}\mathrm{C}(\mathrm{T}_{fp}|fgh) - \sum_{g,p} \mathrm{L}_{gp}\mathrm{C}(\mathrm{T}_{gp}|fgh) = 0, \qquad (9)$$

Metal-insulator transition and Mott insulators

(II). The minimum energy corresponds to a certain $s = s_0$, where $0 < s_0 < n$. This case we have, for instance, when

$$\mathrm{A} + 6(\mathrm{J} - \mathrm{B}) > 0, \quad \mathrm{A} + 6\mathrm{J} - 12\mathrm{L} < 0.$$

Then, so long as s remains small, the lowest energy level *diminishes* as s increases; for a certain $s = s_0$ it attains a minimum and then again begins to increase. For such metals—at not very high temperatures—the number of "free" electrons approximates to twice this s_0 (electrons + holes !) and is therefore *smaller* than the number of atoms. In order to calculate s_0 in terms of our integrals, the energy must be evaluated up to the second approximation in powers of s/n; we shall not, however, make these rather cumbersome calculations here.

Metal

(III). The minimum energy corresponds to $s = 0$. This is the case when

$$\mathrm{A} + 6(\mathrm{J} - \mathrm{B}) > 0, \quad \mathrm{A} + 6\mathrm{J} - 12\mathrm{L} > 0.$$

Insulator

Quantum Hamiltonians: Lattice models

Modern way of treatment (well... for last 70 years): Secondary quantization

$$\hat{H} = \sum_{\sigma} \int d\vec{r} \hat{\psi}_{\sigma}^{+}(\vec{r}) \hat{h}_0 \hat{\psi}_{\sigma}(\vec{r}) + \frac{1}{2} \sum_{\sigma\sigma'} \int d\vec{r} d\vec{r}' \hat{\psi}_{\sigma}^{+}(\vec{r}) \hat{\psi}_{\sigma'}^{+}(\vec{r}') v(\vec{r} - \vec{r}') \hat{\psi}_{\sigma'}(\vec{r}') \hat{\psi}_{\sigma}(\vec{r})$$

$$\hat{h}_0 = \frac{\hat{\vec{p}}^2}{2m} - \sum_l \frac{Z_l e^2}{|\vec{r} - \vec{R}_l|} \qquad v(\vec{r} - \vec{r}') = \frac{e^2}{|\vec{r} - \vec{r}'|}$$

In a single-electron basis: $\{\varphi_{\lambda}(\vec{r})\}$

$$\hat{H} = \sum_{\lambda\mu\sigma} h_{\lambda\mu} \hat{c}_{\lambda\sigma}^{+} \hat{c}_{\mu\sigma} + \frac{1}{2} \sum_{\substack{\kappa\lambda\mu\nu \\ \sigma\sigma'}} v_{\kappa\lambda\mu\nu} \hat{c}_{\kappa\sigma}^{+} \hat{c}_{\lambda\sigma'}^{+} \hat{c}_{\nu\sigma'} \hat{c}_{\mu\sigma}$$

$$h_{\lambda\mu} = \int d\vec{r} \varphi_{\lambda}^{*}(\vec{r}) \hat{h}_0 \varphi_{\mu}(\vec{r})$$

$$v_{\kappa\lambda\mu\nu} = \int d\vec{r} d\vec{r}' \varphi_{\kappa}^{*}(\vec{r}) \varphi_{\lambda}^{*}(\vec{r}') v(\vec{r} - \vec{r}') \varphi_{\mu}(\vec{r}) \varphi_{\nu}(\vec{r}')$$

Fermionic operators:

$$\{\hat{c}_{\lambda\sigma}, \hat{c}_{\lambda'\sigma'}\} = 0, \quad \{\hat{c}_{\lambda\sigma}^{+}, \hat{c}_{\lambda'\sigma'}^{+}\} = 0, \quad \{\hat{c}_{\lambda\sigma}, \hat{c}_{\lambda'\sigma'}^{+}\} = \delta_{\lambda\lambda'} \delta_{\sigma\sigma'}$$

$$\{\hat{A}, \hat{B}\} = \hat{A}\hat{B} + \hat{B}\hat{A}, \quad [\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$$

Quantum Hamiltonians: Lattice models II

For simplicity: single-band model $c_{i\sigma} = \sum_{\vec{k}} c_{\vec{k}\sigma} \exp\left(i\vec{k}\vec{R}_i\right),$ **Band Hamiltonian**

From sites to bands: $c_{\vec{k}\sigma} = \sum_{i} c_{i\sigma} \exp\left(-i\vec{k}\vec{R}_i\right)$ $\hat{H}_0 = \sum_{\vec{k}\sigma} t_{\vec{k}} \hat{c}^{+}_{\vec{k}\sigma} \hat{c}_{\vec{k}\sigma}$

$t_{\vec{k}}$ **is the Fourier transform of the hopping parameters** t_{ij}

In the presence of electromagnetic field: Peierls substitution

$$t_{ij} \to t_{ij} \exp\left\{ \frac{ie}{\hbar c} \int_{\vec{R}_j}^{\vec{R}_i} d\vec{r}\,' \vec{A}(\vec{r}\,', t) \right\}$$

$\vec{A}(\vec{r}\,', t)$ **vector potential; in optics** $\vec{E}(t) = -\frac{1}{c}\frac{\partial \vec{A}}{\partial t}$

Simple models: Hubbard model

$$\hat{H} = \sum_{ij\sigma}{}' t_{ij} \hat{c}^{+}_{i\sigma} \hat{c}_{j\sigma} + U \sum_{i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$

(only on-site Coulomb repulsion)

Extended Hubbard model
(intersite interactions added)

$$\hat{H}_c = U \sum_{i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} + \frac{1}{2} \sum_{ij}{}' V_{ij} \hat{n}_i \hat{n}_j$$

$$\hat{n}_{i\sigma} = \hat{c}^{+}_{i\sigma} \hat{c}_{i\sigma}, \qquad \hat{n}_i = \sum_{\sigma} \hat{n}_{i\sigma}$$

Quantum Hamiltonians: Lattice models III

Half-filled case, $U >> t_{ij}$ **Homopolar state (one electron per atom, spins up and down)**

Bogoliubov perturbation theory (also known as Anderson superexchange, but first results are by Shubin & Vonsovsky)

$$\hat{H} = \hat{H}_0 + \varepsilon \hat{H}_1 + \varepsilon^2 \hat{H}_2$$

$$\hat{H}_{eff} = \varepsilon \hat{P}\hat{H}_1\hat{P} + \varepsilon^2 \left[\hat{P}\hat{H}_2\hat{P} + \hat{P}\left(\hat{H}_1 - \hat{P}\hat{H}_1\hat{P}\right)\frac{1}{E_0 - \hat{H}_0}\left(\hat{H}_1 - \hat{P}\hat{H}_1\hat{P}\right) \right]$$

P is projector to homopolar state

Heisenberg model, antiferromagnetic exchange:

$$\hat{H}_{ex} = -2\sum_{i<j} J_{ij} \hat{\vec{S}}_i \hat{\vec{S}}_j$$

$$\hat{\vec{S}}_i = \frac{1}{2}\sum_{\alpha\beta} \hat{P}\hat{c}^{+}_{i\alpha}\hat{\vec{\sigma}}_{\alpha\beta}\hat{c}_{i\beta}\hat{P}$$

localized spins

$$J_{ij}^{eff} = -\frac{2\left|t_{ij}\right|^2}{U}$$

Spins like to be antiparallel (singlet ground state)

In non-half-filled case: ferromagnetic tendency ("Zener double exchange"), phase separation etc.

Quantum Hamiltonians: Lattice models IV

Many other phenomena, e.g. charge and orbital ordering, etc.

E.g., degenerate orbitals: orbital momentum operator enters the Hamiltonian

E.g., for triple degenerate band:

$$\hat{H}_K = \frac{U - 3J_H}{2}\hat{N}(\hat{N}-1) - 2J_H\hat{\vec{S}}^2 - \frac{J_H}{2}\hat{\vec{L}}^2 + \frac{5J_H}{2}\hat{N}$$

J_H **is Hund exchange**

Two orbitals per site, one electron (quarter filling, Kugel-Khomskii model): Orbital anitiferromagentism and spin ferromagnetism

$$J_{eff} = \frac{2t^2}{U} - \frac{2t^2}{U - J_H} = \frac{2t^2 J_H}{U(U - J_H)} > 0$$

s-d exchange (Vonsovsky-Zener) model: interaction of localized and itinerant electrons

$$\hat{H} = \sum_{ij\sigma}{}' t_{ij}\hat{c}^{+}_{i\sigma}\hat{c}_{j\sigma} - 2I\sum_{i}\hat{\vec{S}}_i\hat{\vec{s}}_i - \sum_{ij\sigma}{}' J_{ij}\hat{\vec{S}}_i\hat{\vec{S}}_j$$

etc.

High-frequency laser fields

Quickly oscillating strong electric field means quickly oscillating effective hopping

$$t_{ij} \to t_{ij} \exp\left\{ \frac{ie}{\hbar c} \int_{\vec{R}_j}^{\vec{R}_i} d\vec{r}\,' \vec{A}(\vec{r}\,', t) \right\}$$

At very high frequency effective *static* Hamiltonian should exist

Classical analog: Kapitza pendulum

One needs to develop efficient perturbative theory in inverse frequency of the laser field

In classical mechanics: Bogoliubov, Krylov …

Development for matrix Hamiltonians:
A. P. Itin & A. I. Neishtadt, Phys. Lett. A 378, 822 (2014)

http://butikov.faculty.ifmo.ru/Russian/ParamPendulumKIO.pdf

General approach to many-body Hamiltonians

A. P. Itin & MIK, Phys. Rev. Lett. 115, 075301 (2015)

$$i\dot{X} = \epsilon \mathcal{H} X$$

where $\epsilon = 1/\omega$ is a small parameter, ω is a frequency of perturbation, $\mathcal{H}(t)$ is the Hamiltonian of the system, X is a column of coefficients of expansion of a quantum state in a certain basis, and fast time was introduced $(t \to t/\epsilon)$,

Unitary transformation to the new wave funstion $X = C\tilde{X}$

The new Hamiltonian: $i\dot{\tilde{X}} = [C^{-1}\epsilon\mathcal{H}C - iC^{-1}\dot{C}]\tilde{X}$

Series expansion: $C = \exp[\epsilon K_1 + \epsilon^2 K_2 + \epsilon^3 K_3 + \cdots]$

K_i **are skrew-Hermitian periodic in time matrices**

Using the average procedure to find a series for the effective Hamiltonian

General approach to many-body Hamiltonians II

$$i\dot{K}_1 = \mathcal{H}(t) - \langle \mathcal{H}(t) \rangle \equiv \{\mathcal{H}\}, iK_1 = \int \{\mathcal{H}\} dt,$$

$$i\dot{K}_2 = \left\{ \mathcal{H}K_1 - K_1\mathcal{H} - \frac{i}{2}(\dot{K}_1 K_1 - K_1 \dot{K}_1) \right\},$$

$$\epsilon \mathcal{H}_{\text{eff}} = [C^{-1}\epsilon \mathcal{H} C - iC^{-1}\dot{C}] = \epsilon \mathcal{H}_0 + \epsilon^2 \mathcal{H}_1 + \cdots$$

$$\{X\} \equiv X - \langle X(t) \rangle \qquad \langle X(t) \rangle \equiv (1/2\pi) \int_0^{2\pi} X(t')dt'$$

The integration constants are choosen in such a way that $\langle K_i \rangle = 0$

Expansion of the effective Hamiltonian:

$$\mathcal{H}_0 = \langle \mathcal{H} \rangle, \qquad \mathcal{H}_1 = \frac{1}{2} \langle [\{\mathcal{H}\}, K_1] \rangle,$$

$$\mathcal{H}_2 = \frac{1}{2} \langle [\{\mathcal{H}\}, K_2] \rangle + \frac{1}{12} \langle [\{[\{\mathcal{H}\}, K_1]\}, K_1] \rangle, \ldots$$

$$[A, B] = AB - BA$$

Hubbard model in strong electric field

We choose the other gauge, $\vec{E}(t) = -\nabla\phi,$ $\vec{A} = 0$ ϕ **- electrostatic potential**

One-dimensional Hubbard model

$$H = H_H + H_d(t),$$

$$H_d(t) = \omega\mathcal{E}(\omega t)\sum_j j n_j,$$

$$H_H = J\sum_{i,\sigma}(c^\dagger_{i,\sigma}c_{i+1,\sigma} + c^\dagger_{i+1,\sigma}c_{i,\sigma}) + U\sum_i n_{i,\sigma}n_{i,-\sigma}$$

Preliminary unitary transformation (to Peierls gauge):

$$U^{(0)}(t) = \exp[if(\omega t)\textstyle\sum_j jn_j],\ \ f(\omega t) \equiv \int_0^t \omega\mathcal{E}(\omega t')dt'$$

$$\mathcal{H} = \sum_{i,\sigma}(\delta_0^+ c^\dagger_{i,\sigma}c_{i+1,\sigma} + \delta_0^- c^\dagger_{i+1,\sigma}c_{i,\sigma}) + U\sum_i n_{i,\sigma}n_{i,-\sigma}$$

$$\delta_0^\pm = Je^{\pm if(t)}$$

Hubbard model in strong electric field II

Notations: $\delta_0^{\pm} = J e^{\pm i f(t)}$ $\delta_1^{\pm} = \int \delta^{\pm}(t')dt'$ $\delta_2^{\pm} = \int \delta_1^{\pm}(t')dt'$

$$\Delta^+ = \frac{1}{2}\langle \delta_2^+ \delta^+ \rangle, \qquad \Delta_0 = \frac{1}{2}\langle \delta^+ \delta_2^- + \delta_2^+ \delta^- \rangle \qquad \Delta^- = (\Delta^+)^*$$

The effective Hamiltonian is $(1/\omega^2)\mathcal{H}_2$ where

$$\mathcal{H}_1 = 0,$$

$$\mathcal{H}_2 = U\Delta_0(-2\mathcal{S} + \mathcal{A} + \mathcal{A}^\dagger + 4\mathbf{V} - 2V) + U[\Delta^-(4\mathbf{R} - 2\mathcal{R} + R_2) + \text{H.c.}],$$

$$\mathcal{S} = \sum_{j,\sigma} c^\dagger_{j+1,\sigma} c_{j,\sigma} c^\dagger_{j,-\sigma} c_{j+1,-\sigma},$$

$$\mathbf{R} = \sum_j c^\dagger_{j+1,\downarrow} c_{j,\downarrow} c^\dagger_{j+1,\uparrow} c_{j,\uparrow},$$

$$\mathcal{A} = \mathcal{A}_{\uparrow,\downarrow} + \mathcal{A}_{\downarrow,\uparrow}, \qquad \mathcal{A}_{\sigma,-\sigma} = \sum_j c^\dagger_{j,\sigma} c_{j-1,\sigma} c^\dagger_{j,-\sigma} c_{j+1,-\sigma},$$

$$R_2 = \sum_{j,\sigma} c^\dagger_{j+1,\sigma} c_{j-1,\sigma}(n_{j-1,-\sigma} - 2n_{j,-\sigma} + n_{j+1,-\sigma}),$$

$$\mathcal{R} = \mathcal{R}_{\uparrow\downarrow} + \mathcal{R}_{\downarrow\uparrow}, \qquad \mathcal{R}_{\sigma,-\sigma} = \sum_j c^\dagger_{j,\sigma} c_{j-1,\sigma} c^\dagger_{j+1,-\sigma} c_{j,-\sigma},$$

$$V = \sum_{j,\sigma} n_{j,\sigma} n_{j+1,-\sigma}, \qquad \mathbf{V} = \sum_j n_{j,\downarrow} n_{j,\uparrow}.$$

Hubbard model in strong electric field III

Density-dependent hopping (as in the general polar model);
Induced interaction on different sites;
Attraction on site;
Modification of exchange interaction (from AFM to FM)

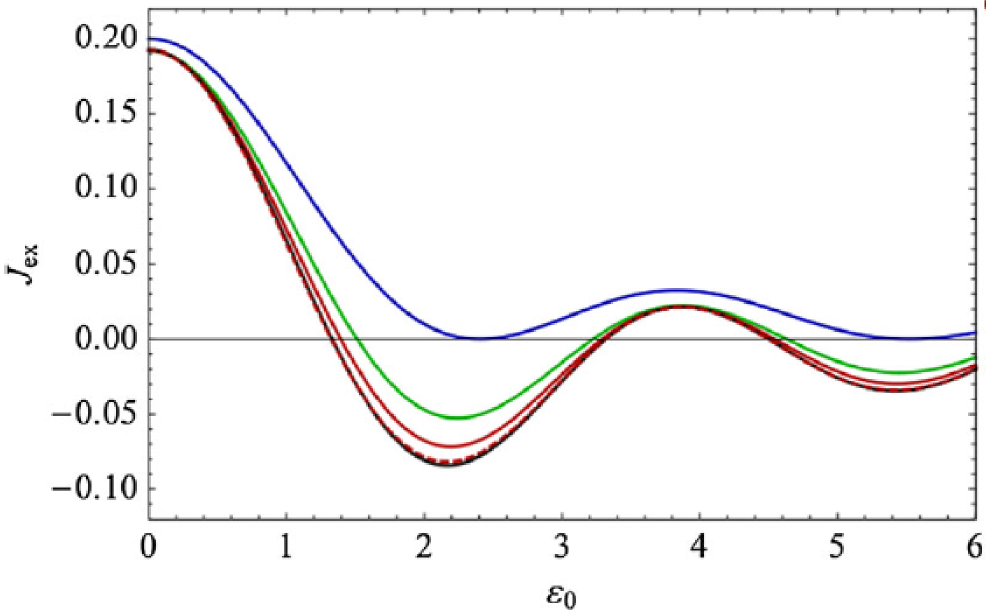
Monochromatic field: $f(\omega t) \propto \sin(\omega t)$ **Effective hopping:** $J \to J_e = J J_0(\mathcal{E}_0)$

Second-order correction to exchange integral $-(4UJ^2/\omega^2)\sum_1^\infty [J_m^2(\mathcal{E}_0)/m^2]$

Total formula for ω comparable with U but >> J

$$A = -4J^2 U \sum_{m=1}^{\infty} J_m^2(\mathcal{E}_0)/[m^2\omega^2 - U^2]$$ **(*)** **(change of sign is unavoidable)**

$U = 10$, "bare" tunneling $J = -1$, $\omega = 16$



Color solid curves, from top to bottom:

- **Bare exchange interaction** $2J_e^2(\mathcal{E}_0)/U$
- **Second order expansion;**
- **Fourth order expansion**
- **Formula (*)**

Dashed line shows numerical results for nonequilibrium exchange (J. Mentink et al)

Dynamical control of electron-phonon interactions

Hamiltonian:

C. Dutreix & MIK, Phys. Rev. B 95, 024306 (2017)

$$H(t) = H_e(t) + H_p + H_{ep}, \text{ with}$$

$$\epsilon_k(t) = 2\nu \cos(k + z \sin \Omega t)$$

$$H_e(t) = \sum_k \epsilon_k(t)\, c_k^\dagger c_k, \quad H_p = \sum_q \omega_q\, b_q^\dagger b_q,$$

$$z = eE_0/\Omega$$

$$H_{ep} = \sum_{k,q} g_q\, c_{k+q}^\dagger c_k B_q.$$

ν nearest-neighbour hopping amplitude

Peierls substitution $A(t) = -E_0 \sin(\Omega t)/\Omega$ $\quad B_q = b_{-q}^\dagger + b_q$

$b_q^\dagger$ and b_q phonon creation and annihilation operators (bosons)

Interesting problem: polaron formation (dressing of electrons by virtual excitations of bosonic field)

At equilibrium, well studied; what happens under a strong high-frequency field?

Electron-phonon interactions II

$$i\,\partial_\tau \phi(\tau) = \lambda\, H(\tau)\,\phi(\tau) \qquad \tau = \Omega t \text{ and } \lambda = \delta E/\Omega$$

Unitary transformation

$$\tilde{\phi}(\tau) = \exp\{-i\,\Delta(\tau)\}\,\phi(\tau) \qquad \Delta(\tau) = \sum_{n=1}^{+\infty} \Delta_n(\tau)\lambda^n$$

New Hamiltonian

$$\tilde{H} = \lambda e^{i\Delta(t)} H(t) e^{-i\Delta(t)} - i\,e^{i\Delta(t)} \partial_t e^{-i\Delta(t)}$$

$$i\,\partial_\tau \tilde{\phi}(\tau) = \tilde{H}\tilde{\phi}(\tau) \qquad \tilde{H} = \sum_{n=1}^{+\infty} \tilde{H}_n \lambda^n$$

$$\tilde{H}_1 = H(\tau) - \partial_\tau \Delta_1(\tau),$$

$$\tilde{H}_2 = \frac{i}{2}[\Delta_1(\tau), H(\tau)] + \frac{i}{2}[\Delta_1(\tau), \tilde{H}_1] - \partial_\tau \Delta_2(\tau),$$

$$\tilde{H}_3 = \frac{i}{2}[\Delta_2(\tau), H(\tau)] + \frac{i}{2}[\Delta_1(\tau), \tilde{H}_2] + \frac{i}{2}[\Delta_2(\tau), \tilde{H}_1] + \frac{1}{12}[[\Delta_1(\tau), \partial_t \Delta_1(\tau)], \Delta_1(\tau)] - \partial_\tau \Delta_3(\tau),$$

Electron-phonon interactions III

By construction $\tilde{H}$ **should be static – the way to choose** $\Delta(\tau)$

$$\tilde{H}_1 = H_0, \quad \tilde{H}_2 = -\frac{1}{2}\sum_{m\neq 0}\frac{[H_m, H_{-m}]}{m},$$

$$\tilde{H}_3 = \frac{1}{2}\sum_{m\neq 0}\frac{[[H_m, H_0], H_{-m}]}{m^2} + \frac{1}{3}\sum_{m\neq 0}\sum_{n\neq 0,m}\frac{[[H_m, H_{n-m}], H_{-n}]}{mn},$$

$$H_m = \int_{-\pi}^{+\pi}\frac{d\tau}{2\pi}e^{im\tau}H(\tau)$$

In the third-order approximation (second-order is trivial)

$$\tilde{H} = \tilde{H}_e + \tilde{H}_p + \tilde{H}_{ep} + o(\lambda^3), \text{ where}$$

$$\tilde{H}_e = \sum_k 2\tilde{t}_1(z)\cos(k)\, c_k^\dagger c_k, \quad \tilde{H}_p = \sum_q \tilde{\omega}_q b_q^\dagger b_q,$$

$$\tilde{H}_{ep} = \sum_{k,q}\gamma_{k,q}(z)c_{k+q}^\dagger c_k B_q,$$

$$\tilde{t}_1(z) = \tilde{\nu} J_0(z), \quad \tilde{\nu} = \nu/\Omega, \quad \text{and} \quad \tilde{\omega}_q = \omega_q/\Omega$$

Electron-phonon interactions IV

$$\gamma_{k,q}(z) = \tilde{g}_q(1 - \eta_{k,q}(z)\,\lambda^2)$$

$$\eta_{k,q}(z) = \sum_{m>0} \left(\frac{\bar{\epsilon}_{k+q,m}(z) - \bar{\epsilon}_{k,m}(z)}{m} \right)^2$$

$$\tilde{g}_q = g_q/\Omega$$

$$\bar{\epsilon}_{k,2n} = \epsilon_{k,2n} \text{ or } \bar{\epsilon}_{k,2n+1} = 2\nu\, J_{2n+1}(z) \sin(k)/\delta E$$

$$\epsilon_{k,m}(z) = 2\nu\, J_m(z) \cos(k)/\delta E$$

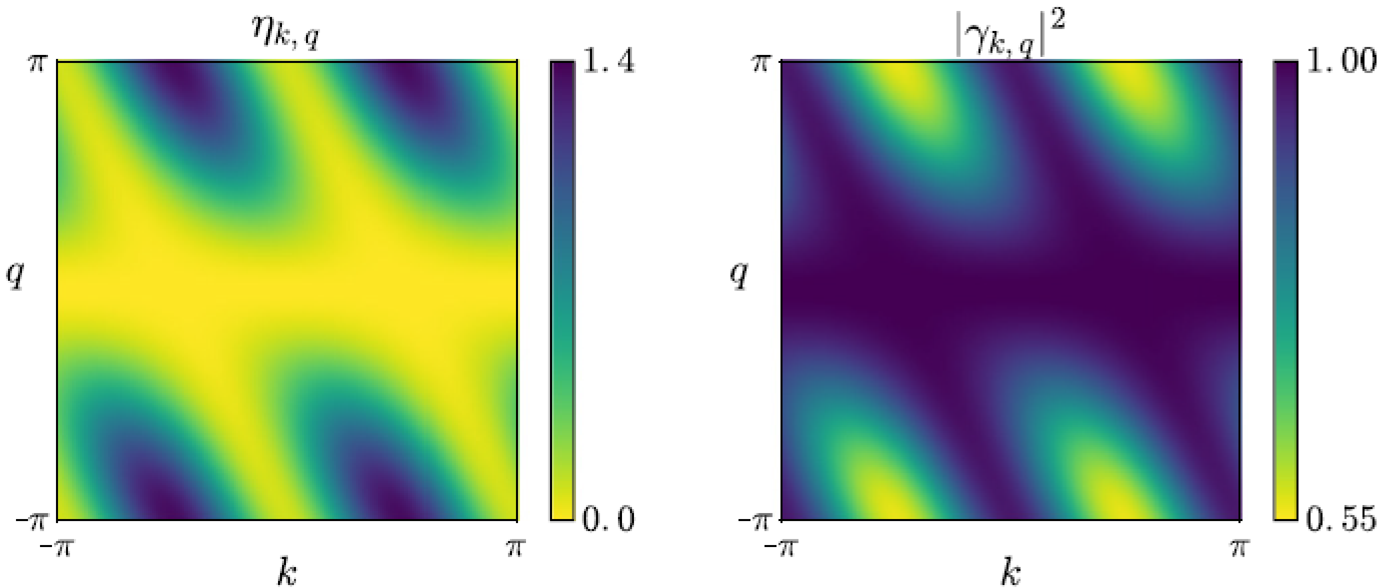


FIG. 1. Third-order correction $\eta_{k,q}$ (left) and effective electron-phonon coupling $\gamma_{k,q}$ in units of g_q (right) for $\Omega = 5\nu$ and $z = 1.8$.

Electron-phonon interactions V

The effective interaction Hamiltonian in real space (if the bare one is local), $g_q = g_0$

$$\tilde{H}_{ep} = \tilde{g}_0 \sum_n c_n^\dagger c_n \, B_n + \tilde{g}_1(z) \sum_n c_n^\dagger c_n (B_{n-1} - 2B_n + B_{n+1})$$

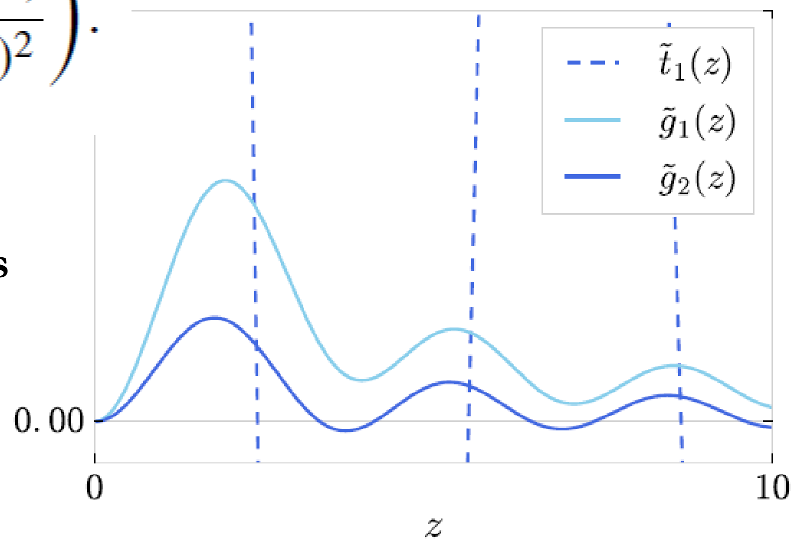
$$+ \tilde{g}_2(z) \sum_n c_n^\dagger c_{n+2} (B_n - 2B_{n+1} + B_{n+2}) + \text{H.c.},$$

$$\tilde{g}_0 = \frac{g_0}{\Omega}, \quad \tilde{g}_1(z) = \frac{1}{2}\frac{g_0}{\Omega}\left(\frac{2\nu}{\Omega}\right)^2 \sum_{m>0} \frac{J_m^2(z)}{m^2},$$

$$\tilde{g}_2(z) = \frac{1}{4}\frac{g_0}{\Omega}\left(\frac{2\nu}{\Omega}\right)^2 \sum_{m>0}\left(\frac{J_{2m-1}^2(z)}{(2m-1)^2} - \frac{J_{2m}^2(z)}{(2m)^2}\right).$$

Renormalized coupling constants

$\Omega = 5\nu$ and $g_0 = \nu$



Electron-phonon interactions VI

Peierls-Feynman-Bogoliubov variational principle $F \le F^* + \left\langle \hat{H} - \hat{H}^* \right\rangle^*$

F – **free energy, corresponding to the Hamiltonian** H, H^* - **trial Hamiltonian,** F^* - **its free energy**

Mapping to polaronic Hamiltonian

$$H^* = \tilde{\omega}_0 \sum_q b_q^\dagger b_q - \tilde{\Delta} \sum_n c_n^\dagger c_n + t_1^* \sum_n (c_{n+1}^\dagger c_n + \text{H.c.})$$
$$+ t_2^* \sum_n (c_{n+2}^\dagger c_n + \text{H.c.}). \qquad (46)$$

Effective energy shift (polaronic shift); renormalization of the first- and second-neighbour hoppings

But first, for H **- Lang-Firsov canonical transformation** $H = e^S \tilde{H} e^{-S}$

$$S = -\sum_{mq} u_q \, e^{-iqm} c_m^\dagger c_m \, (b_q - b_{-q}^\dagger), \quad u_q = \frac{\tilde{g}_q}{\tilde{\omega}_q}$$

Electron-phonon interactions VII

Polaron dispersion $$\xi_k^*(z) = 2t_1^*(z)\cos(k) + 2t_2^*(z)\cos(2k) - \tilde{\Delta}(z)$$

$$\tilde{\Delta}(z) = \frac{\tilde{g}_0^2 - 4\tilde{g}_0\tilde{g}_1(z)}{\tilde{\omega}_0}$$

$$t_1^*(z) = \tilde{t}_1(z)\exp\left(-(2N_0+1)\frac{\tilde{g}_0^2 - 6\tilde{g}_0\tilde{g}_1(z)}{\tilde{\omega}_0^2}\right)$$

$$t_2^*(z) = \tilde{t}_2(z)\exp\left(-(2N_0+1)\frac{\tilde{g}_0^2 - 4\tilde{g}_0\tilde{g}_1(z)}{\tilde{\omega}_0}\right)$$

$\tilde{t}_2(z) = 2\frac{\tilde{g}_0\tilde{g}_2(z)}{\tilde{\omega}_0}$ **induced NNN hopping** $\tilde{t}_1(z) = \tilde{v}\,J_0(z)$ N_0 **Planck funtion**

Electron-phonon interactions VIII

Floquet spectrum (quasienergies are conserving modulo Omega)

Spectral density: electron spectrum is both renormalized and broaden)

Effective spectral density: for effective static Hamiltonian

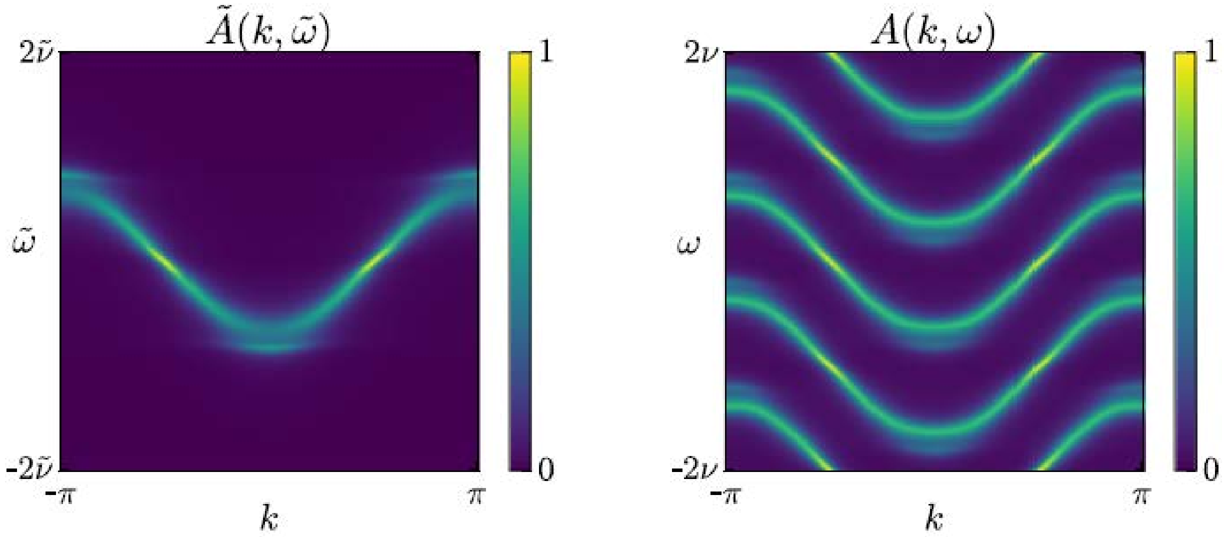
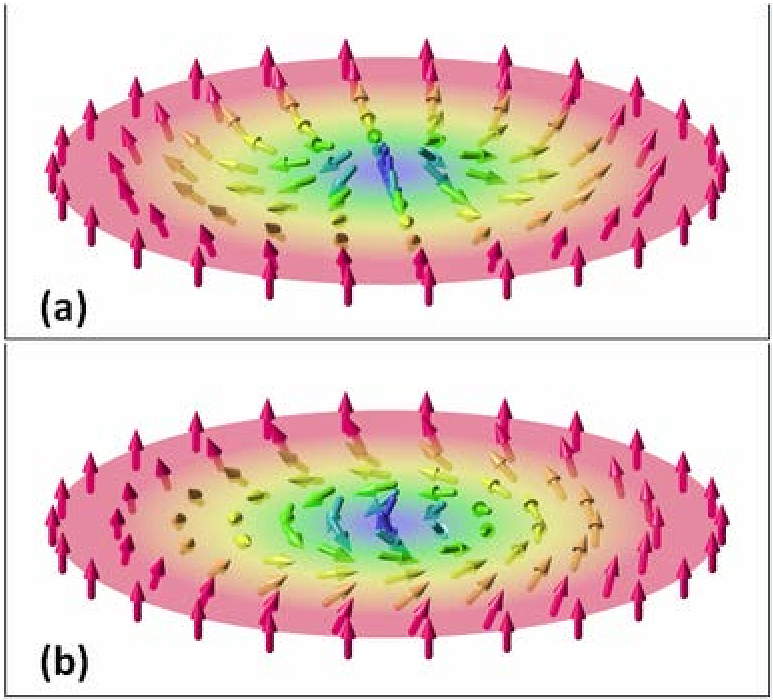


FIG. 5. Effective and Floquet spectral functions for $\Omega = 5\nu$ (left) and $\Omega = \nu$ (right), respectively. Both spectral functions have been computed for zero temperature with the following parameters: $\omega_0 = 0.1\nu$, $g_0 = 0.2\nu$, $z = 1.8$, and $\delta = 0.01$.

Dynamical control of spin textures

Motivation: **magnetic skyrmions, topological magnetic defects supposed to be useful for ultradense information storage**



(Magnetic skyrmion – Wikipedia)

A hot subject (e.g., Europhysics Prize 2016)

Experimentally observed in MnSi, (Fe,Co)Si, Fe:Ir(111), etc.

Importantly: in the most of cases (not always) they result from competition of exchange and Dzialoshinskii-Moriya (DM) magnetic interactions

$$\hat{H} = \sum_{ij} J_{ij} \hat{\vec{S}}_i \hat{\vec{S}}_j + \sum_{i\mu\nu} \hat{S}_i^{\mu} A_i^{\mu\nu} \hat{S}_i^{\nu} + \sum_{ij} \vec{D}_{ij} [\hat{\vec{S}}_i \times \hat{\vec{S}}_j]$$

The last term (DMI) has a smallness in spin-orbit coupling

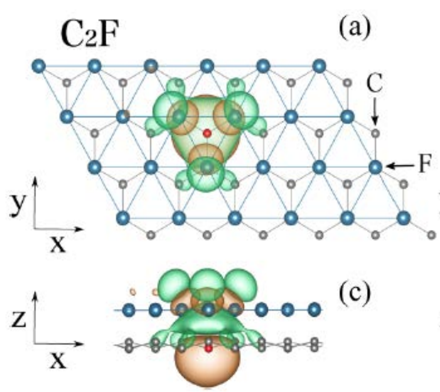
Dynamical control of spin textures II

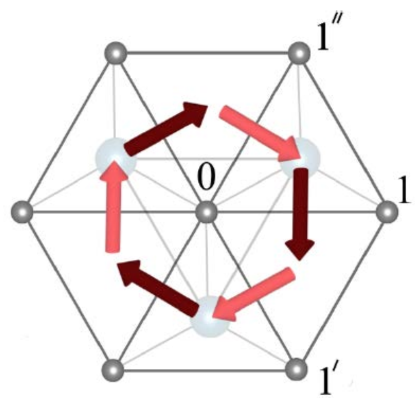
Model systems (single-band, strongly correlated): C_2F, Pb:Si(111), Sn:Si(111),Sn:SiC(0001)

PHYSICAL REVIEW B **94**, 214411 (2016)

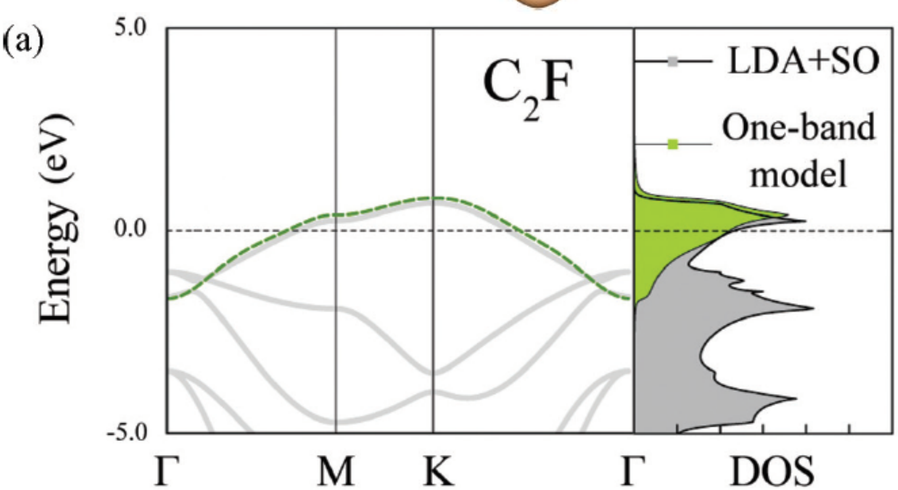
Role of direct exchange and Dzyaloshinskii-Moriya interactions in magnetic properties of graphene derivatives: C_2F and C_2H

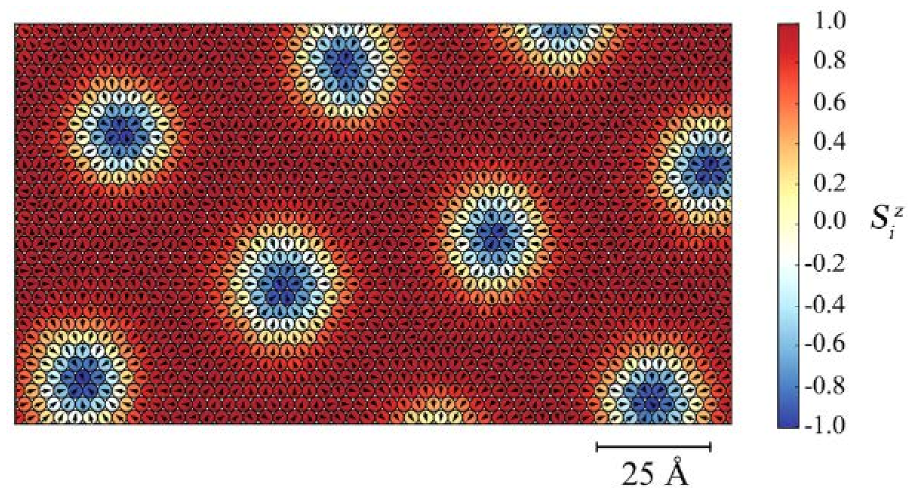
V. V. Mazurenko,[1] A. N. Rudenko,[1,2] S. A. Nikolaev,[1] D. S. Medvedeva,[1] A. I. Lichtenstein,[1,3] and M. I. Katsnelson[1,2]





Calculated DMI vectors (light and dark – positive and negative z components)



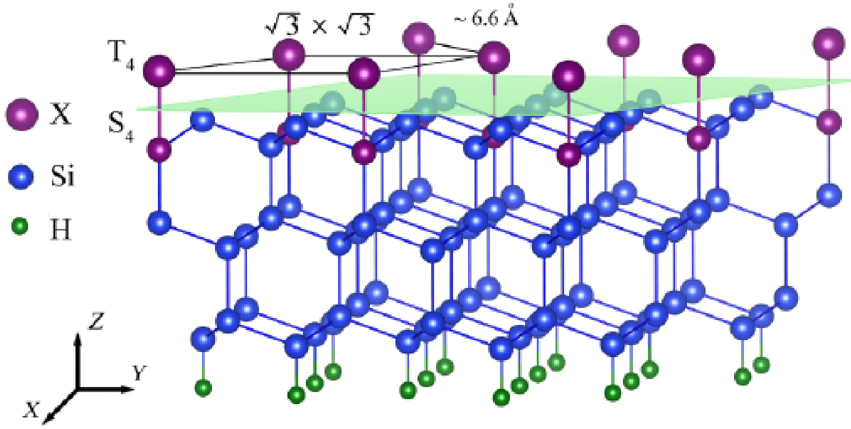


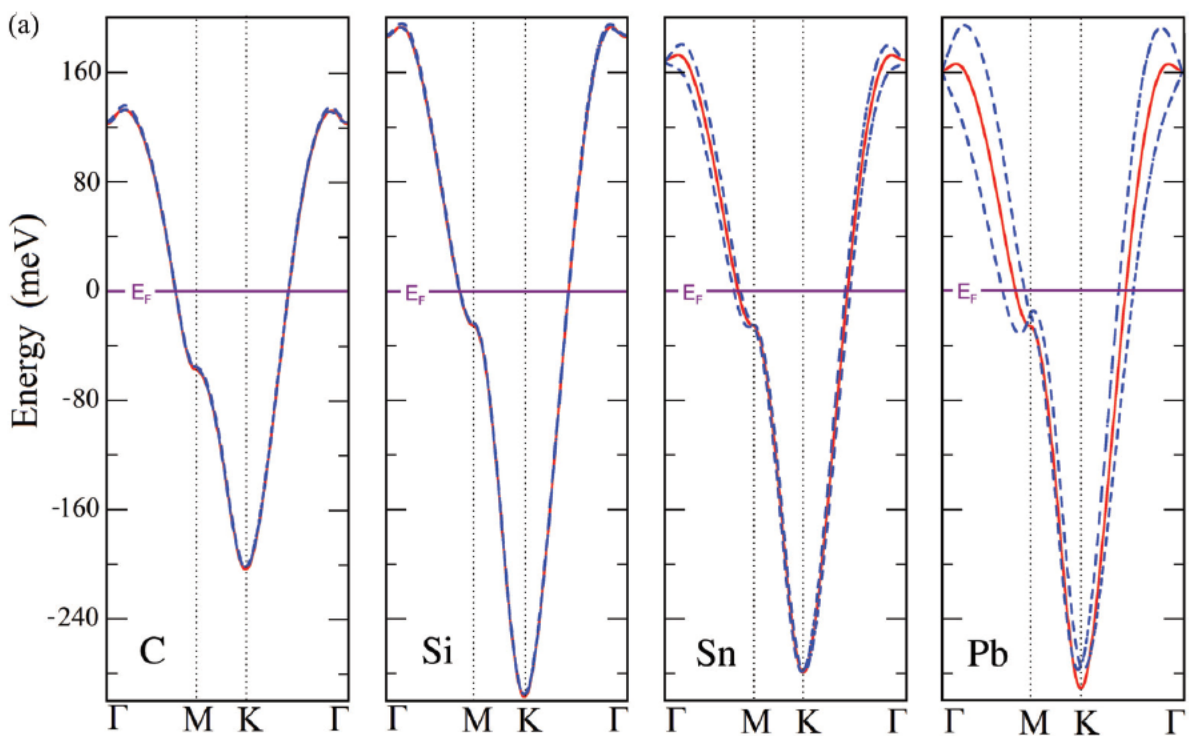
Dynamical control of spin textures III

PHYSICAL REVIEW B **94**, 224418 (2016)

Spin-orbit coupling and magnetic interactions in Si(111):{C,Si,Sn,Pb}

D. I. Badrtdinov,[1] S. A. Nikolaev,[1] M. I. Katsnelson,[1,2] and V. V. Mazurenko[1]



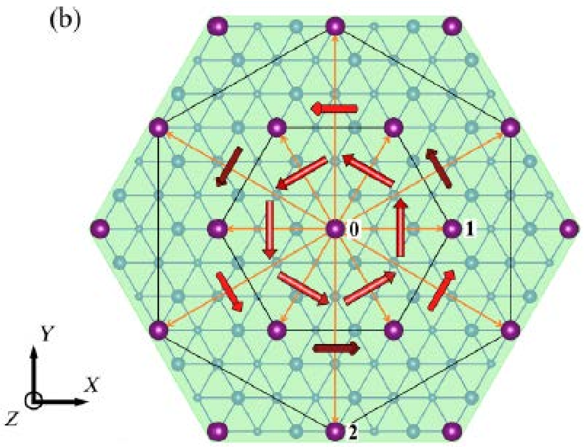


Single narrow band nea the Fermi energy

Red – without SO
Blue – with SO

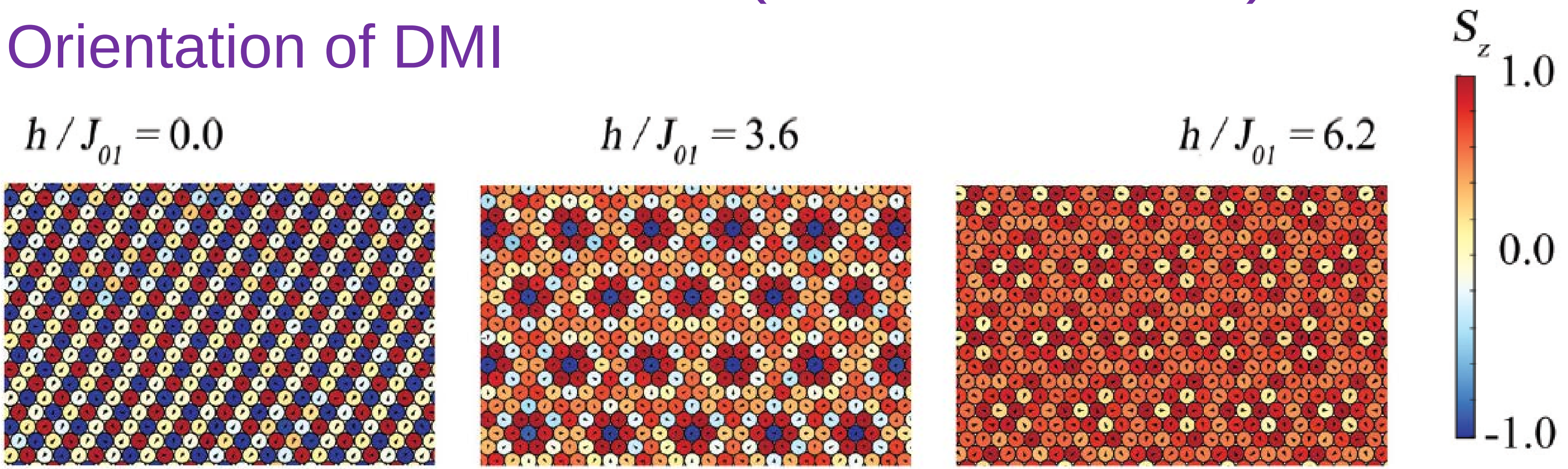
Dynamical control of spin textures IV

Mott insulator if take into account Hubbard U



Orientation of DMI

Ground state magnetic configurations for Si(111):Pb in magnetic field (MC simulations)



Dynamical control of spin textures V

E. A. Stepanov, C. Dutreix & MIK, Phys. Rev. Lett. 118, 157201 (2017)

The model:

$$H = \sum_{\langle ij\rangle,\sigma\sigma'} c^*_{i\sigma}(t\delta_{\sigma\sigma'} + i\varDelta_{ij}\boldsymbol{\sigma}_{\sigma\sigma'})c_{j\sigma'} + \sum_i U_{00} n_{i\uparrow} n_{i\downarrow}$$

$$+ \frac{1}{2}\sum_{\langle ij\rangle,\sigma\sigma'} U_{\langle ij\rangle} n_{i\sigma} n_{j\sigma'} - \frac{1}{2}\sum_{\langle ij\rangle,\sigma\sigma'} J^{\mathrm{D}}_{\langle ij\rangle} c^*_{i\sigma} c_{i,\sigma'} c^*_{j,\sigma'} c_{j\sigma},$$

(spin-orbit coupling Δ is inluded!) $\varDelta_{ij} = (\Delta^x_{ij}, \Delta^y_{ij}, 0) = -\boldsymbol{\Delta}_{ji}$

High-frequency laser field

$\mathbf{k} \to \mathbf{k} - e\mathbf{A}(t)$ $\mathbf{A} = (A_x a_0 \cos(\Omega t), A_y a_0 \sin(\Omega t - \phi), 0)$

light polarization elliptic for $\phi = 0$ and linear for $\phi = \pi/2$

The lowest-order renormalization): $t' = t\mathcal{J}_0(Z)$ $\boldsymbol{\Delta}'_{ij} = \boldsymbol{\Delta}'_{ij}\mathcal{J}_0(Z)$

$$Z = eE_0 a_0/\Omega$$

Dynamical control of spin textures VI

Effective spin Hamiltonian (via operator perturbatuon theory)

$$H_{\text{spin}} = -\sum_{\langle ij \rangle} J_{ij} \hat{\mathbf{S}}_i \hat{\mathbf{S}}_j + \sum_{\langle ij \rangle} \mathbf{D}_{ij} [\hat{\mathbf{S}}_i \times \hat{\mathbf{S}}_j].$$

$$\mathbf{D}_{ij} = 4t' \mathbf{\Delta}_{ij}' / \tilde{U}, \text{ where } \tilde{U} = U_{00} - U_{\langle ij \rangle}$$

Plus: renormalization of exchange interactions via Itin & MIK, 2015

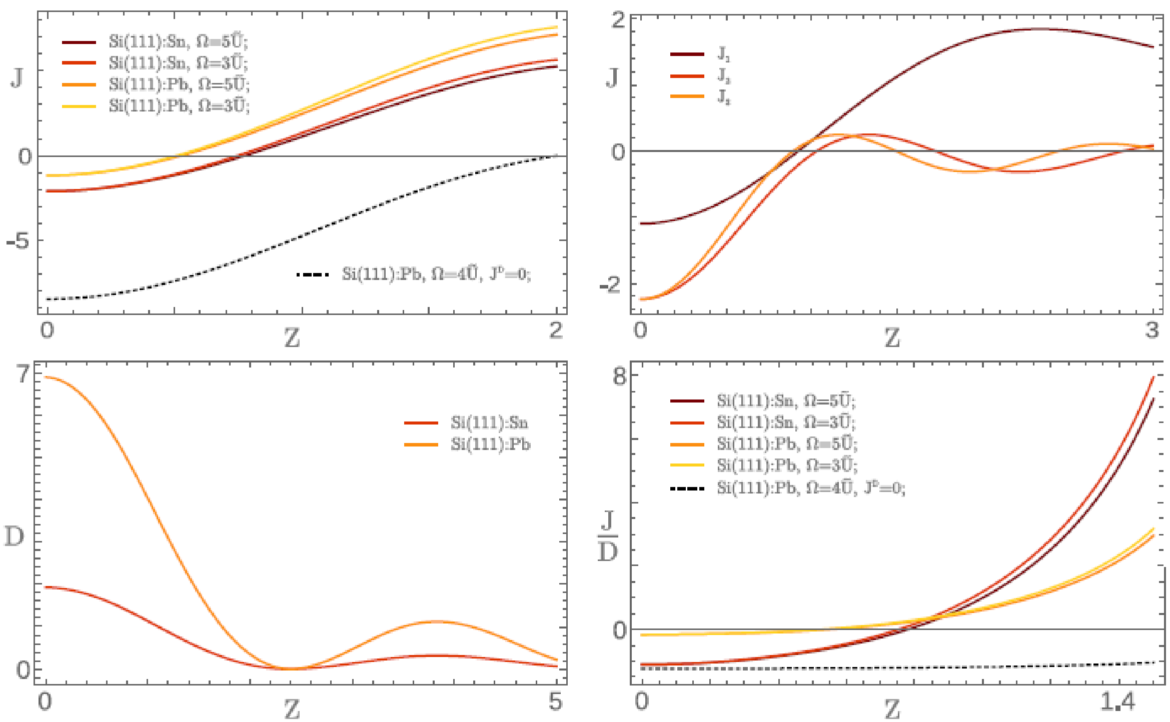


FIG. 1. Magnetic properties of the Si(111):{Sn, Pb} systems as functions of the laser field strength Z for different frequencies $\Omega = 3\tilde{U}, 5\tilde{U}$: exchange interactions J (top left), DMI (bottom left), ratio J/D, which is proportional to a Skyrmion radius (bottom right). Dashed black curve corresponds to the case of zero direct exchange and shows the important role that J^D plays in a phase transition and manipulation of the Skyrmionic structure. Top right panel shows NN and next-NN exchange interactions of Si(111):C, where we take "unrealistic" case of $t_1 = t_2 = t_3$ to make the difference in anti-FM–FM transition more visible. All units are given in meV.

Dynamical control of spin textures VII

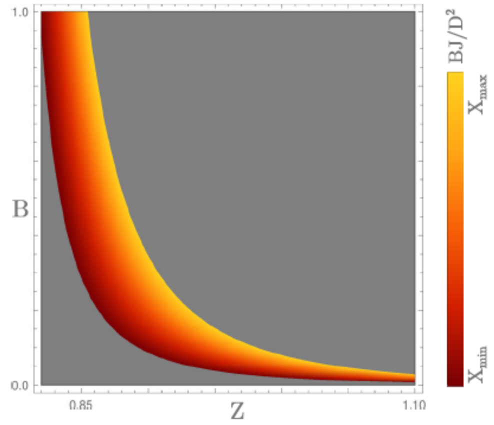


FIG. 2. Stable Skyrmionic phase for the Si(111):Sn as a function of laser field amplitude Z and magnetic field $\tilde{B} = B/J_{A=0}$ given in units of the initial exchange interaction $J_{A=0}$, $\Omega = 4\tilde{U}$.

Other way to stabilize skyrmions: via competing exchange interactions

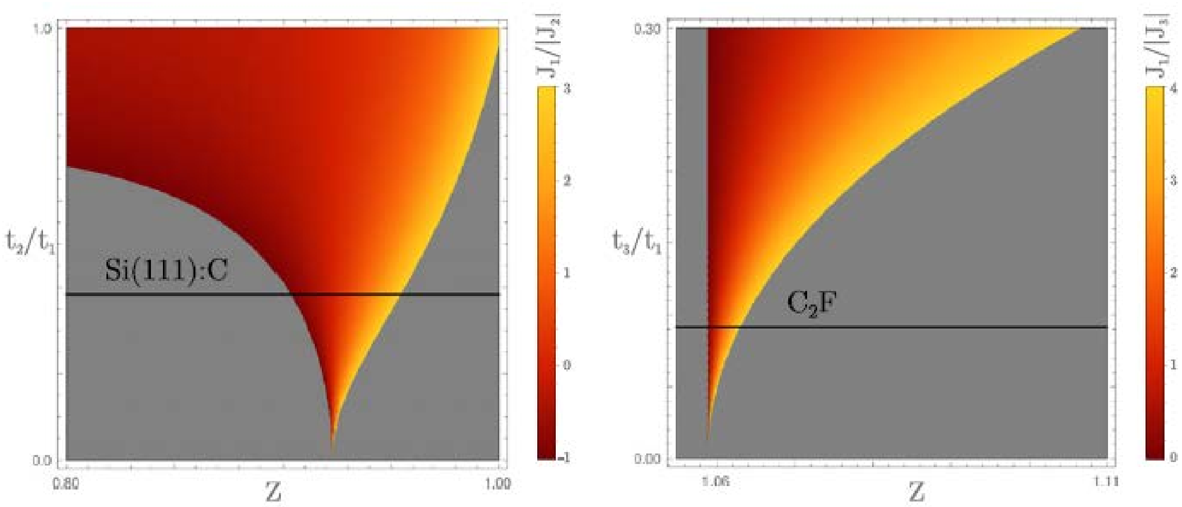


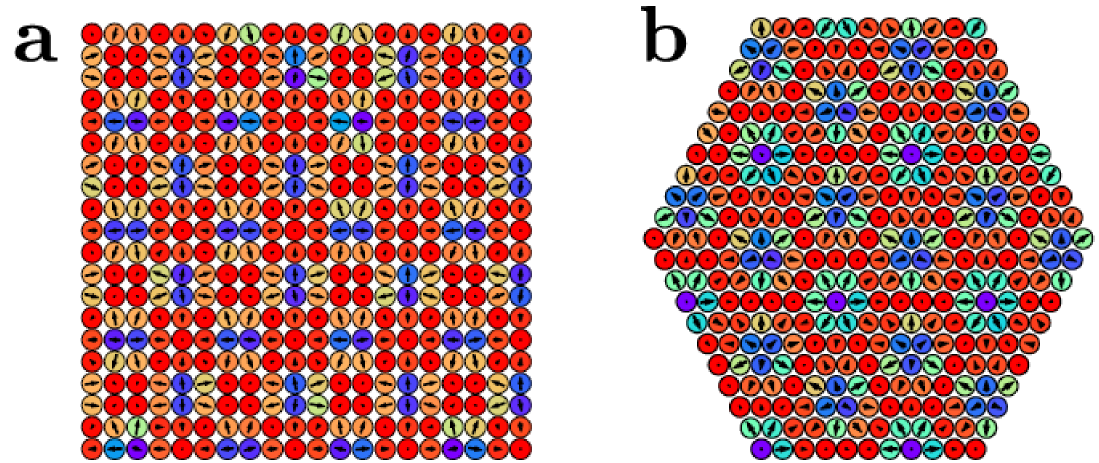
FIG. 3. Hopping amplitudes $t_{2(3)}/t_1$ as the function of the amplitude Z of the laser field for the values $J_1/|J_{2(3)}|$ that correspond to the Skyrmionic phase. Frequency of the laser field is $\Omega = 3\tilde{U}$.

Dynamical control of spin textures VIII

Stepanov, Nikolaev, Dutreix, MIK & Mazurenko, arXiv:1710.03044

Usually *J* >> *D*; with laser field one can inverse this and even reach the regime *J* = 0

Exchange-free nanoslyrmion mozaik



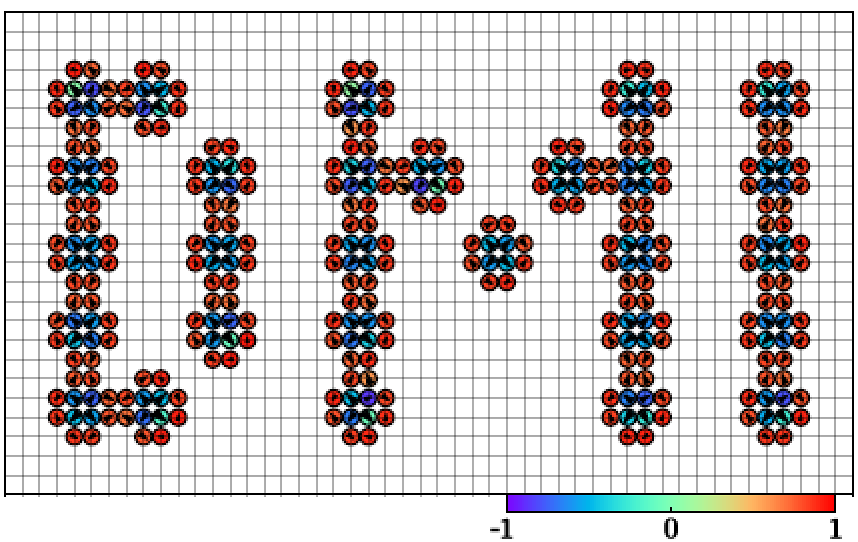
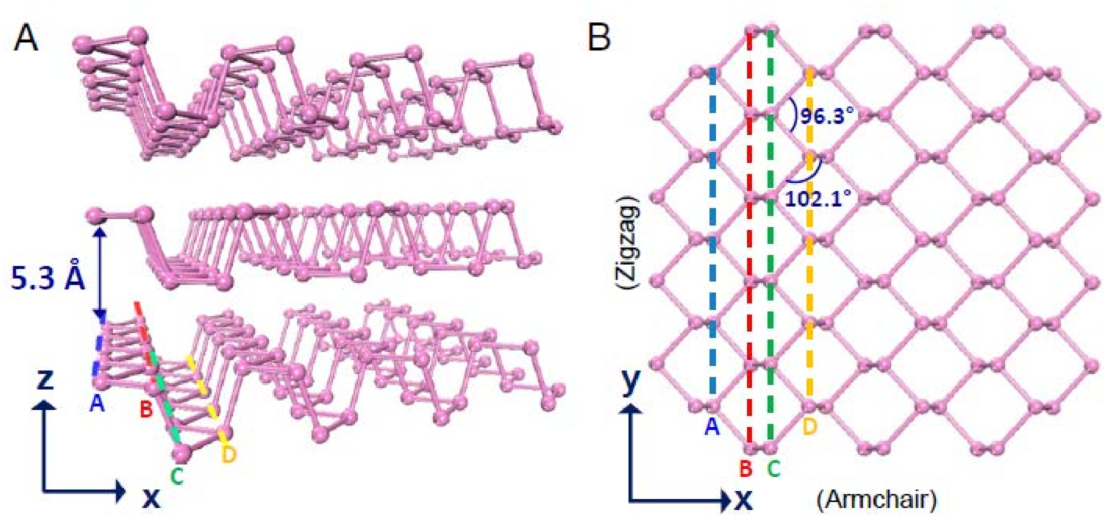


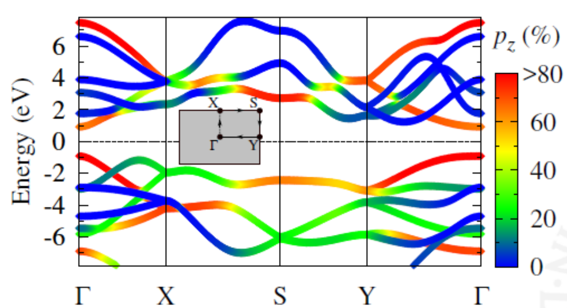
FIG. 1. Stable nanoskyrmion-designed DMI abbreviation resulting from the Monte Carlo simulation of the Heisenberg-exchange-free model on the non-regular square lattice with B_z = 1.2. Arrows and color depict the in- and out-of-plane spin projection, respectively.

Laser-induced topological transitions

C. Dutreix, E. A. Stepanov & MIK, Phys. Rev. B 93, 241404(R) (2016)

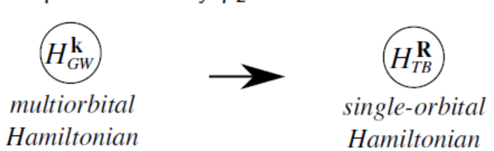
Black phosphorus: novel two-dimensional semiconductor





Electronic structure: semiconductor

- Valence and conduction band edges are isolated
- ...and have predominantly p_z character



In bilayer, electric bias creates insulator-semimetal transition; but with high-frequency laser field one can make it for the single layer

Laser-induced topological transitions II

Mapping to tight-binding model

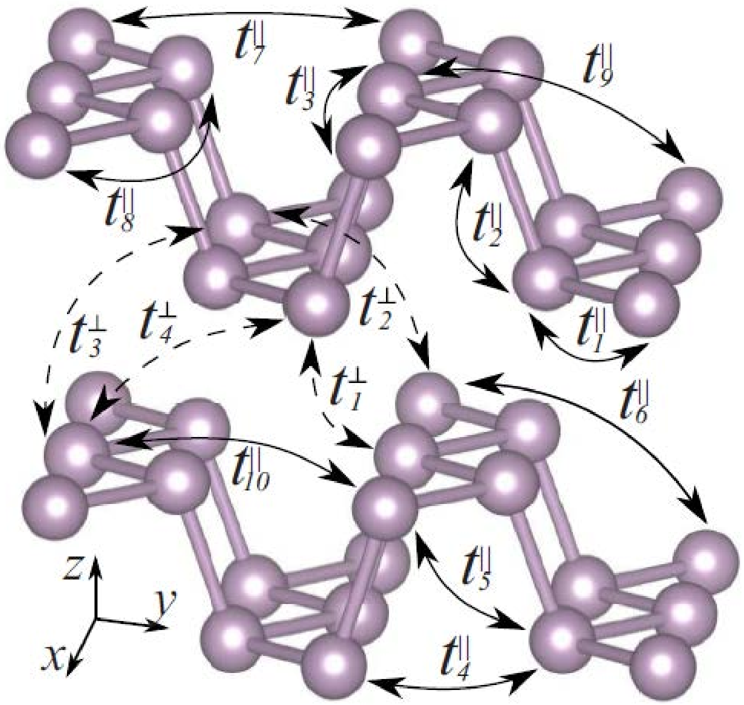


TABLE II. Intralayer ($t^{\parallel}$) and interlayer ($t^{\perp}$) hopping parameters (in eV) obtained in terms of the TB Hamiltonian [Eq. (1)] for multilayer BP. d and N_c denote the distances between the corresponding interacting lattice sites and coordination numbers for the given distance, respectively. The hoppings are schematically shown

Intralayer				Intralayer				Interlayer			
No.	$t^{\parallel}$ (eV)	d (Å)	N_c	No.	$t^{\parallel}$ (eV)	d (Å)	N_c	No.	$t^{\perp}$ (eV)	d (Å)	N_c
1	−1.486	2.22	2	6	0.186	4.23	1	1	0.524	3.60	2
2	3.729	2.24	1	7	−0.063	4.37	2	2	0.180	3.81	2
3	−0.252	3.31	2	8	0.101	5.18	2	3	−0.123	5.05	4
4	−0.071	3.34	2	9	−0.042	5.37	2	4	−0.168	5.08	2
5	−0.019	3.47	4	10	0.073	5.49	4	5	0.000	5.44	1

The main difference with graphene: a very large and positive second-neighbour hopping in plane; interlayer hopping is roughly of the same order of magnitude

A. Rudenko & MIK, Phys. Rev. B 89, 201408 (2014); A. Rudneko, S. Yuan & MIK, Phys. Rev. B 92, 085419 (2015)

Laser-induced topological transitions III

Single-particle Hamiltonian (only bands), Peierls substitution

$$\mathbf{A}(t) = (A_x \cos \Omega t, A_y \sin[\Omega t - \phi], 0)$$

Second-order effective static Hamiltonian

On can pass from band insulator to topological insulator or to semimetal

Elliptic polarization: topological insulator
Linear polarization: semimetal, no gap

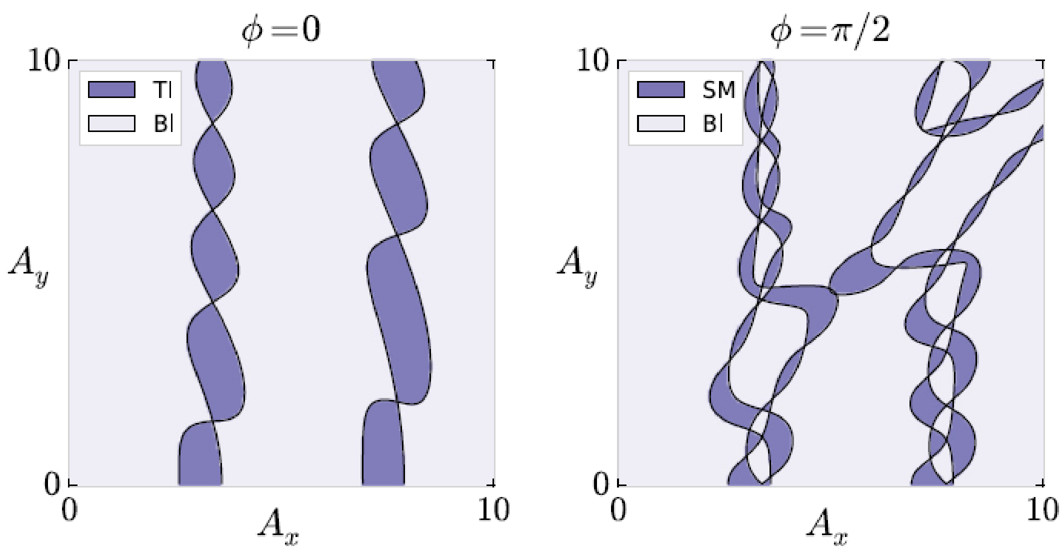
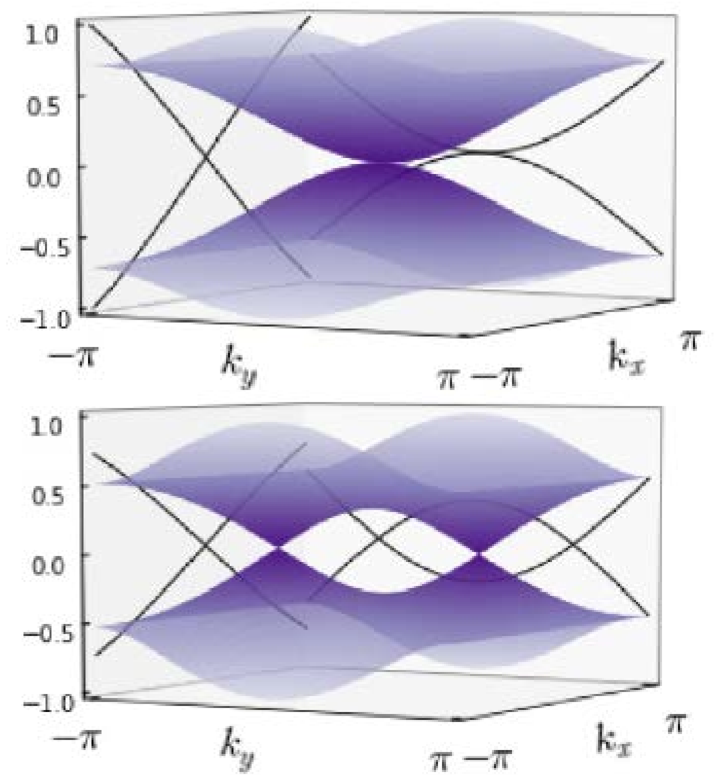


FIG. 3. Phase diagrams for electric fields with elliptic (left) and linear (right) polarizations. Light purple areas refer to band insulating (BI) phases characterized by $e^{i\gamma c} = +1$. Dark purple areas correspond to semimetallic (SM) and topological insulating (TI) phases in which $e^{i\gamma c} = -1$. Components A_x and A_y are given in $Å^{-1}$.

Lowest-energy bands in semimetallic phase



Resume

"Kapitza pendulum" has analog for quantum many-body systems: one can engineer quantum Hamiltonians by high-frequency modulation of the Hamiltonian parameters

Problem: heating by strong laser field

Systems with narrow defect bands (like C_2H or Sn:Si(111)) may be a solutionL frequency is much higher than the defect band width but stil within the gap of host semiconductor, weak light absortption (*exponentially* weak in simple models)

The other application: ultracold gases in optical lattices ("quantum simulators"). Mathematics is the same, physical realization can be easier (may be not so interesting for potential applications but.... quantum computing?!)

MANY THANKS FOR YOUR ATTENTION