Metallicity and superconductivity of the hydrogen-rich compounds

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supercomputing
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Auckland, February 5, 2019

Kraków, Department of Condensed Matter Theory

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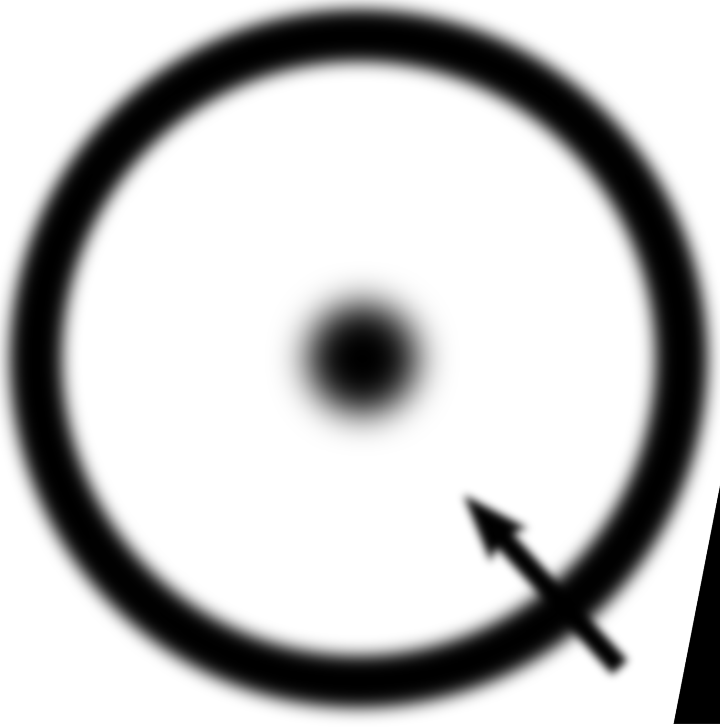


QMT

Quantum Metallization Tools

Sources

`https://bitbucket.org/azja/qmt`

♠ J. Spałek et al., Phys. Rev. B **61**, 15676 (2000);

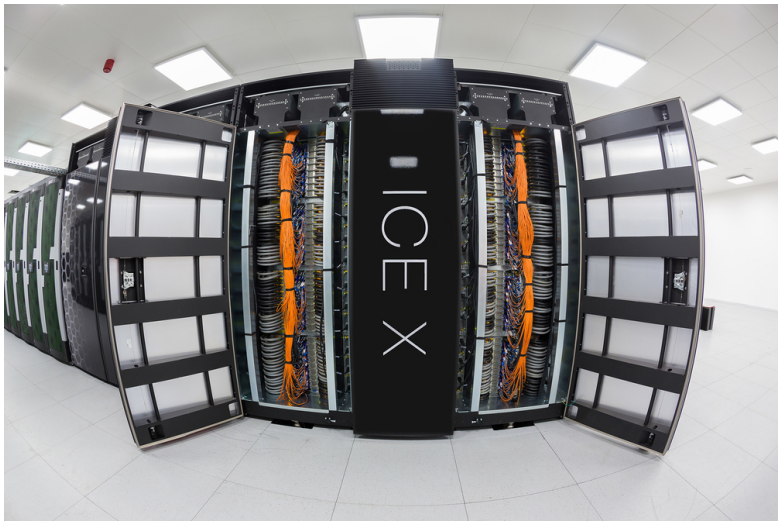
♣ APK et al., Eur. Phys. J. B **86**, 252 (2013);

♦ A. Biborski, APK, J. Spałek, Comput. Phys. Commun. **197**, 7 (2015);

♡ A. Biborski, APK, J. Spałek, Phys. Rev. B **98**, 085112 (2018).

Ostrava, IT4Innovations - Czech National Supercomputing Center

Three clusters: Anselm, Salomon (**TOP500**, peak performance 2.011 PFLOPS DP) and [ ] ($\sim$ 1.8 PFLOPS DP; GPU on each node).



Research - Leading Directions

1. Design of materials for the fission, fussion and nuclear fuels
2. Protective and thermal coatings, ultrahard materials and 2D films
3. Magneto-optical, laser induced and multiferroic phenomena
4. Dimensionality reduced magnetic interactions

People

Dominik Legut (Team leader), Sergiu Arapan, Jaroslav Chovan, Stella Skiadopulou, Lukaš Kyvala, Michal Farana, Petr Dvoracek

Utilization of HPC resources

Quantum mechanical calculations of electronic structure
$\rightarrow$ material properties, physical phenomena

- 100 *MCh* in last 5 years;
- more than 50 publications;
- $\sim 25 - 30\%$ of IT4I's total computational power

Methods

- Pseudopotential and all electron codes (VASP, Wien2k, Elk)
- Genetic predictive algorithms (USPEX, Calypso)
- Machine learning (TensorFlow)
- Original code - Xray optics, transport, annealing, magnetic properties
- Molecular dynamics (LAMMPS)

Outline

R. P. Dias, I. F. Silvera, Science 10.1126/science.aal1579 (2017)

The New York Times


Mount Etna, Europe's Most Active Volcano, Puts On a Show


In California, a Move to Ease the Pressures on Aging Dams


Edward E. David Jr., Who Elevated Science Under Nixon, Dies at 92


Before Vaquitas Vanish, a Desperate Bid to Save Them

SCIENCE

Hydrogen Squeezed Into a Metal, Possibly Solid, Harvard Physicists Say

By KENNETH CHANG JAN. 26, 2017

Frankfurter Allgemeine Wissen

MATERIALFORSCHUNG EXTREM

Wasserstoff zu Metall gequetscht?

VON MANFRED LINDINGER

Ingeniøren

Nyheder Blogs Debat Jobfinder Avisen Mere

VORES FOKUS | KUNSTIG INTELLIGENS | 3D-PRINT | DIESELSKANDALEN | KAMPFLY FOR MILLI

Metallisk hydrogen sætter forskerverdenen i kog

Påstand om fremstilling af metallisk hydrogen mødes med meget hård kritik fra forskere. Lige til skraldepanden, lyder det. Andre bakker dog de kritiserede forskere op.

Af Jens Ramskov 2. feb 2017 kl. 12:03

ВЕСТИ.RU Новости Видео Фотолента Трансляции Сервисы

Тема: Сверхпроводники и изучение сверхпроводимости

Новости | Наука

30 января 2017 15:00 | Дарья Загорская

Прорыв в физике? Твёрдый металлический водород, возможно, стал реальностью

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TECH HOME COMPUTERS GOOGLE VIDEO GAMES MILITARY TECH WAR GAMES SLIDESHOWS

INNOVATION

Scientific breakthrough lost? Unique

Le Scienze

EDIZIONE ITALIANA DI SCIENTIFIC AMERICAN

Le Scienze | Mente&cervello | comportamento | epidemiologia | onde gravitazional

31 gennaio 2017

Idrogeno solido metallico, un annuncio e molti dubbi

Due ricercatori hanno annunciato di aver prodotto per la prima volta idrogeno solido metallico, previsto per via teorica circa ottant'anni fa, un traguardo che aprirebbe la strada a nuove applicazioni, dai superconduttori ai propellenti per razzi. Ma non pochi scienziati nutrono dubbi riguardo alle modalità con cui è stato svolto l'esperimento e dunque al suo risultato *(red)*

Credit: Ranga P. Dias/Isaac F. Silvera

indiatoday in NEWS Live TV

INDIA TODAY CONCLAVE 2017 ASSEMBLY ELECTIONS 2017 MAIL TODAY INDIA TODAY

World's first metallic hydrogen sample disappears

Last month physicists from Harvard University in the US had claimed to have successfully turned hydrogen into a metal - something researchers had been struggling to achieve for more than 80 years.

PTI | Posted by Bijin Jose

Boston, February 27, 2017 | UPDATED 19:20 IST

A+ A-

INDEPENDENT News Voices Culture Lifestyle Tech Sport Daily Edition Charity Appeal

News › Science

World's only piece of a metal that could revolutionise technology has disappeared, scientists reveal

Exclusive: Harvard University physicists say first-ever piece of metallic hydrogen on Earth has been lost after catastrophic failure of diamond holding it under enormous pressure

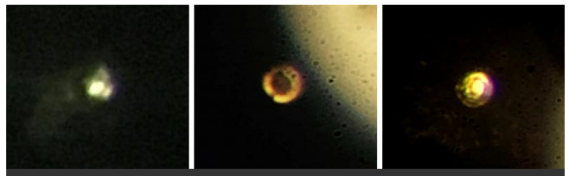
EDITION: INDIA REUTERS

Business Markets India World Tech Commentary Breakingviews Money Sport & Life

TECHNOLOGY NEWS | Fri Jan 27, 2017 | 10:02am IST

U.S. scientists create metallic hydrogen, a possible superconductor, ending quest

FULL COVERAGE: INDIA ELECTIONS 2017



RMF 24 NAJBLIŻEJ FAKTÓW

FAKTY OPINIE AKCJE RMF FM ROZRYWKA ZDJĘCIA FILMY

RMF 24 › Fakty › Nauka › Metaliczny wodór, materiał marzeń, stał się rzeczywistością

Metaliczny wodór, materiał marzeń, stał się rzeczywistością

Czwartek, 26 stycznia (23:40)

Jego istnienie fizycy przewidywali od 80 lat. Teraz wreszcie stał się faktem. Naukowcy z Uniwersytetu Harvarda ogłosili właśnie, że udało im się stworzyć metaliczny wodór, materiał o potencjalnie rewolucyjnych właściwościach. Na razie jego wytworzenie wymaga skrajnie niskiej temperatury i olbrzymiego ciśnienia, większego, niż w samym środku Ziemi, jeśli okazałby się stabilny w normalnych warunkach, mógłby być w temperaturze pokojowej nadprzewodnikiem. To oznaczałoby rewolucję w wielu

Metalization of Hydrogen

Prediction: Metalic state

E. Wigner i H. B. Huntington, J. Chem. Phys. **3**, 764 (1935):

- $H - H$ distance (d_{HH}),
- Wigner-Seitz radius ($r_s \equiv (\frac{3}{4\pi n})^{1/3}$).

Metalization at $p \approx 25 GPa$:

$$2r_s > d_{HH}.$$

Prediction: Superconductivity in $300K$

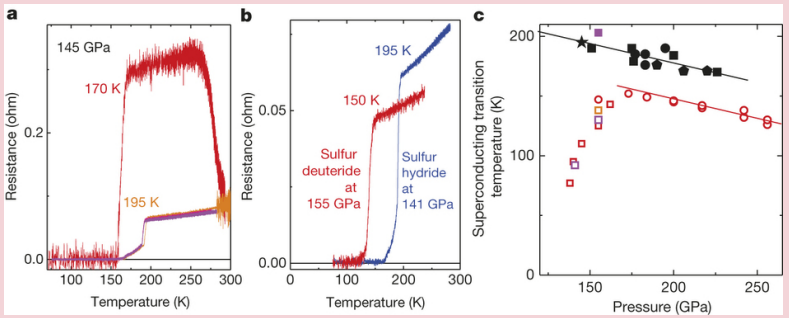
N. Ashcroft, PRL **21**, 1748 (1968)

$$T_C = \Theta_D \mathcal{F}(\text{el.-ph.})$$

	T_C (K)
Jupiter surface	$\sim 10^{-27}$
Jupiter core	~ 290

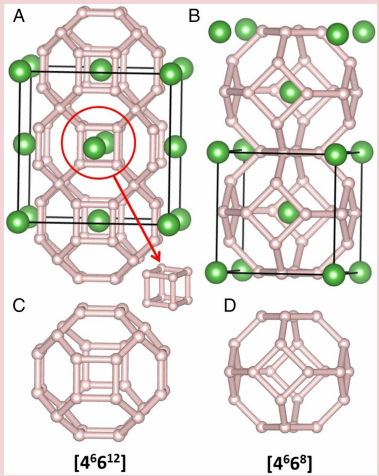
Hydrogen in 2D - superconductivity?

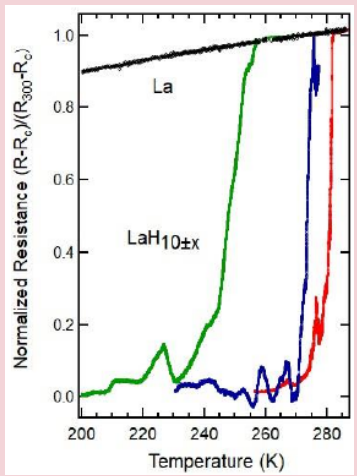
$H_{2|3}S$



A. P. Drozdov et al., Nature **525**, 73 (2015)

$LaH_{10 \pm x}$





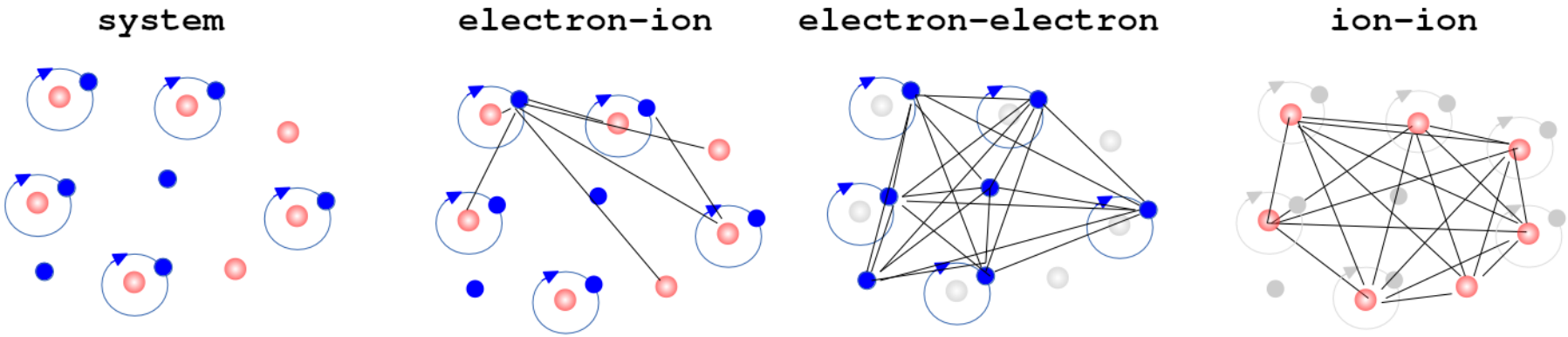
$L_{th.}$: Hanyu Liu et al., PNAS 114, 27 (2017)

$R_{exp.}$: M. Somayazulu et al., arXiv:1808.07695 (2018)

Picture

Born–Oppenheimer Approximation

$$\psi^{\text{total}} = \psi^{\text{electrons}} \otimes \psi^{\text{nuclei}}$$

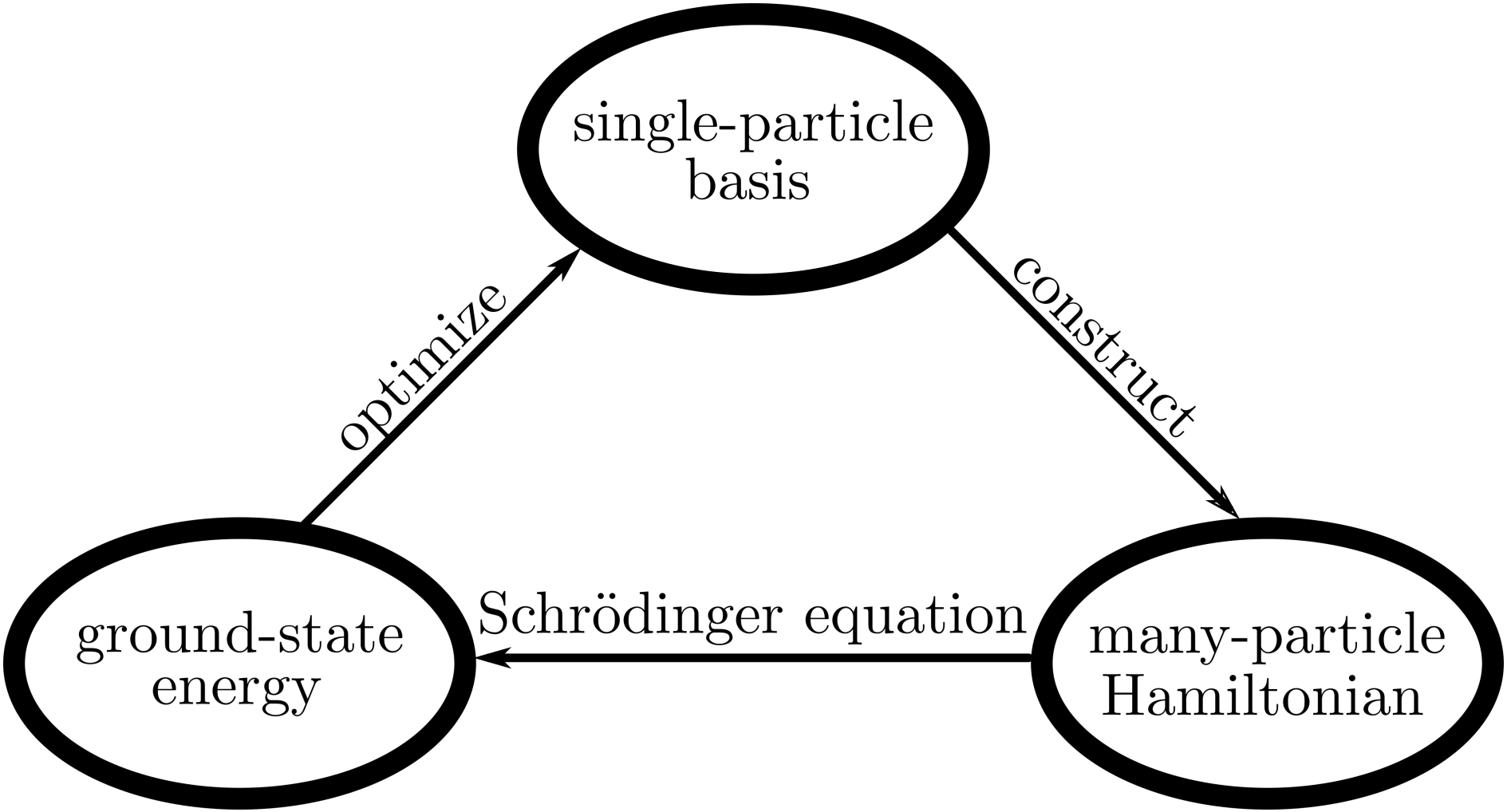


Hamiltonian

Rydberg atomic units $\hbar = 2m_e = \frac{e}{\sqrt{2}} = 1$

$$\mathcal{H} = \mathcal{T} + \mathcal{V}_{\text{el.–ion}} + \mathcal{V}_{\text{el.–el.}} + \mathcal{V}_{\text{ion–ion}}$$
$$-\sum_i \nabla_i^2 - \sum_{ij} \frac{2}{|\mathbf{r}_i - \mathbf{R}_j|} + \sum_{i>j} \frac{2}{|\mathbf{r}_i - \mathbf{r}_j|} + \sum_{i>j} \frac{2}{|\mathbf{R}_i - \mathbf{R}_j|}$$

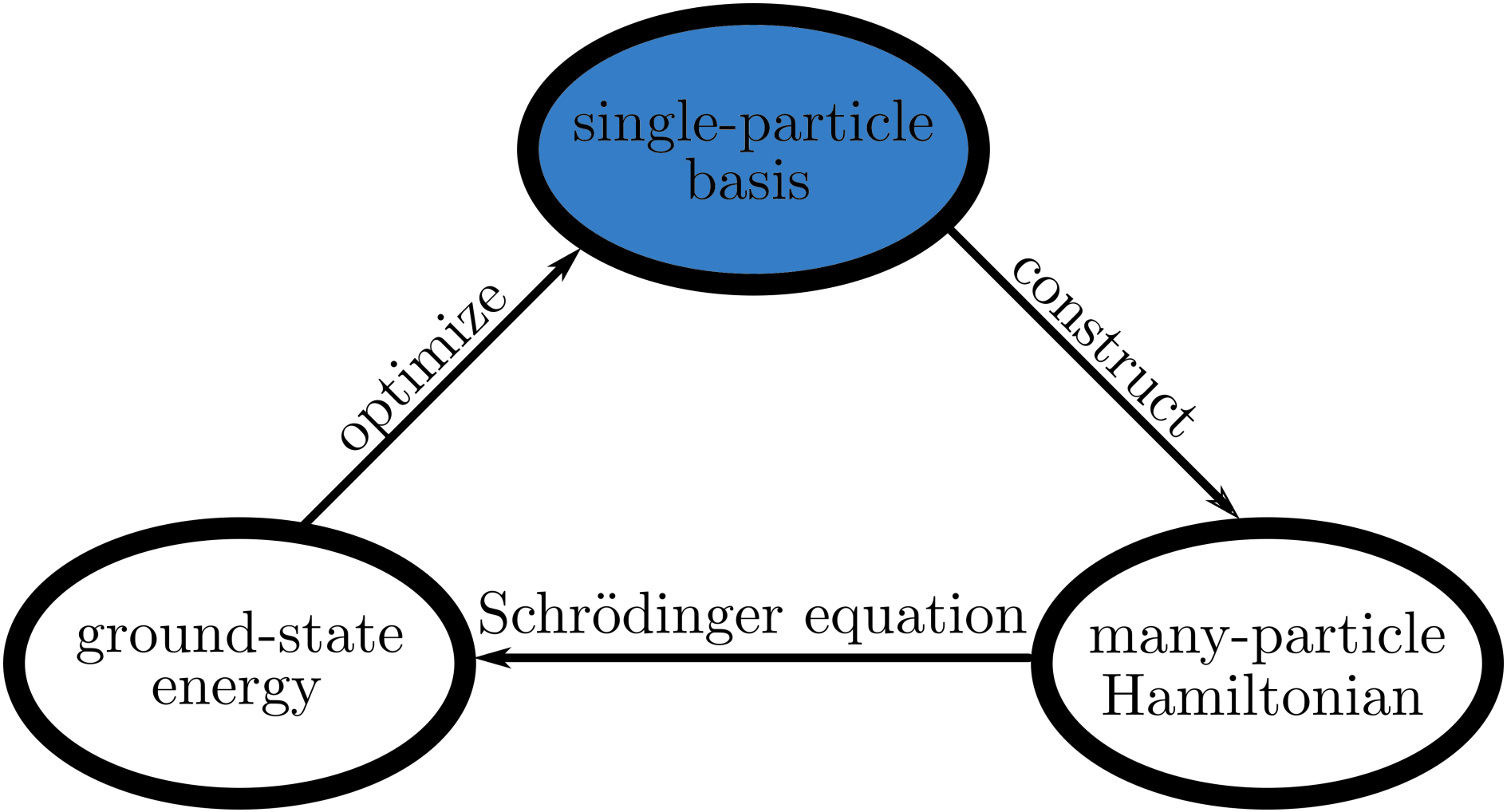
Exact Diagonalization Ab Initio (EDABI++)



Spiritus Movens: Using second quantization

Decoupling of single-particle picture and wavefunctions' algebra

Exact Diagonalization Ab Initio++ I



Single-particle basis

Conservation of complexity

Switching to the second quantization is effective only for the orthogonal bases (otherwise either $\left\{\hat{c}_i, \hat{c}_j^\dagger\right\} = \mathbb{S}_{ij}$ or $\hat{c}^{\,i} \equiv \mathbb{S}^{ij}\hat{c}_j^\dagger$).

LCAO

Orthogonal basis $\{w_i\}$ can be expressed as a linear combination of Slater orbitals $\{\psi_i\}$:

$$w_i(\mathbf{r}) \sum_k \beta_j \psi_j(\mathbf{r}),$$

satisfying orthonormality condition

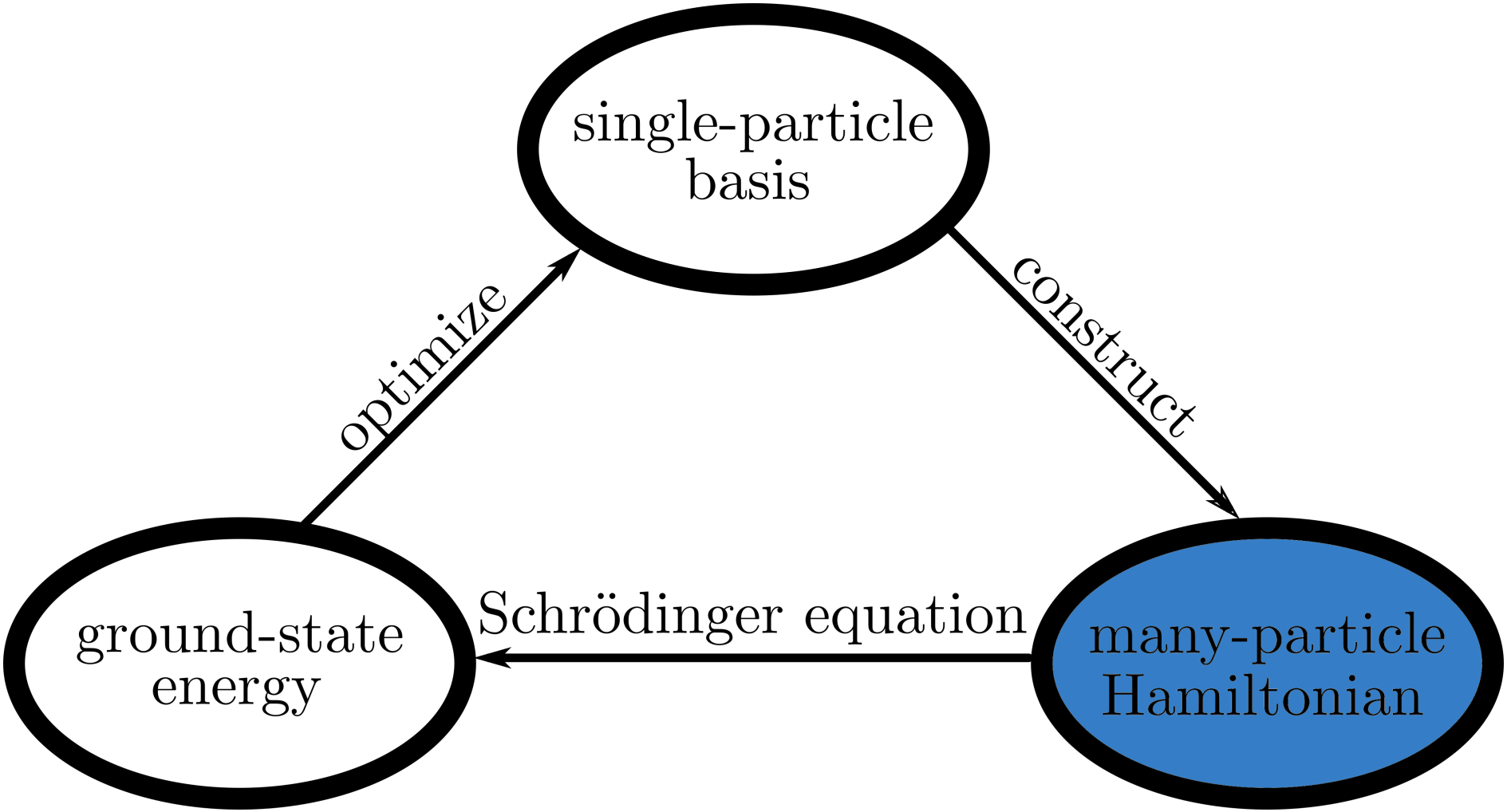
$$\langle w_i | \, w_j \rangle = \delta_{ij}.$$

Suitable methods

Let us define mixing matrix $\mathbb{W}_{ij} \equiv \langle w_i | \, \psi_j \rangle$.

- Löwdin orthogonalization
  - ♪ one solution close to starting orbitals
  - ∅ dense $\mathbb{W}$
  - ∅ requires sharp cut-off for infinite systems
- quadratic forms
  - ∅ many solutions
  - ♪∅ allows/requires symmetry constrains
  - ♪ sparse $\mathbb{W}$
  - ♪ systematic approach to infinity

Exact Diagonalization Ab Initio++ II



Hamiltonian

Hamiltonian and its parameters

By acting on the starting, first-quantization Hamiltonian with the field operator: $\Psi_i \equiv w_i(\mathbf{r})\chi_\sigma \hat{c}^\dagger_{i\sigma}$ we get the second-quantization Hamiltonian

$$\mathcal{H} = \sum_{\substack{i,j \\ \sigma}}^{\text{(P|A|R)BC}} t_{ij}\hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma} + \sum_{\substack{i,j,k,l \\ \sigma,\sigma'}}^{\text{(P|A|R)BC}} V_{ijkl}\hat{c}^\dagger_{i\sigma}\hat{c}^\dagger_{j\sigma'}\hat{c}_{l\sigma'}\hat{c}_{k\sigma} + \mathcal{H}_{\text{ext}} + \mathcal{V}_{\text{ion-ion}}$$

with fermionic creation/annihilation operators

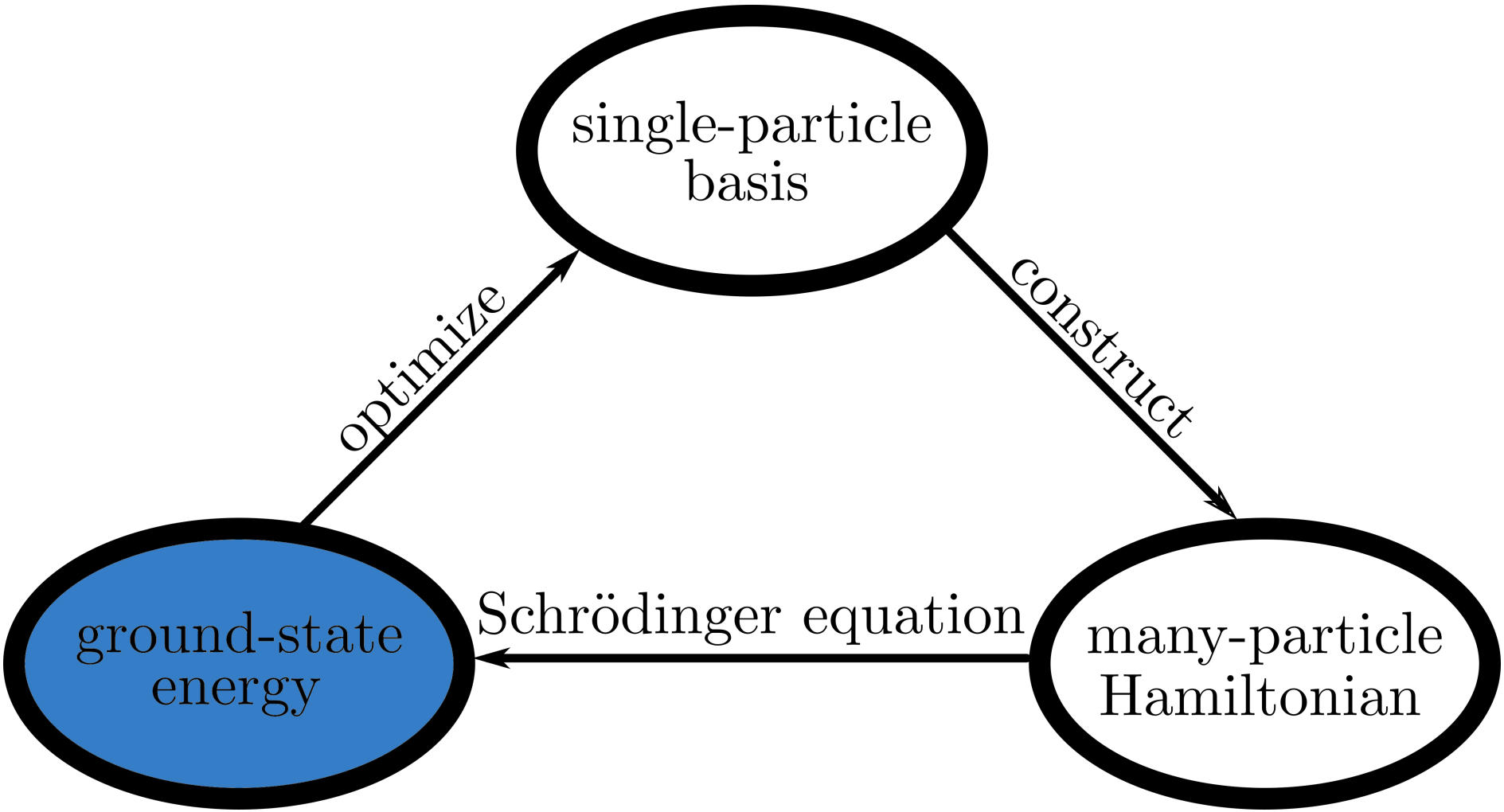
$$\{\hat{c}^\dagger_{i\sigma}, \hat{c}^\dagger_{j\sigma'}\} \equiv \{\hat{c}_{i\sigma}, \hat{c}_{j\sigma'}\} \equiv 0 \quad \text{and} \quad \{\hat{c}^\dagger_{i\sigma}, \hat{c}_{j\sigma'}\} \equiv \delta_{ij}\delta_{\sigma\sigma'}.$$

Hence, all of the information about single-particle wavefunction exists only in the microscopic parameters

$$t_{ij} = \left\langle w(\mathbf{r})_i \right| -\nabla^2 - \sum_{k=1}^{n} \frac{2}{|\mathbf{r} - \mathbf{R_k}|} \left| w(\mathbf{r})_j \right\rangle,$$

$$V_{ijkl} = \left\langle w(\mathbf{r})_i w(\mathbf{r}')_j \right| \frac{2}{|\mathbf{r} - \mathbf{r}'|} \left| w(\mathbf{r}')_k w(\mathbf{r})_l \right\rangle.$$

Exact Diagonalization Ab Initio++ III



Diagonalization core

Advantage

No constrains on diagonalization method

Already applied:

- Lanczos
- Truncated Lanczos
- Variational Monte Carlo
- Gutzwiller Wavefunction
- Gutzwiller Approximation

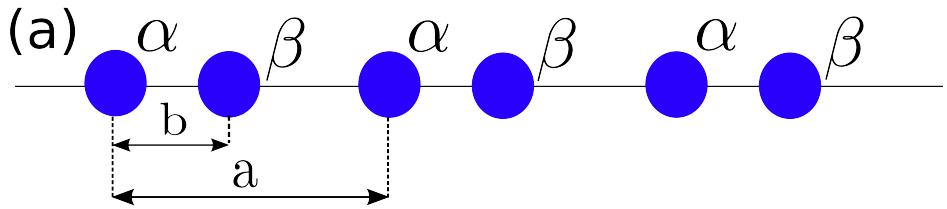
Whatever provides us with:

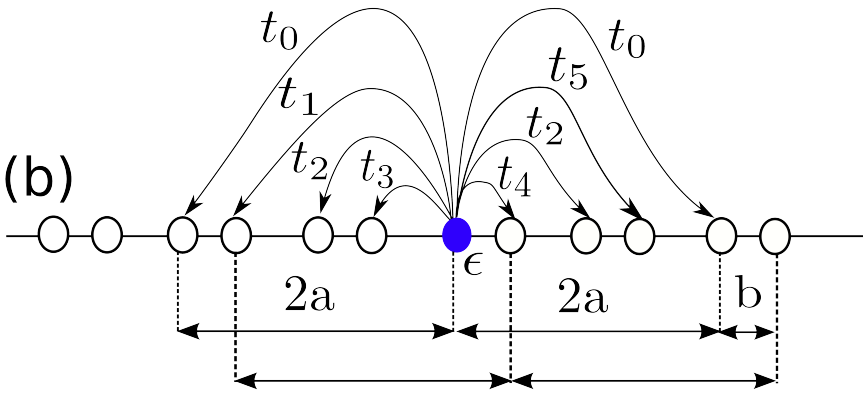
- ground-state energy (E_g)
- (ideally) excited states close to E_g
- (in)direct correlation picture
- observables for comparison with experiment
- scalability

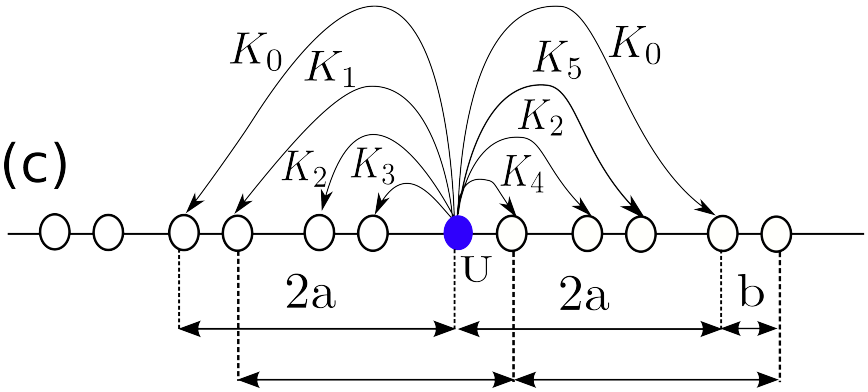
2^{nd}-quantization states

$$|\Psi\rangle_N = \mathcal{N} \sum_k A_k |\Phi_k\rangle, \quad |\Phi_k\rangle = \prod_{i \in \Omega_{\uparrow k}} \hat{c}^\dagger_{i\uparrow} \prod_{j \in \Omega_{\downarrow k}} \hat{c}^\dagger_{j\uparrow} |0\rangle, \langle \Phi_k | \Phi_l \rangle = \delta_{kl}$$

For details see: Phys. Rev. B **98**, 085112 (2018)







Assumptions

(a) two hydorgen atoms in the unit cell (α, β), with the lattice parameter a and bond length b;
(b) range of the hoppings terms extends up to $2a$;
(c) interactions counted up to the range of $2a$.

"Infinite" crystal

- Periodic Boundary Conditions;
- supercell of 17, 21, 25, 33 and 37 unit cells;

Hamiltonian

Second quantization

$$\mathcal{H} = \sum_i \epsilon_i(\hat{n}_{i\uparrow} + \hat{n}_{i\downarrow}) + \sum_{i\neq j} t_{ij}(\hat{c}^\dagger_{i\uparrow}\hat{c}_{j\uparrow} + \hat{c}^\dagger_{i\downarrow}\hat{c}_{j\downarrow}) \qquad \text{// free electrons}$$

$$+ \sum_i U_i \hat{n}_{i\uparrow}\hat{n}_{i\downarrow} + \sum_{i\neq j} K_{ij}\hat{n}_i\hat{n}_j \qquad \text{// interactions}$$

First-to-second-quantization calculation step

$$t_{ij} \equiv \left\langle w_i(\mathbf{r}) \right| -\nabla^2 - \textstyle\sum_{I\in\text{ions}} \frac{2Z}{|\mathbf{R_I}-\mathbf{r}|} \left| w_j(\mathbf{r}) \right\rangle \qquad \epsilon_i \equiv t_{ii}$$

$$V_{ijkl} \equiv \left\langle w_i(\mathbf{r})w_j(\mathbf{r}') \right| \frac{2}{|\mathbf{r}-\mathbf{r}'|} \left| w_k(\mathbf{r})w_l(\mathbf{r}') \right\rangle \qquad U_i \equiv V_{iiii},\ K_{ij} \equiv V_{ijij}$$

Dimensionality - 1D chain in 3D space

- $w_i(\mathbf{r})$ build from 1s Slater orbitals;
- Coulomb potential $V_C(\mathbf{R}) \propto |\mathbf{R}|^{-1}$;

Proper state function

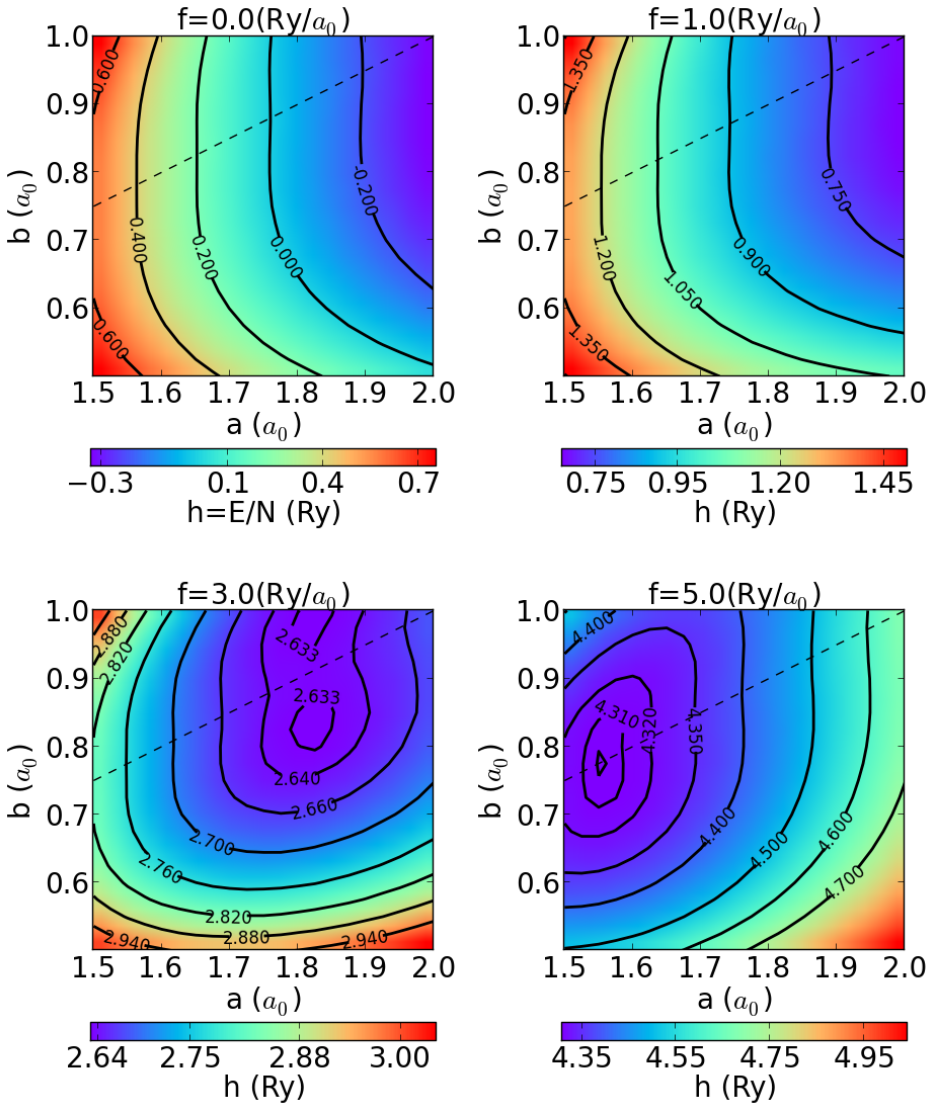
One-dimensional enthalpy

$$h \equiv f\frac{a}{2} + \frac{E}{N},$$

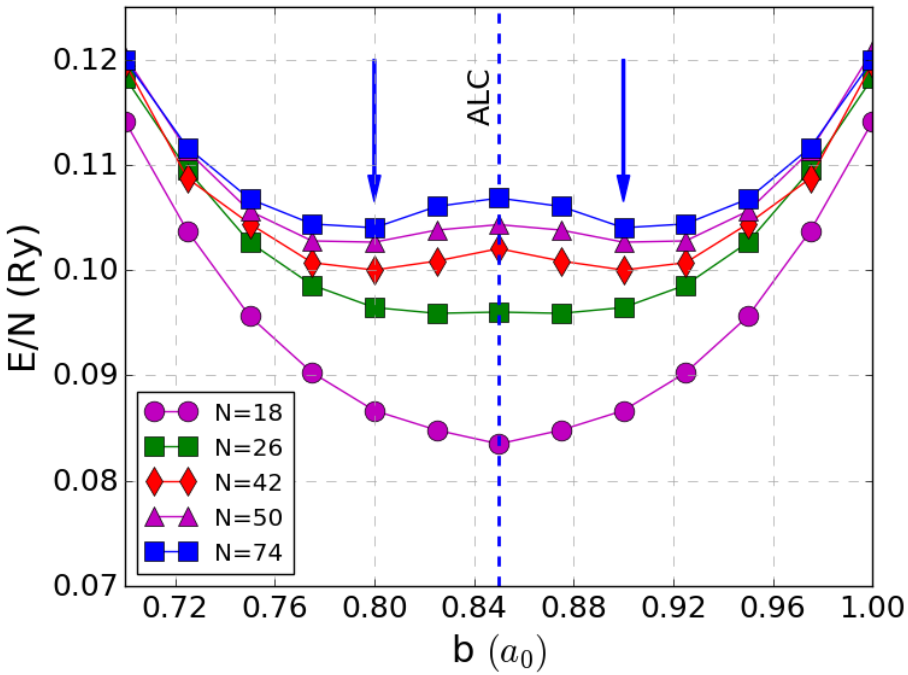
with f as an external force (analogue of the pressure), the lattice parameter a, and ground-state energy E for the N-particle supercell.

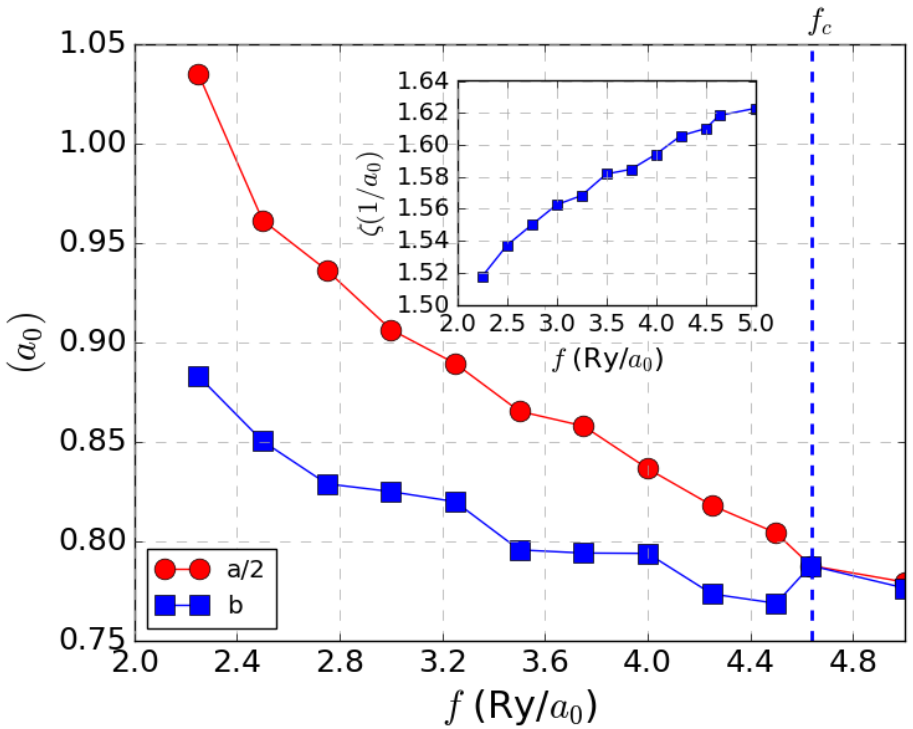
Run for given f

- opt. structure
  - opt. wavefunction
    - opt. Jastrow



Results for finite systems



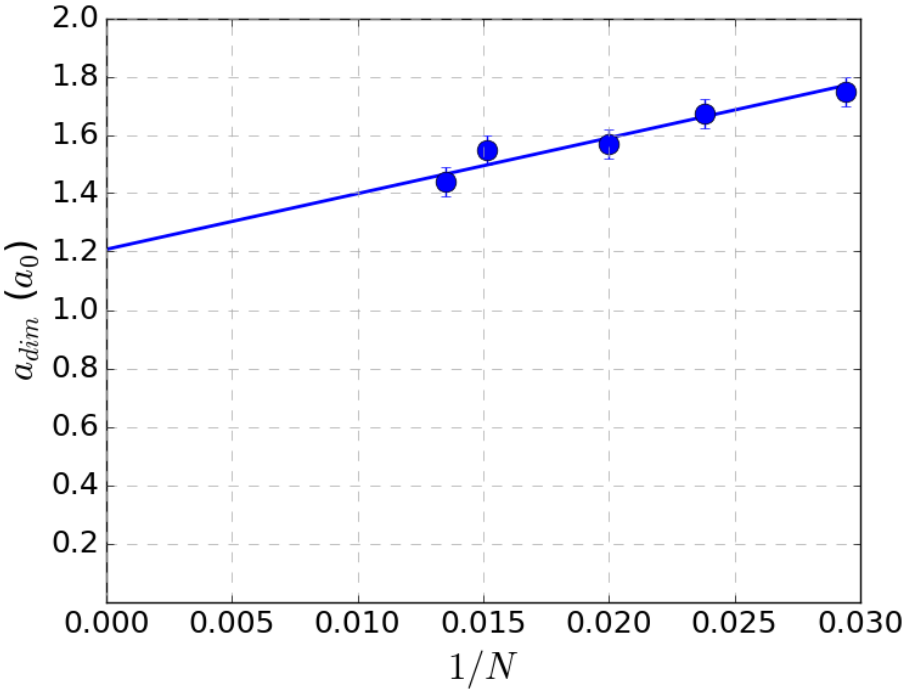


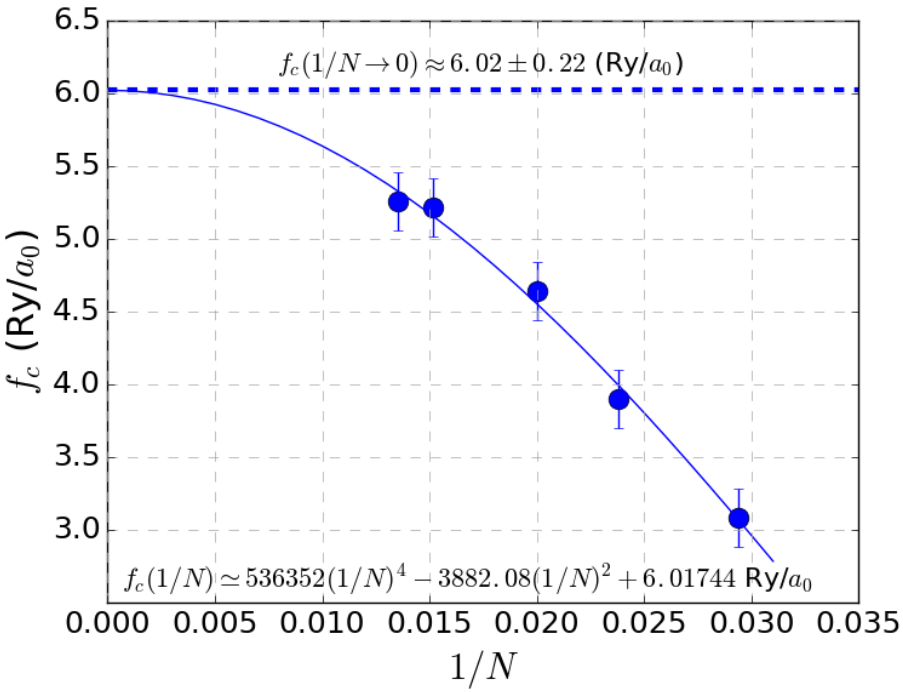
Peierls-like distortion from First Principles for a correlated system

- **No distortion for small systems.**
- Molecular $\rightarrow$ atomic transition at high "pressure"
  $\hookrightarrow$ reverse Peierls-like transition.

for finite systems cf. also E. Giner *et al.*, J. Chem. Phys. **138**, 074315 (2013).

Thermodynamic limit





Conditions of molecular-to-atomic transition for $N \to \infty$

- finite-size scaling of atomization lattice parameter $a_{dim} \approx 1.17 a_0 > 0$;
- finite-size scaling of atomization force $f_c \approx 6.02 \frac{Ry}{a_0} < \infty$.

Metallicity of hydrogen chain

Point of reference

We use the equilibrium microscopic parameters of the Hamiltonian for $N = 50$ as a point of reference.

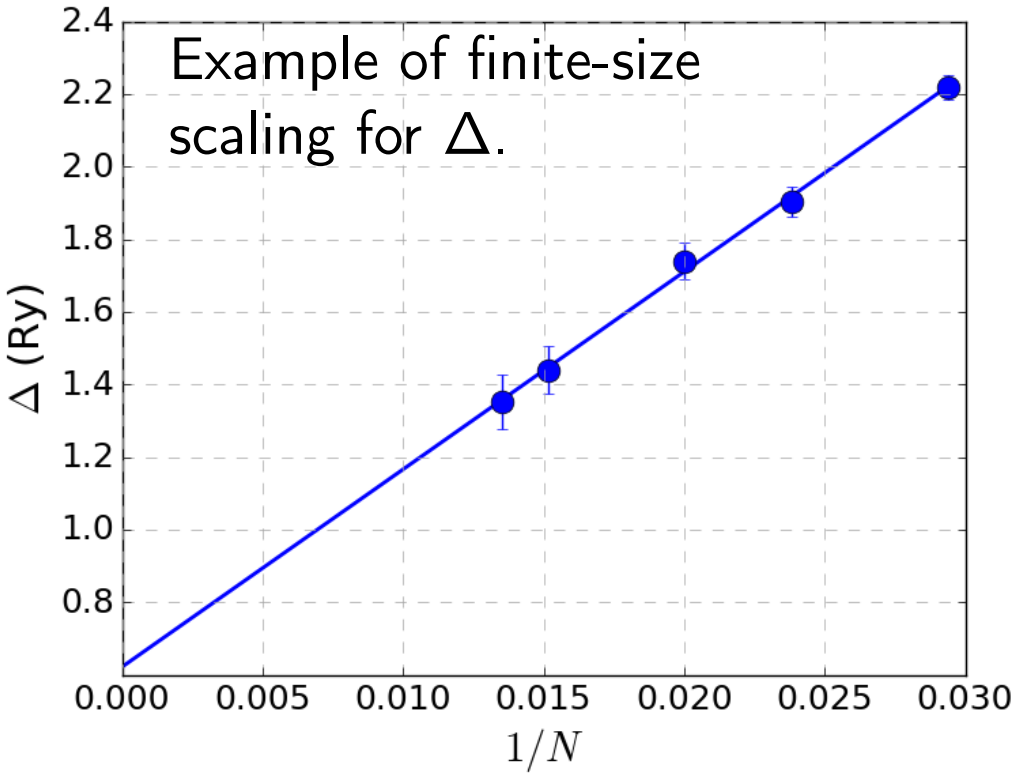
Charge gap

$$\Delta_N \equiv \left. \frac{E_{N+4} - 2E_N + E_{N-4}}{4} \right|_{@h(f)}$$

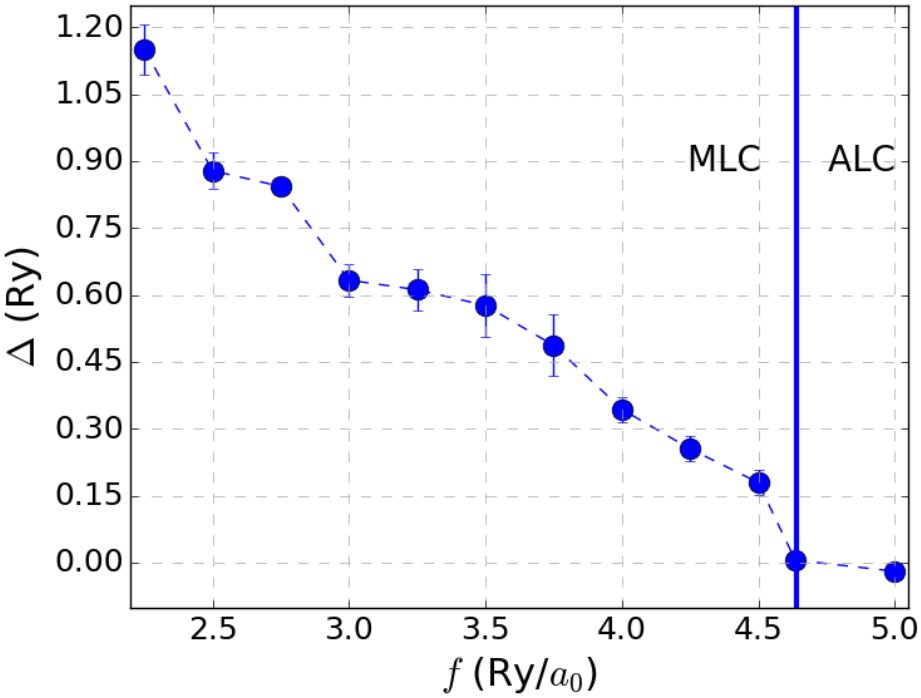
E_N - the ground state of the N-particle system described by the reference Hamiltonian with the structure minimizing the effective enthalpy.

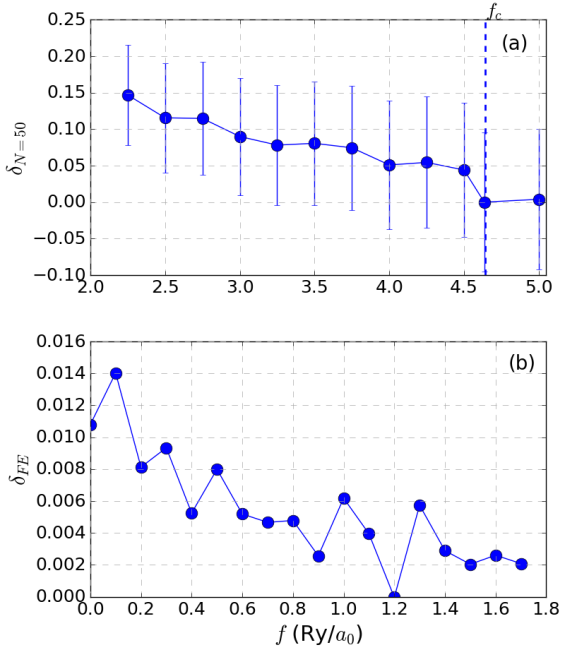
Thermodynamic limit

$$\Delta \equiv \Delta_\infty = \lim_{N \to \infty} \Delta_N$$



Closing of the charge gap





Apparent metallicity of the hydrogen chain in the atomic phase

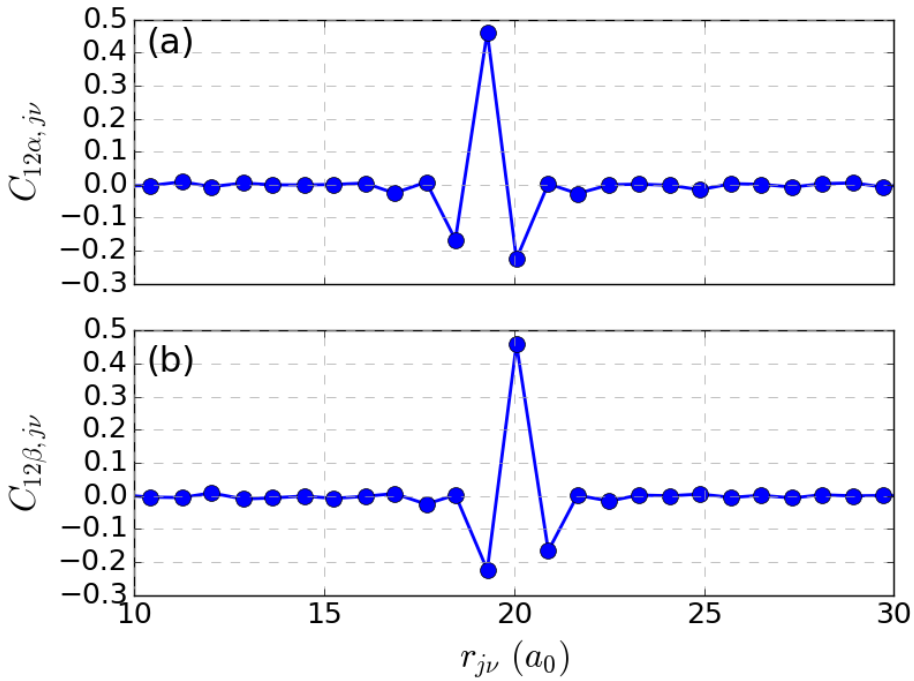
- charge gap closed at the MLC $\rightarrow$ ALC transition;
- further-than-nearest neighbor hoppings;
- chain exist in 3D (both single-particle wavefunctions and Coulomb potential are taken for $D = 3$);

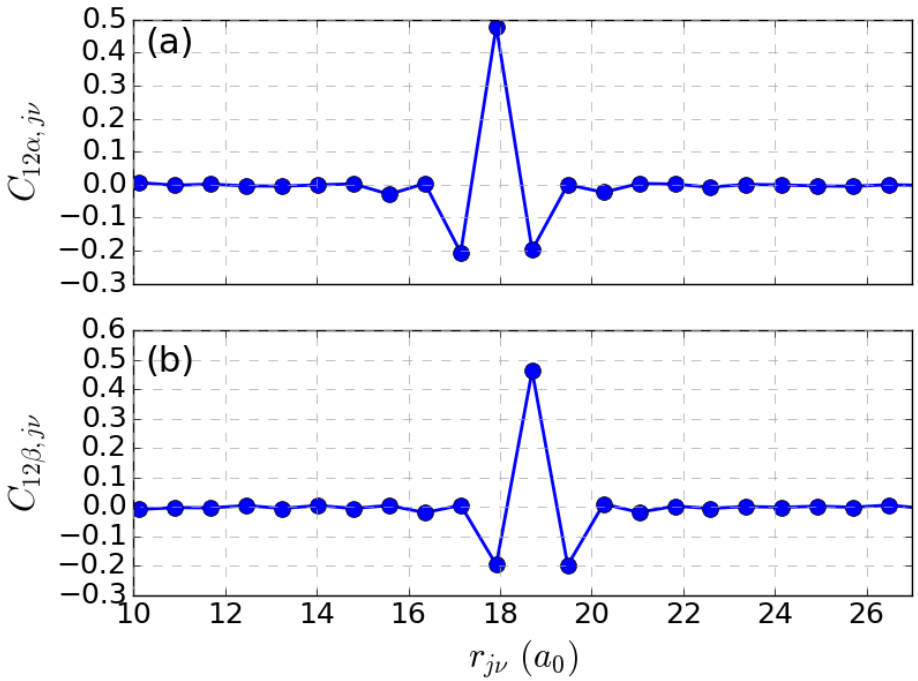
in agreement with L. Stella *et al.*, Phys. Rev. B **84**, 245117 (2011)

Density-density correlation

Density-density correlation

$$C_{i,j} \equiv \langle \hat{n}_i \hat{n}_j \rangle - \langle \hat{n}_i \rangle \langle \hat{n}_j \rangle$$



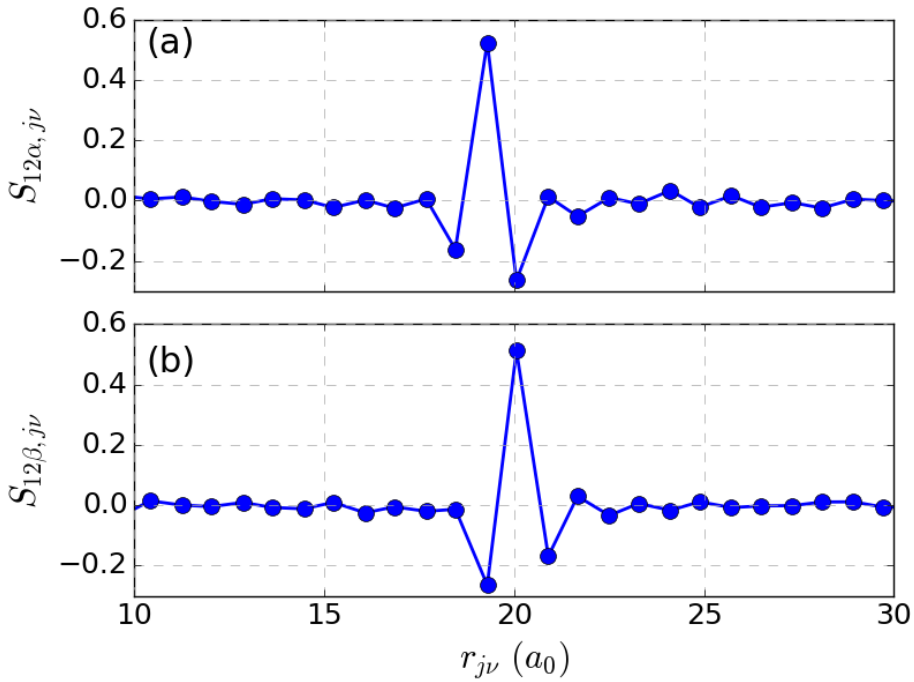


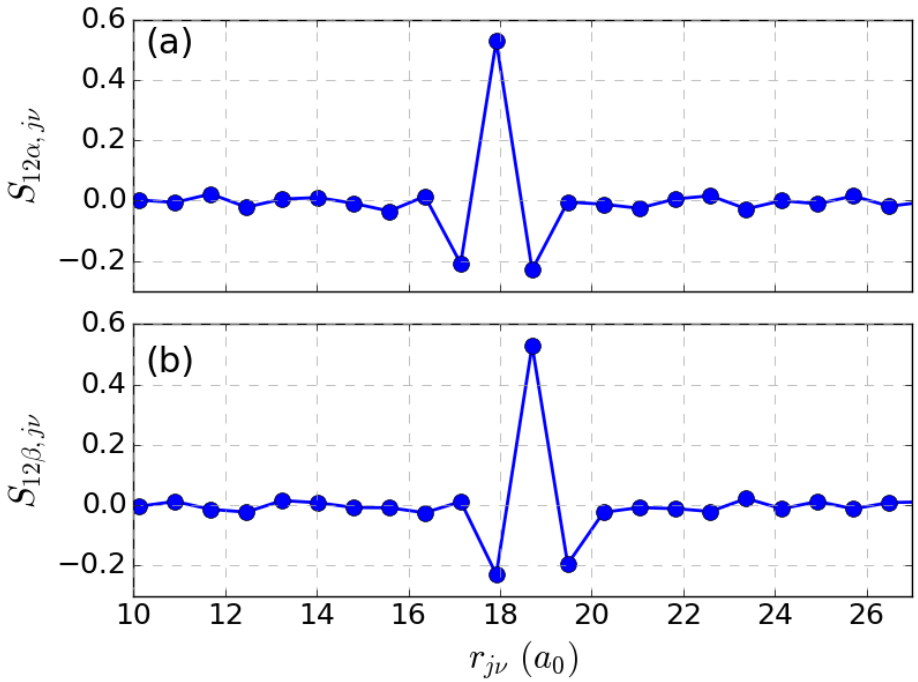
(LEFT) $f = 4.5$ Ry/a_0; (RIGHT) $f = 5.0$ Ry/a_0

Spin-spin correlation

Spin-spin correlation

$$S_{i,j} \equiv \left\langle (\hat{n}_{i\uparrow} - \hat{n}_{i\sigma})(\hat{n}_{j\uparrow} - \hat{n}_{j\sigma}) \right\rangle = \langle \hat{S}_i^z \hat{S}_j^z \rangle$$



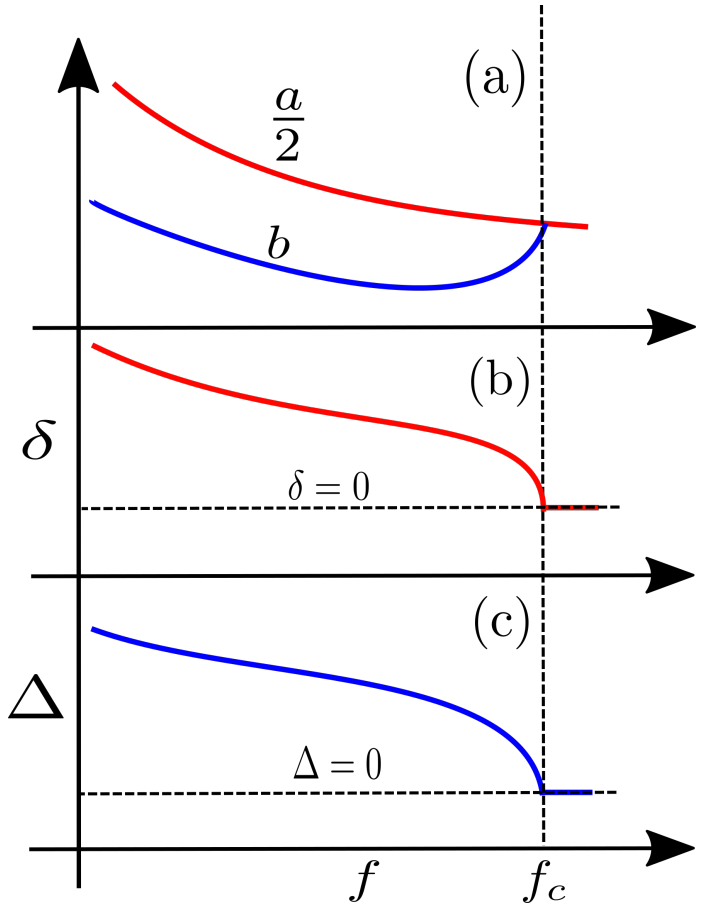


(LEFT) $f = 4.5$ Ry/a_0; (RIGHT) $f = 5.0$ Ry/a_0

Conclusions 1D

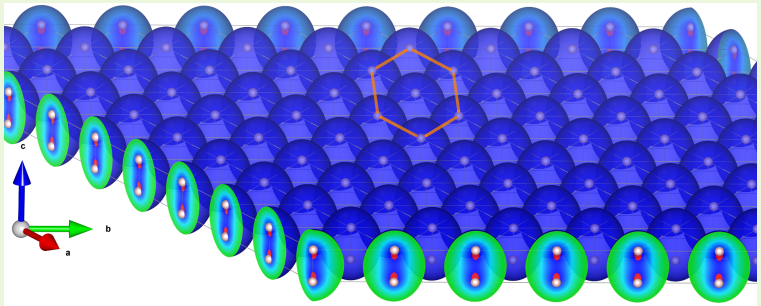
Hydrogen chain

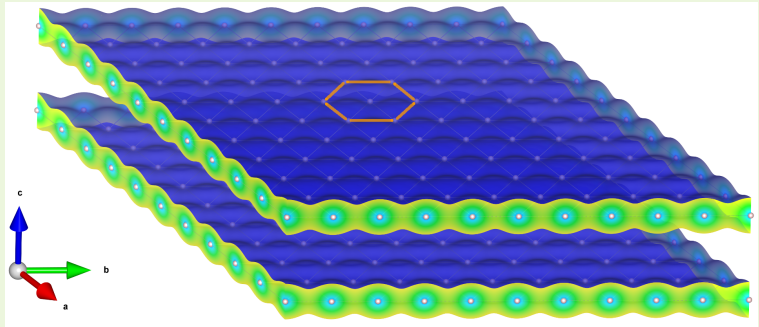
- Peierls-like distortion at ambient "pressure";
- correlations do not weaken distortion;
- external force induces molecular $\rightarrow$ atomic transition;
- concomitant atomization and metallization ;
- no long-range order;



Triangular lattice

Two-dimensional crystal





- periodic boundary conditions in xy plane;
- Lanczos algorithm for the diagonalization core of 6 and 8 atoms (to comply with proper Néel 120° and 90° phases);
- wavefunction constructed from 10 classes of nodes

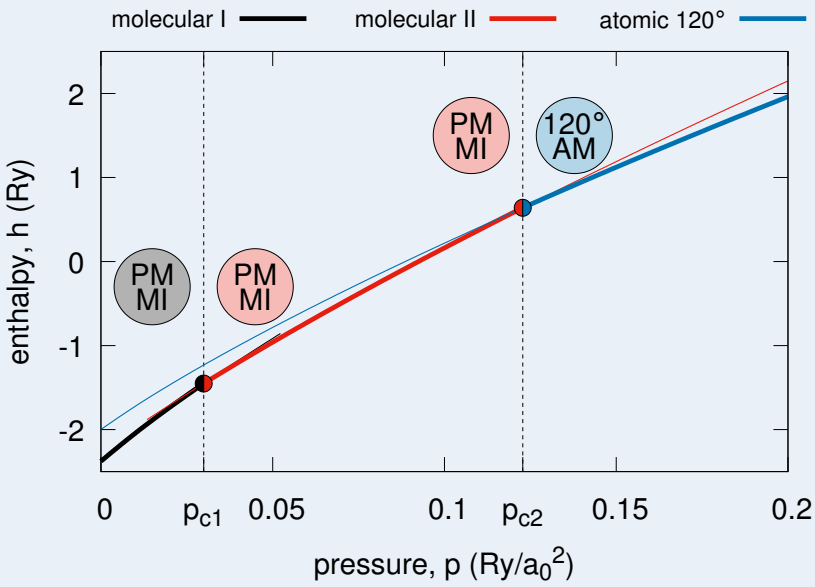
$$\mathcal{H} = \sum_{i\sigma} \epsilon_i \hat{n}_{i\sigma} + \sum_{i\neq j\sigma} t_{ij} \hat{c}^{\dagger}_{i\sigma} \hat{c}_{i\sigma}$$
$$+ \sum_i U_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} + \sum_{i\neq j} K_{ij} \hat{n}_i \hat{n}_j$$
$$- \sum_{i\neq j} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j - \tfrac{\mathbf{1}}{\mathbf{4}} \sum_{i\neq j} J_{ij} \hat{n}_i \hat{n}_j$$
$$+ \sum_{i\neq j} J_{ij} \hat{c}^{\dagger}_{i\uparrow} \hat{c}^{\dagger}_{i\downarrow} \hat{c}_{j\downarrow} \hat{c}_{j\uparrow}$$

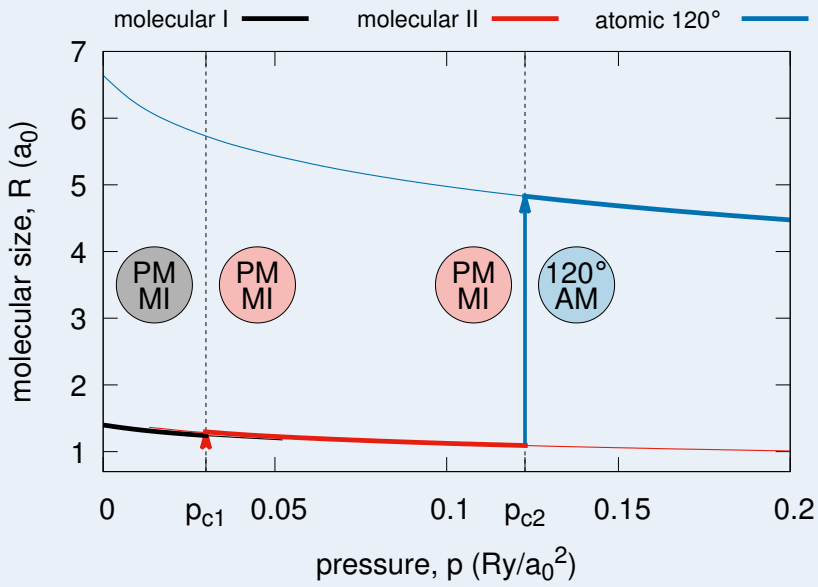
$\hookrightarrow$ hoppings t_{ij} up to 10^{th} neighbor;

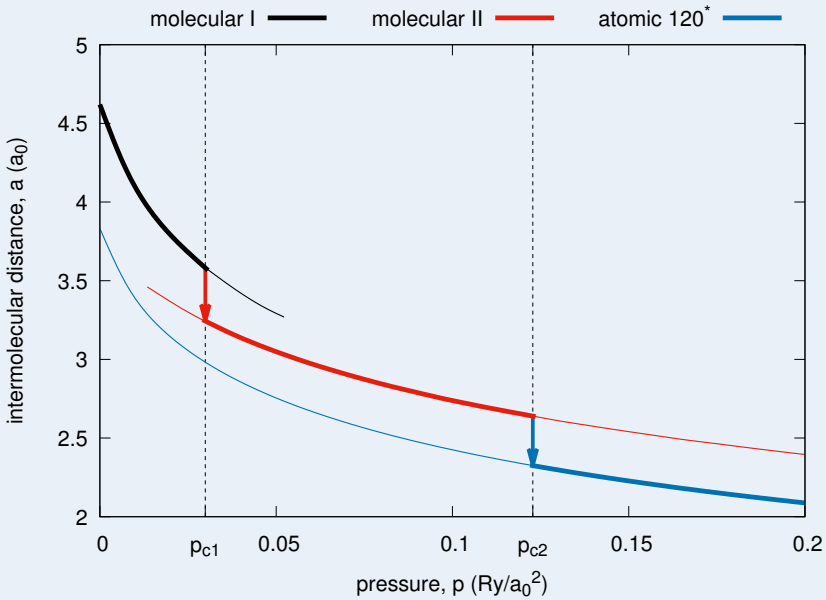
$\hookrightarrow$ Coulomb repulsion K_{ij} up to 10^{th} neighbor;

$\hookrightarrow$ ferromagnetic exchange J_{ij} up to 3^{rd} neighbor;

2D enthalpy and lattice parameters







Question:

What is the quantum equivalent of $R_{eff} \longrightarrow \infty$?

Atomicity

Classically

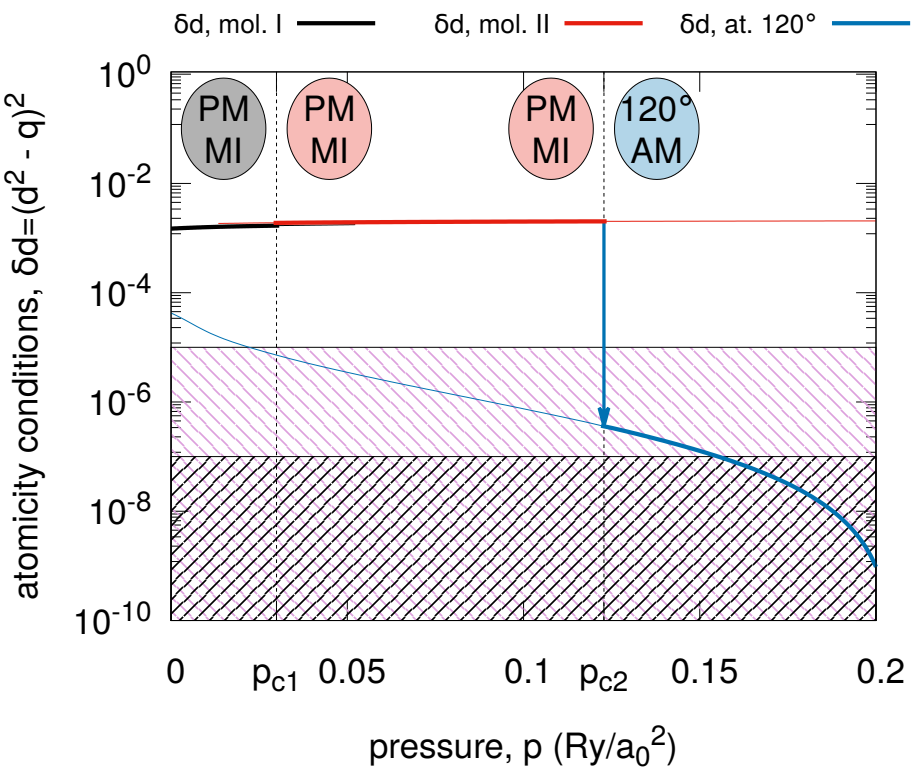
Interplanar distance $R_{eff} \longrightarrow \infty \Leftarrow$ **Not necessarily in the quantum realm!**

(van-der-Waals-like behavior)

Independence of classical probability

$$\delta d \equiv \left(P \begin{bmatrix} * \\ \uparrow\downarrow \end{bmatrix} P \begin{bmatrix} \uparrow\downarrow \\ * \end{bmatrix} - P \begin{bmatrix} \uparrow\downarrow \\ \uparrow\downarrow \end{bmatrix} \right)^2$$

$$\equiv \left(\langle \Phi_0 | \, \hat{n}_{1\uparrow} \hat{n}_{1\downarrow} \, | \Phi_0 \rangle \, \langle \Phi_0 | \, \hat{n}_{2\uparrow} \hat{n}_{2\downarrow} \, | \Phi_0 \rangle - \langle \Phi_0 | \, \hat{n}_{1\uparrow} \hat{n}_{1\downarrow} \hat{n}_{2\uparrow} \hat{n}_{2\downarrow} \, | \Phi_0 \rangle \right)^2$$



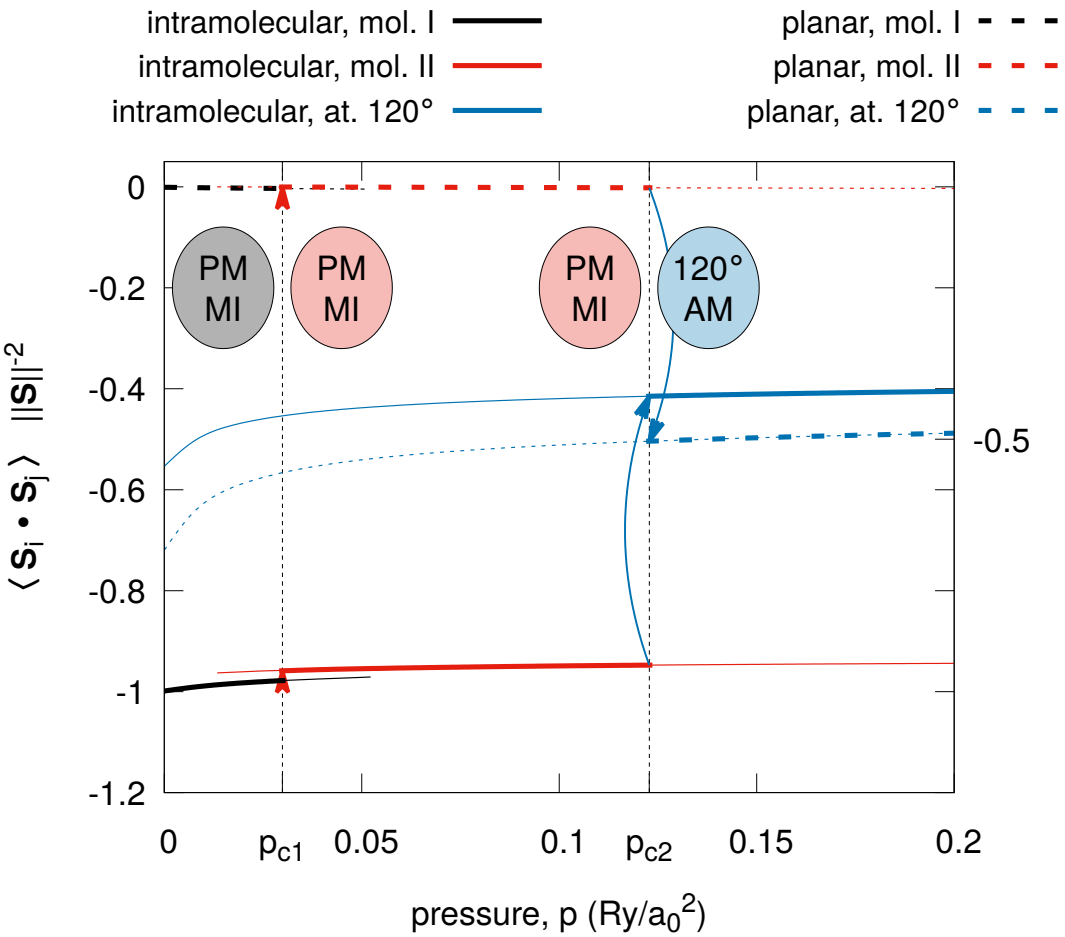
Magnetic order

FM vs. AFM exchange

$J_{\text{FM, Hund-like}} \ll J_{\text{AFM, kinetic}}$
Required for the ambient pressure stability of the atomic phase!

Spin correlation

1. Molecular phases:
   molecular H_2,
   near-spin-singlet
2. Atomic phase:
   120° Néel order



Total spin

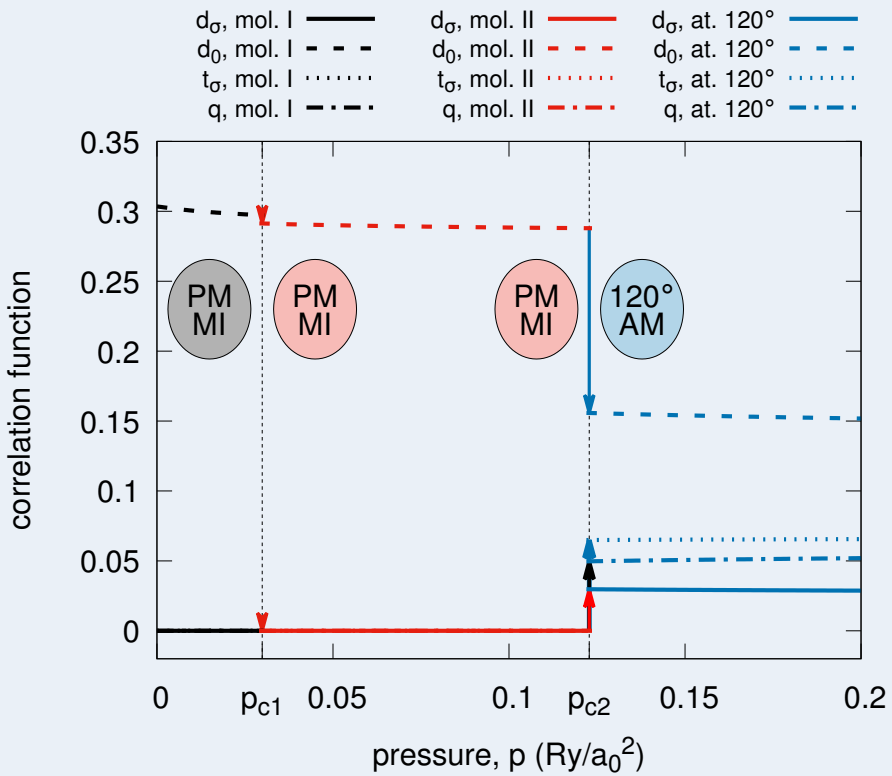
	mol. I → II		mol. II → atomic	
$\|\|\mathbf{S}\|\|_{\text{molecule}}$	0.10	0.14	0.16	0.54
$\|\|\mathbf{S}\|\|_{\text{triangle}}$	0.86	0.87	0.86	0.077

$$||\mathbf{S}||_{\mathbf{molecule}} \equiv ||\mathbf{S}(\mathbf{x_{2D}}, -\tfrac{R}{2}) + \mathbf{S_2}(\mathbf{x_{2D}}, \tfrac{R}{2})||$$

$$||\mathbf{S}||_{\mathbf{triangle}} \equiv ||\mathbf{S}(\mathbf{x_{2D}}, \tfrac{R}{2}) + \mathbf{S}(\mathbf{x_{2D}} + \mathbf{e_1}, \tfrac{R}{2}) + \mathbf{S}(\mathbf{x_{2D}} + \mathbf{e_2}, \tfrac{R}{2})||$$

Two-step metallization

Metallicity of atomic phase



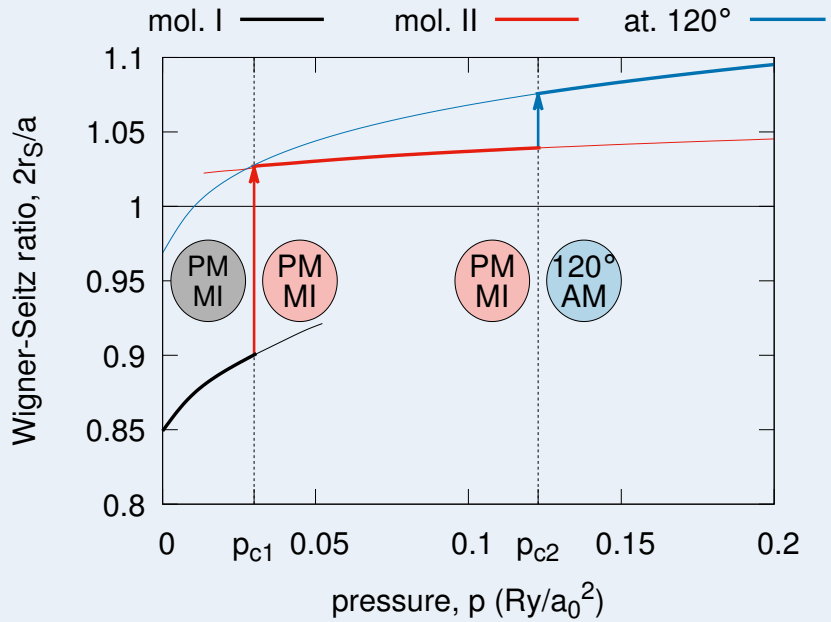
$\Uparrow$ occupancy correlation functions

$\Rightarrow$ Wigner-Seitz metallicity condition $r_S > \frac{a}{2}$, where WS radius $r_S \equiv \sqrt[3]{\frac{3}{4\pi n}}$.

$$q \equiv P \begin{bmatrix} \uparrow\downarrow \\ \uparrow\downarrow \end{bmatrix} \qquad d_0 \equiv P \begin{bmatrix} \uparrow & \\ & \downarrow \end{bmatrix}$$

$$t_\uparrow \equiv P \begin{bmatrix} \uparrow & \\ \uparrow\downarrow & \end{bmatrix} \qquad d_\uparrow \equiv P \begin{bmatrix} \uparrow & \\ \uparrow & \end{bmatrix}$$

$$t_\downarrow \equiv P \begin{bmatrix} \downarrow & \\ \uparrow\downarrow & \end{bmatrix} \qquad d_\downarrow \equiv P \begin{bmatrix} & \downarrow \\ & \downarrow \end{bmatrix}$$



Band structure

Bare bands

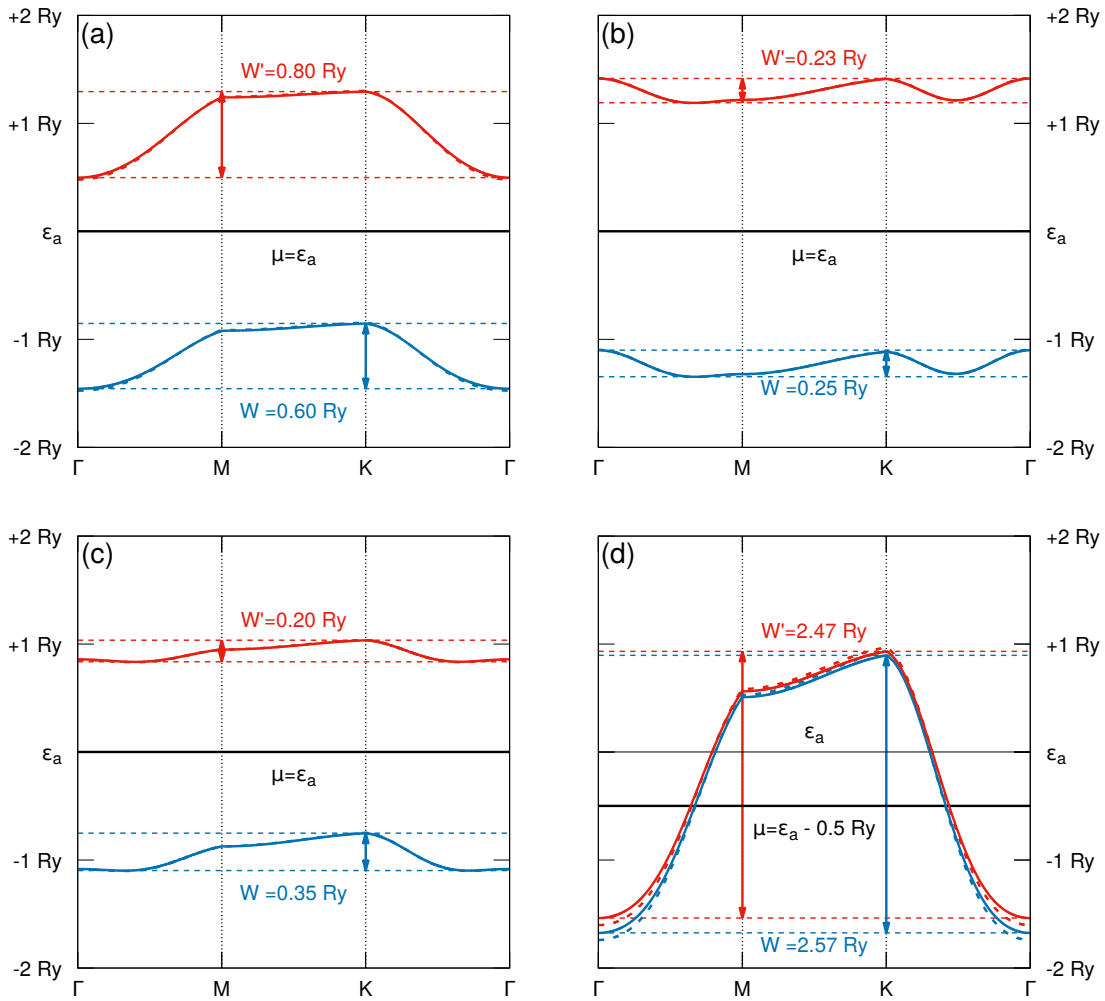
- easily calculable
- depend only on $\mathcal{H}_{\text{free}}$

Correlated bands

- full $\mathcal{H}$ dependence
- no generic method

Bare bands with a correlator

- calculable
- local interaction
- ∅ correlator physics



Possibility of superconducting state

Wigner-Seitz radia

$r_S = r_S(V)$

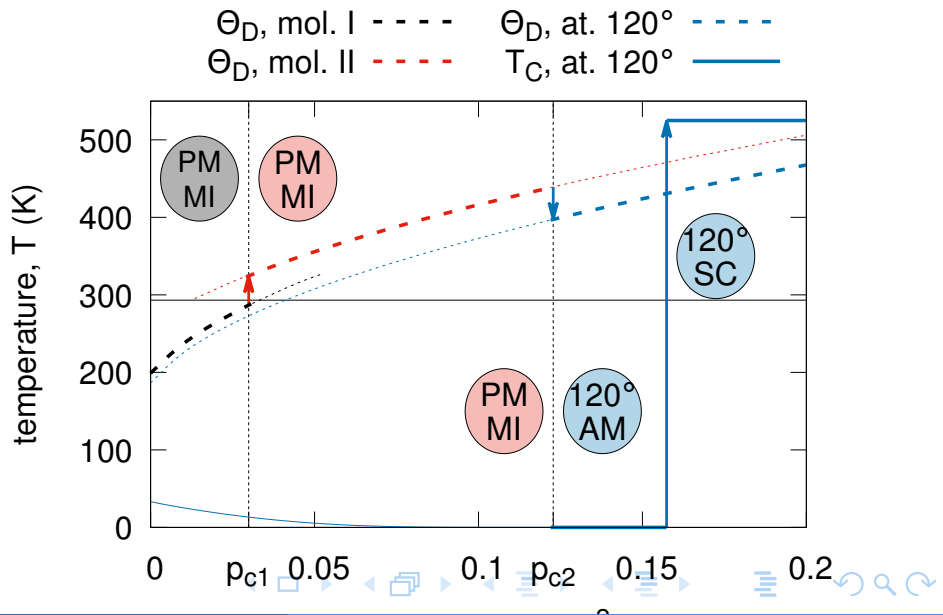
- volume of an electron in phases I & II:
  $V_e = \frac{V_{\mathbf{mol}}}{2} \equiv \frac{1}{2} a^2 (R + \frac{2}{\zeta})$,
- volume of an **atom** in atomic phase:
  $V_e = a^2 \frac{2}{\zeta}$,

source	method	r_s (a_0)
J. McMinis et al. (arXiv:1309.7051)	DMC	2.27
G. Mazzola et al. (Nat. Commun. **5**, 3487 (2014))	DMC	**1.28**
J.-L. Li et al. (Phys. Rev. B **66**, 035102 (2002))	LSDA	2.78
J.-L. Li et al. (Phys. Rev. B **66**, 035102 (2002))	GGA	2.50
B. I. Min et al. (Phys. Rev. B **33**, 324 (1986))	LMTO-LSDA	2.85
A. Svane et al. (Solid State Commun. **76**, 851 (1990))	SIC-LSDA	2.45
B. G. Pfrommer et al. (Phys. Rev. B **58**, 12680 (1998))	GGA-PW91	2.5
APK, AB, JS (2018)	EDABI	**1.265**
R. P. Dias et al. (Science: 10.1126/science.aal1579 (2017))	eksperyment	**1.255 – 1.34**

McMillana formula

T_C depends on

- Θ_D (from phonon spectra)
  - ∅ always a soft mode $\perp$ to the plane
- $\alpha \approx 1.0$
- $\lambda^2 \approx 0.166 r_S$
  - ∅ tolerable (?) approx.



Conclusions

Physics of hydrogen planes

- concomitant atomization & metallization;
- long-range interactions ($\sim ||\mathbf{R}||^{-p}$)
- London-like interactions in insulating molecular phases;
- benchmark for infinite-system quantum chemistry (EDABI + QMT Quantum Metallization Tools);

Hydrogen-induced superconductivity

- **medianly** correlated system (playground for a physicist)
- (most probably)[citation needed] **anharmonic** phonons;
- (but maybe)[citation needed] correlation driven;
- extreme pressure (chemical?);
- record high T_C;