Metallicity and superconductivity of the hydrogen-rich compounds

Andrzej P. Kądzielawa
Institute of Theoretical Physics, Jagiellonian University,
Kraków, Poland
IT4Innovations, Vysoká škola báňská - Technical University of Ostrava,
Ostrava, Czech Republic

andrzej.piotr.kadzielawa@vsb.cz

VŠB TECHNICKÁ UNIVERZITA OSTRAVA | IT4INNOVATIONS NÁRODNÍ SUPERPOČÍTAČOVÉ CENTRUM

NARODOWE CENTRUM NAUKI

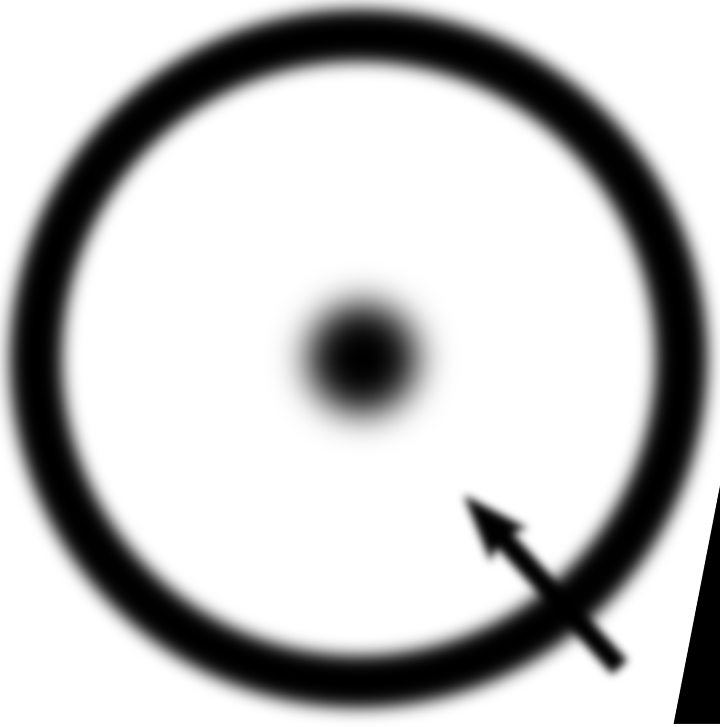
GAČR
GRANTOVÁ AGENTURA ČESKÉ REPUBLIKY

Team

Andrzej Biborski (left),
Academic Centre for Materials and Nanotechnology, AGH University of Science and Technology, Kraków

Józef Spałek (right),
Institute of Theoretical Physics, Jagiellonian University, Kraków

Dominik Legut (bottom),
IT4Innovations, Vysoká škola báňská Technical University of Ostrava



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).

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

Wasserstoff zu Metall gequetscht?

VON MANFRED LINDINGER - AKTUALISIERT AM 02.02.2017

Ingeniøren

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

Сверхпроводники и изучение сверхпроводимости

30 января 2017 15:00 | Дарья Загорская

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

FOX NEWS Tech

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


Credit: Ranga P. Dias/Isaac F. Silvera

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)*

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

INDEPENDENT

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

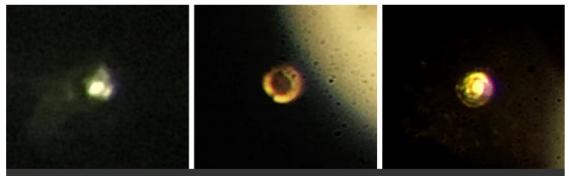
Exclusive: Harvard University physicists say first-ever piece of metallic hydrogen on Earth has been lost after catastrophic failure of diamond holding it under enormous pressure

REUTERS

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

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 własnie, 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 $300K$

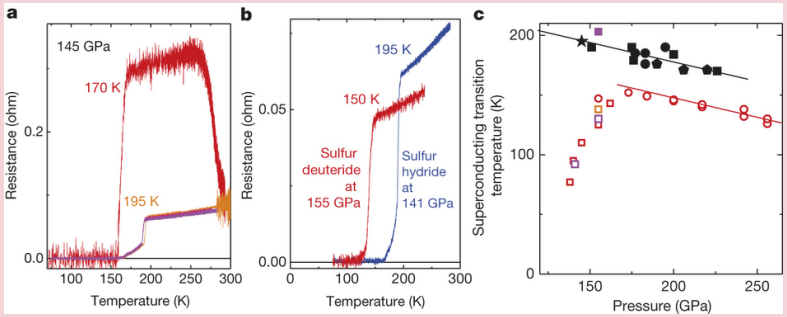
N. Ashcroft, PRL **21**, 1748 (1968)

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

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

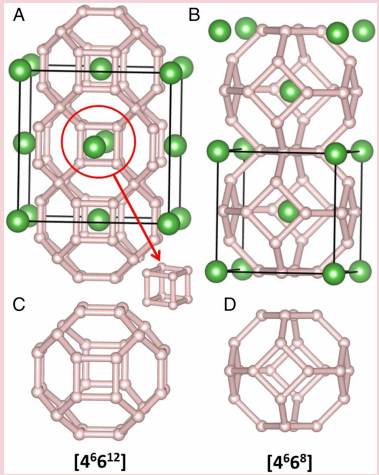
Hydrogen in 2D - superconductivity?

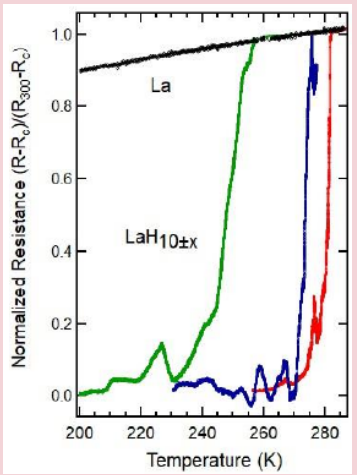
$H_{2|3}S$



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

$LaH_{10 \pm x}$





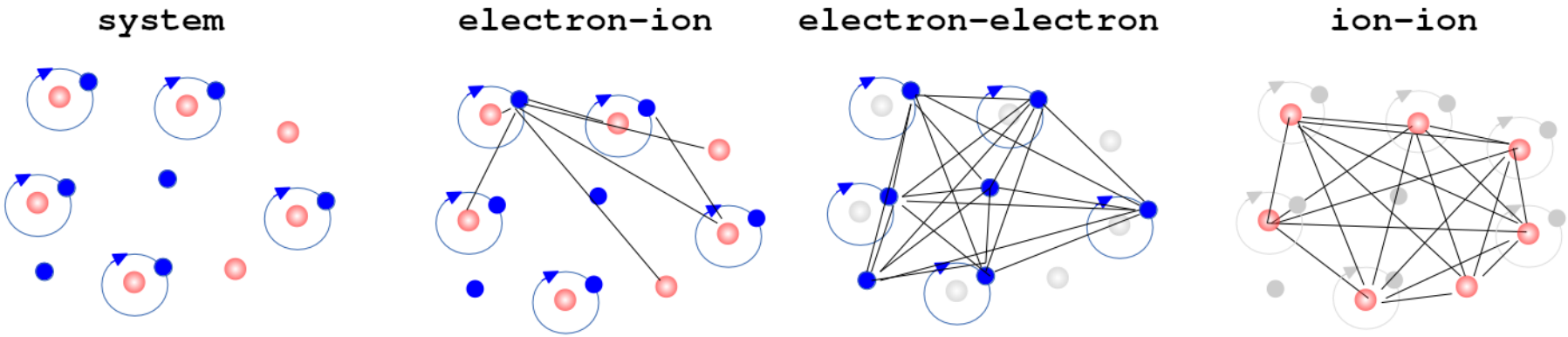
$L_{th.}$: Hanyu Liu et al., PNAS 114, 27 (2017)

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

Picture

Born–Oppenheimer Approximation

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

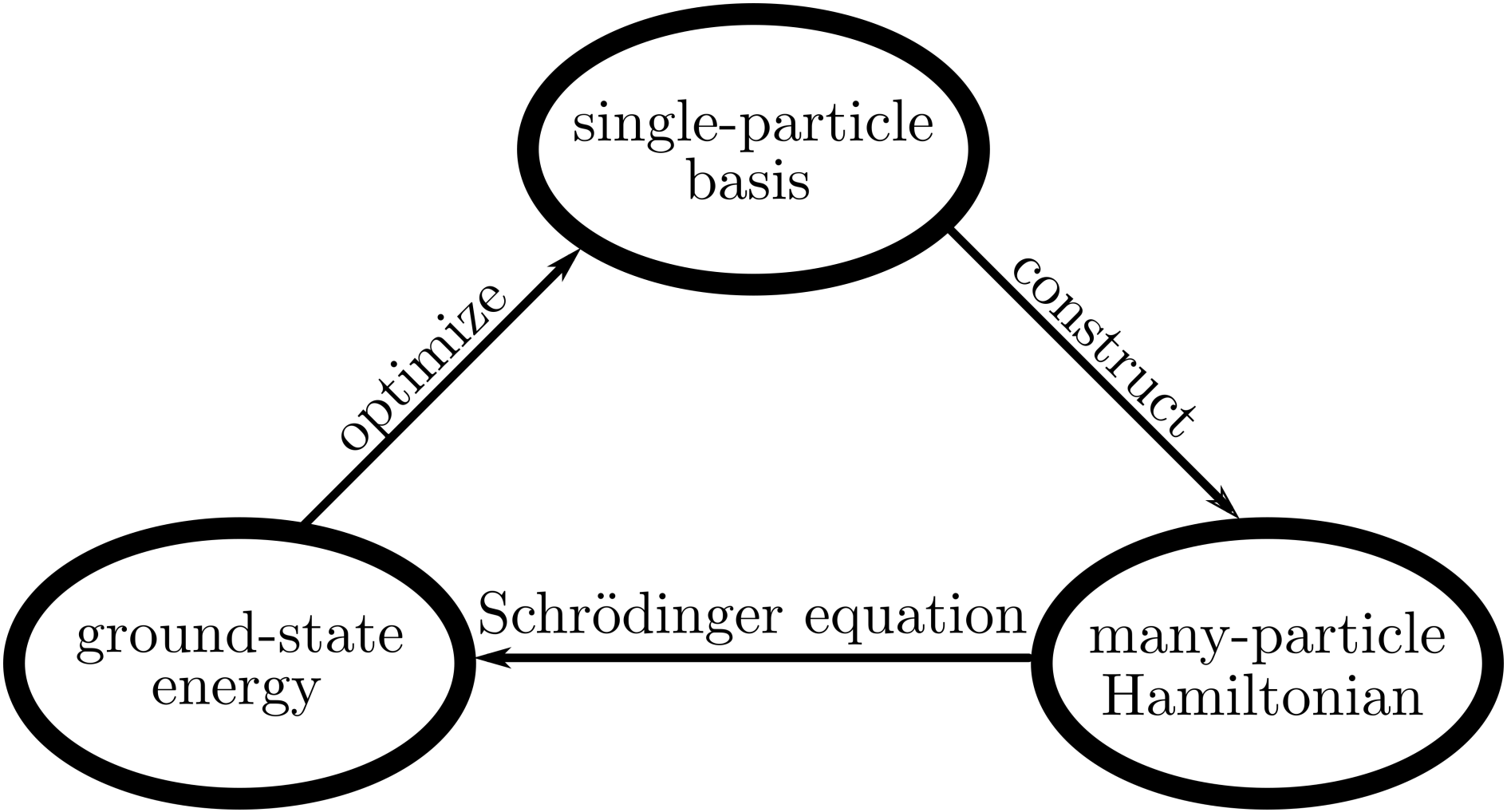


Hamiltonian

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

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

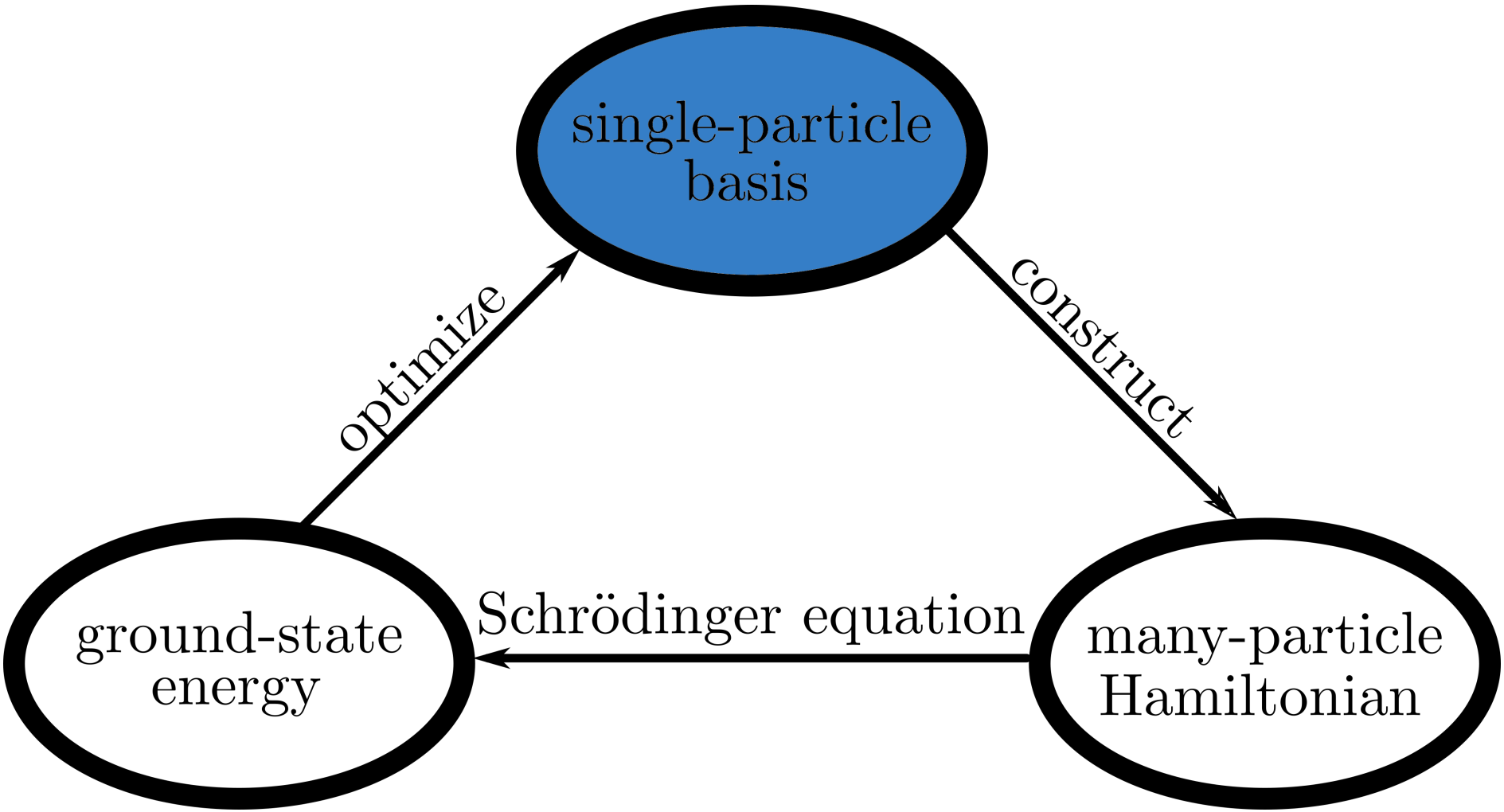
Exact Diagonalization Ab Initio (EDABI++)



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 $\{\psi_i\}$:

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

satisfying orthonormality condition

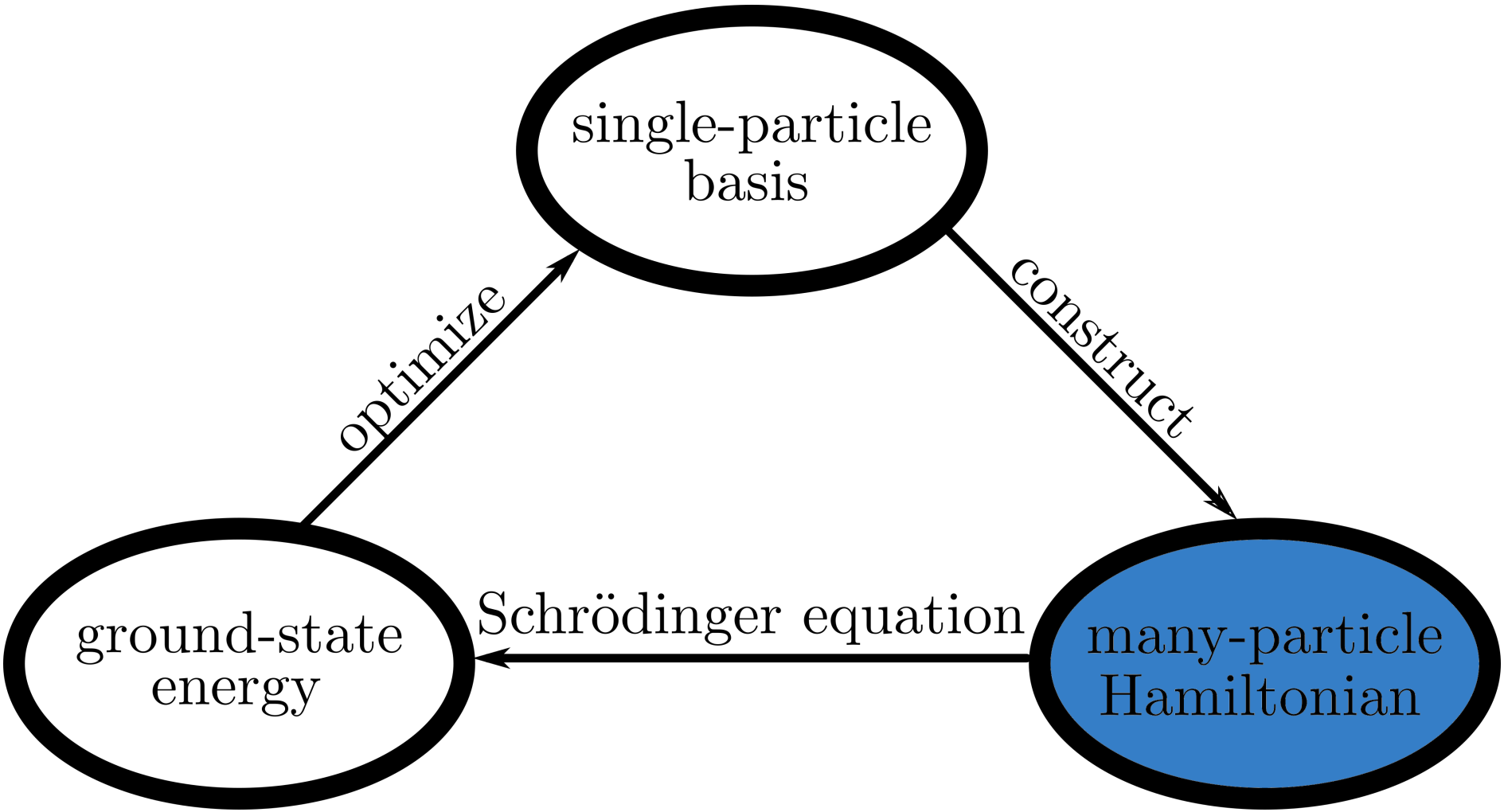
$$\langle w_i |\ w_j \rangle = \delta_{ij}.$$

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: $\Psi_i \equiv w_i(\mathrm{r})\chi_\sigma \hat{c}^\dagger_{i\sigma}$ we get the second-quantization Hamiltonian

$$\mathcal{H} = \sum_{\substack{i,j \\ \sigma}}^{\text{bound. con.}} t_{ij}\hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma} + \sum_{\substack{i,j,k,l \\ \sigma,\sigma'}}^{\text{bound. con.}} V_{ijkl}\hat{c}^\dagger_{i\sigma}\hat{c}^\dagger_{j\sigma'}\hat{c}_{l\sigma'}\hat{c}_{k\sigma} + \mathcal{H}_{\text{ext}} + \mathcal{V}_{\text{ion–ion}}$$

with fermionic creation/annihilation operators

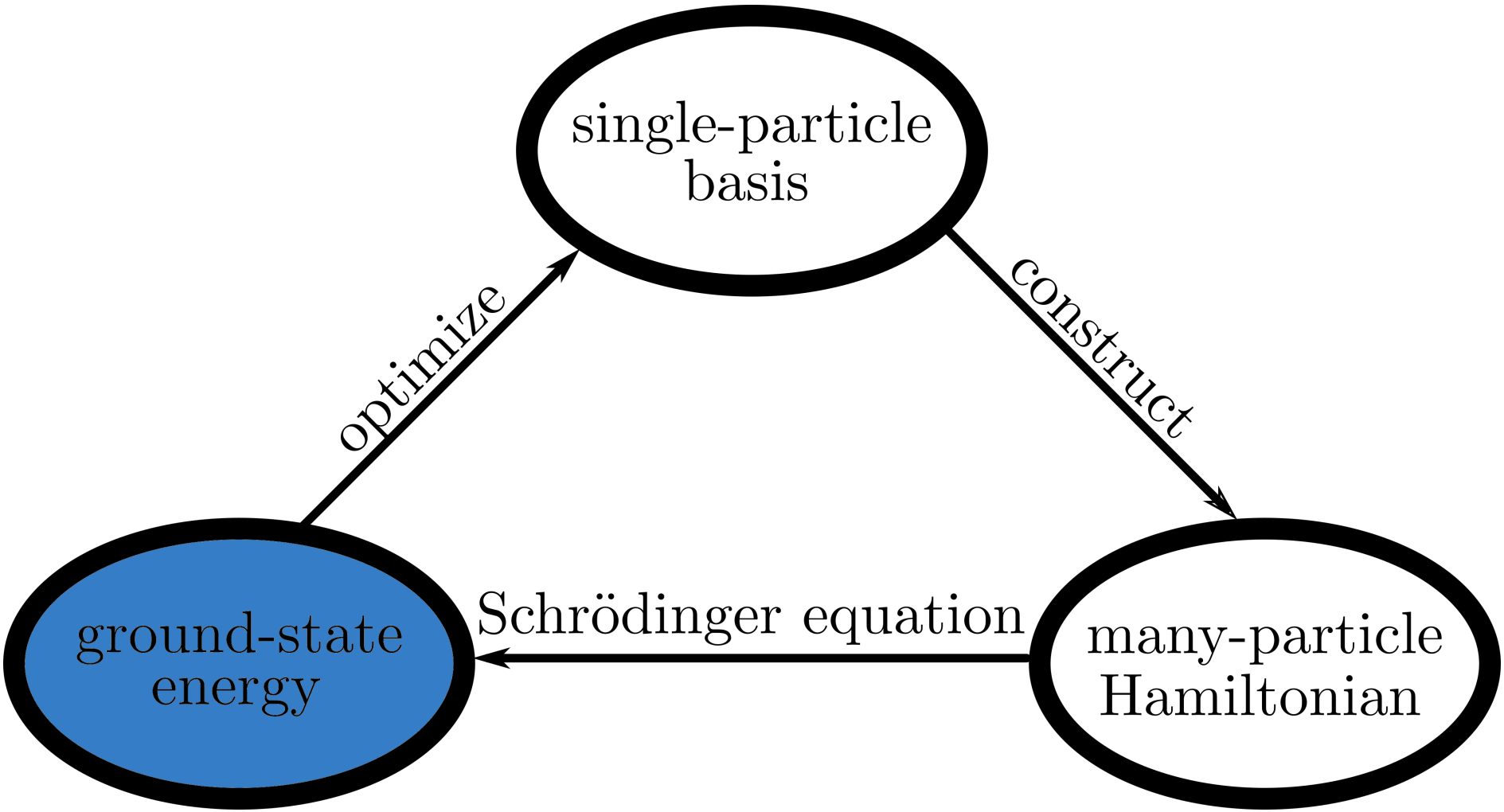
$$\{\hat{c}^\dagger_{i\sigma}, \hat{c}^\dagger_{j\sigma'}\} \equiv \{\hat{c}_{i\sigma}, \hat{c}_{j\sigma'}\} \equiv 0 \quad \text{and} \quad \{\hat{c}^\dagger_{i\sigma}, \hat{c}_{j\sigma'}\} \equiv \delta_{ij}\delta_{\sigma\sigma'}.$$

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

$$t_{ij} = \left\langle w(\mathrm{r})_i \right| -\nabla^2 - \sum_{k=1}^{n} \frac{2}{|\mathrm{r}-\mathrm{R_k}|} \left| w(\mathrm{r})_j \right\rangle, \qquad \text{"Rydberg" Atomic Units}$$

$$V_{ijkl} = \left\langle w(\mathrm{r})_i w(\mathrm{r}')_j \right| \frac{2}{|\mathrm{r}-\mathrm{r}'|} \left| w(\mathrm{r}')_k w(\mathrm{r})_l \right\rangle. \qquad \hbar = 2m_e = \frac{e}{\sqrt{2}} = 1$$

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

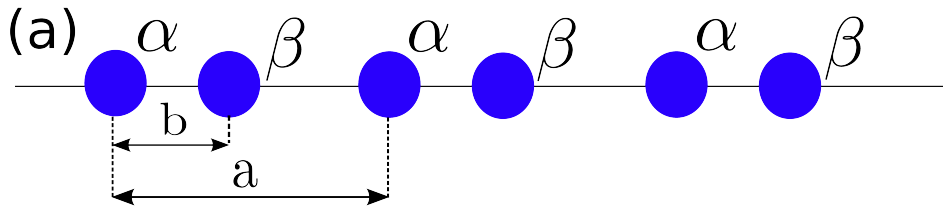
Whatever provides us with:

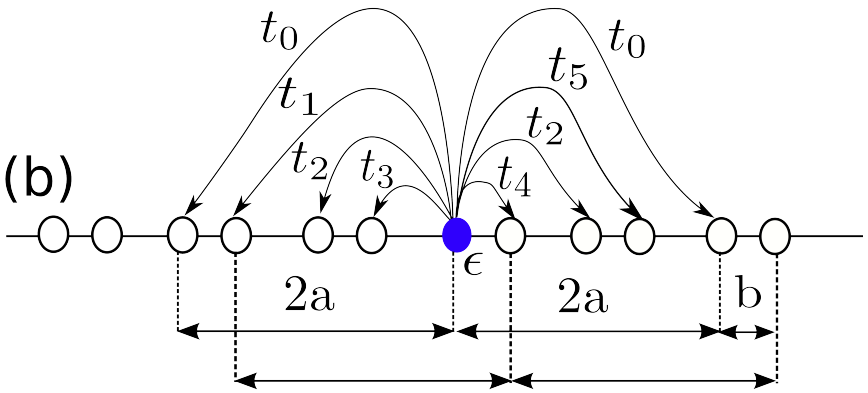
- ground-state energy (E_g)
- (ideally) excited states close to E_g
- (in)direct correlation picture
- observables for comparison with experiment
- scalability

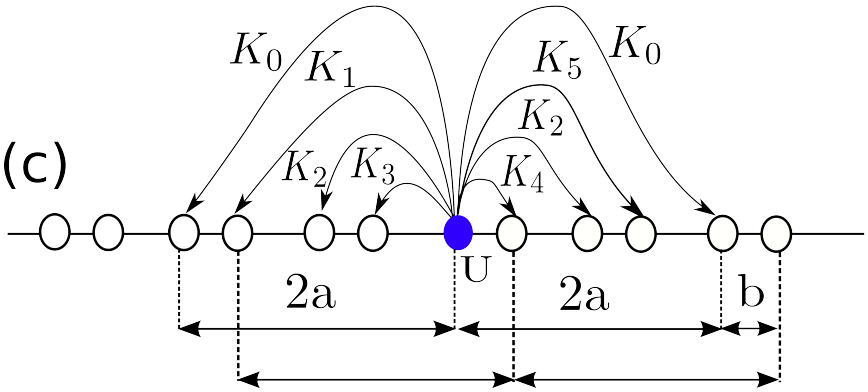
2^{nd}-quantization states

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

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

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

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

Dimensionality - 1D chain in 3D space

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

Proper state function

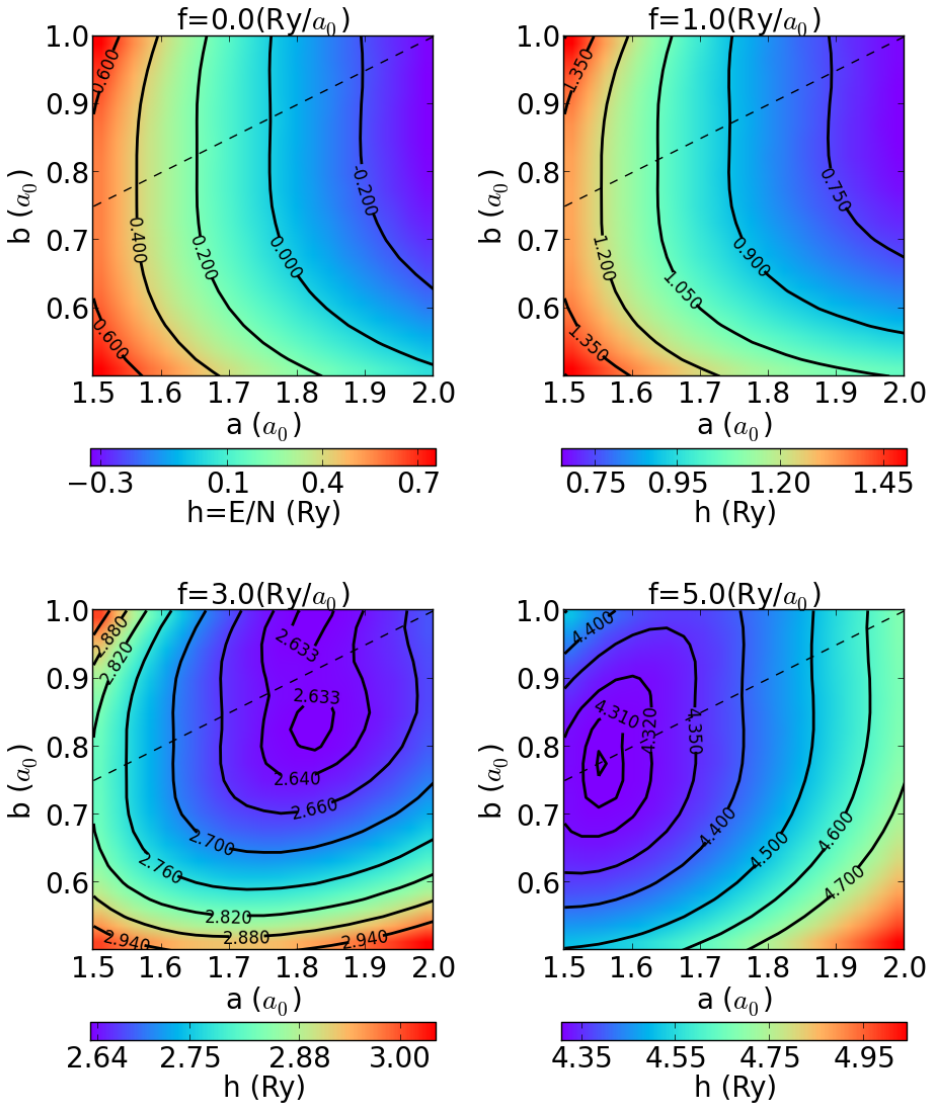
One-dimensional enthalpy

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

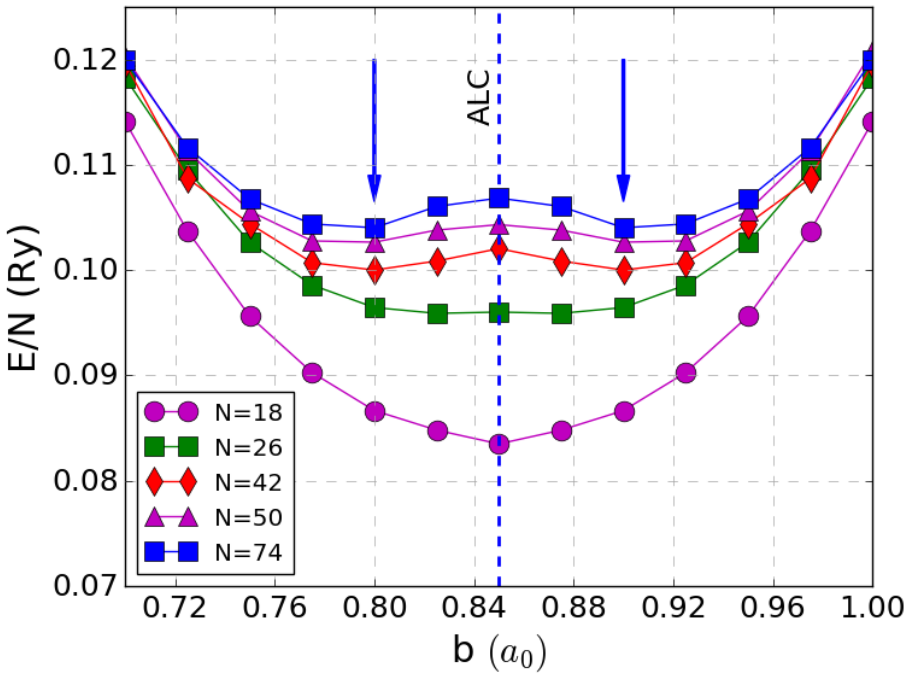
with f as an external force (analogue of the pressure), the lattice parameter a, and ground-state energy E for the N-particle supercell.

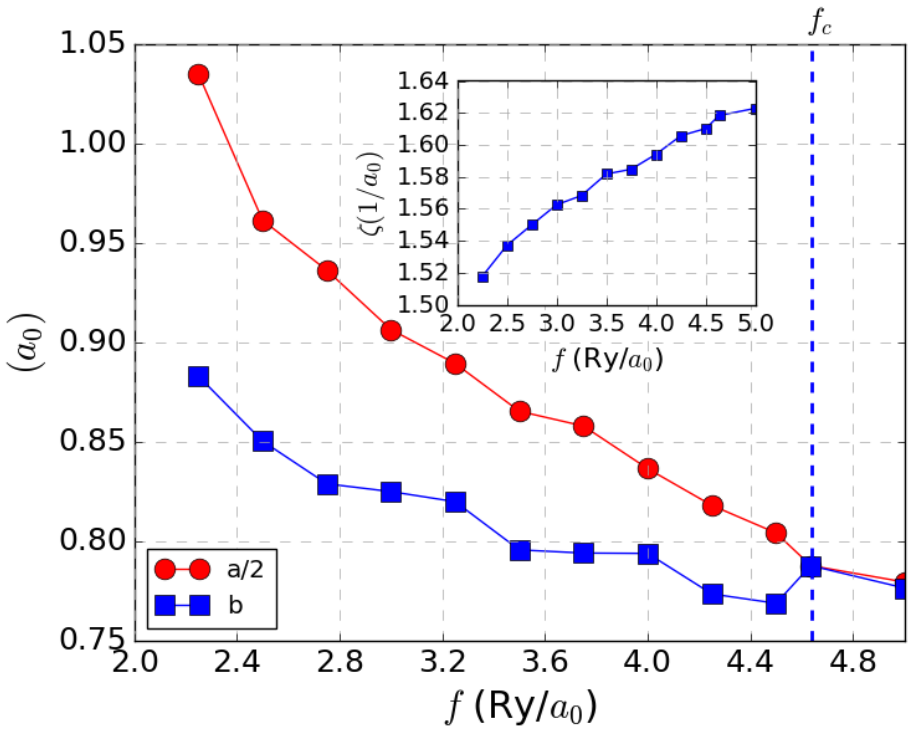
Run for given f

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



Results for finite systems



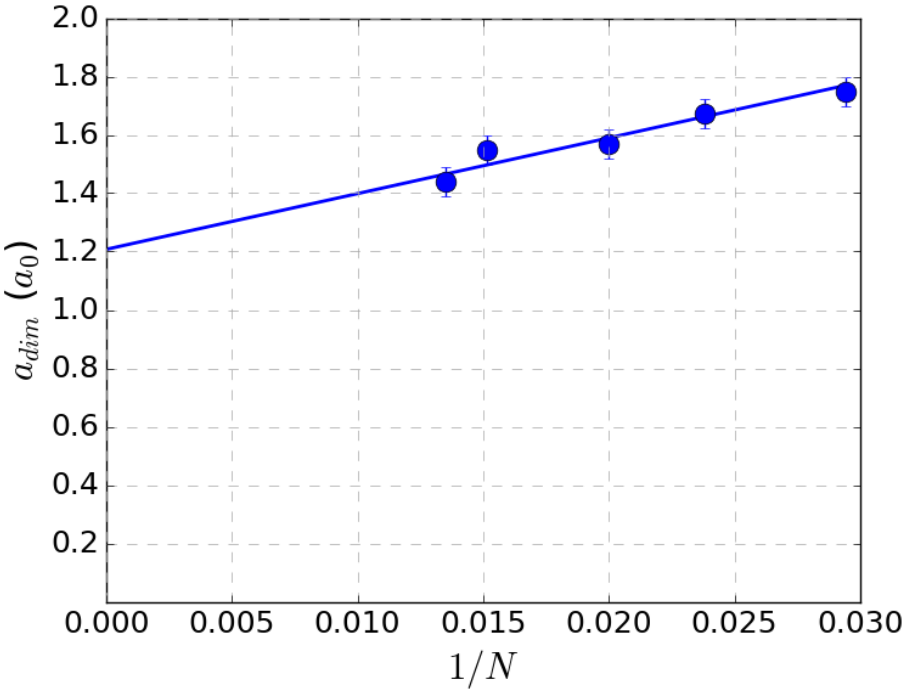


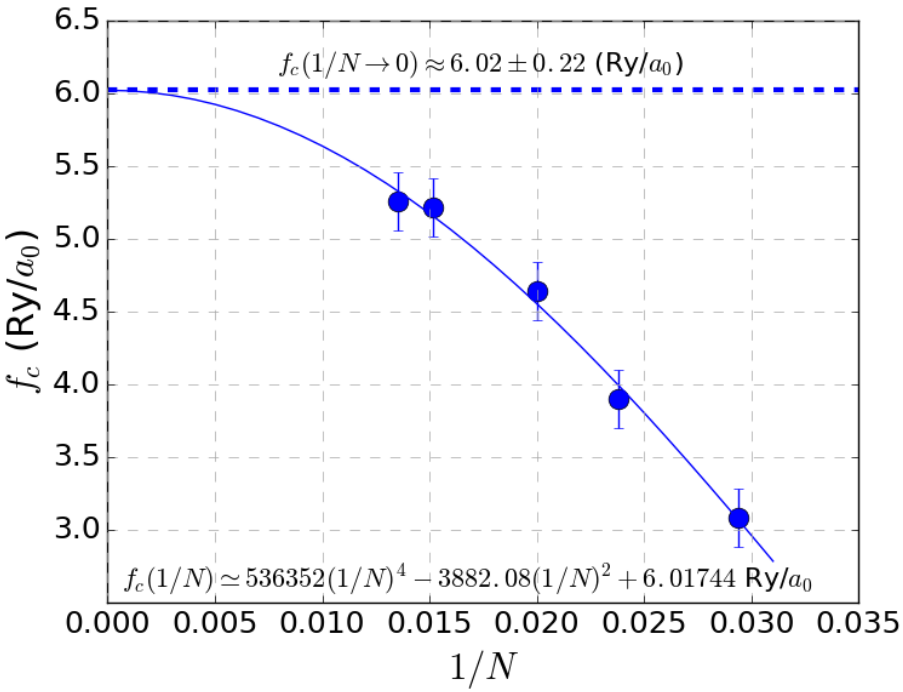
Peierls-like distortion from First Principles for a correlated system

- **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.

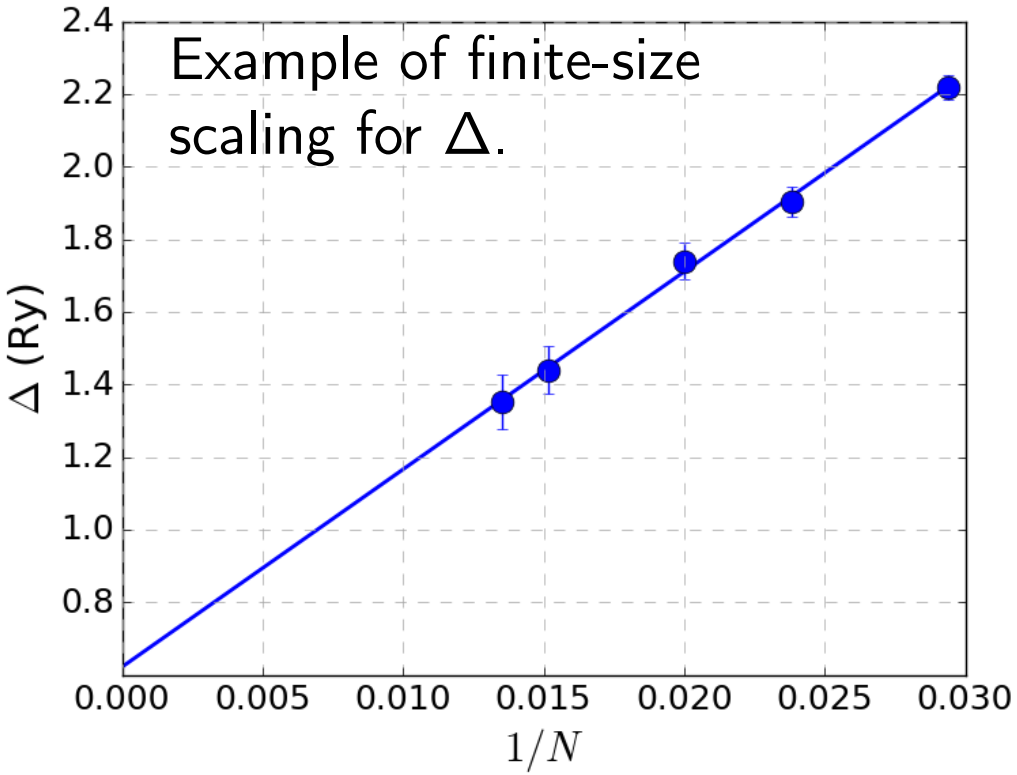
Charge gap

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

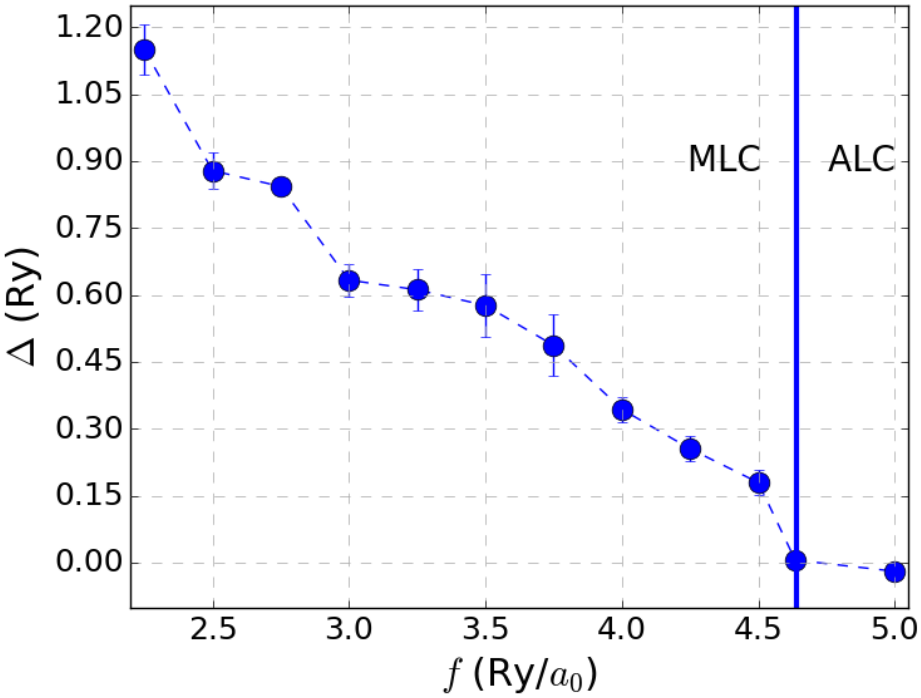
E_N - the ground state of the N-particle system described by the reference Hamiltonian with the structure minimizing the effective enthalpy.

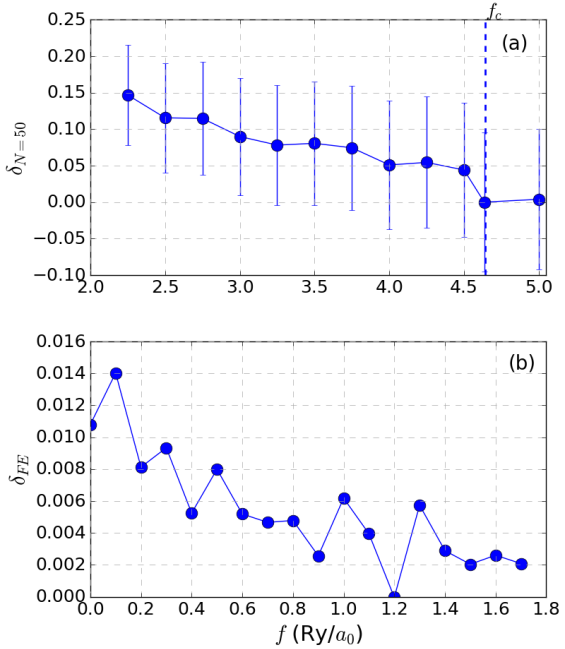
Thermodynamic limit

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



Closing of the charge gap





Apparent metallicity of the hydrogen chain in the atomic phase

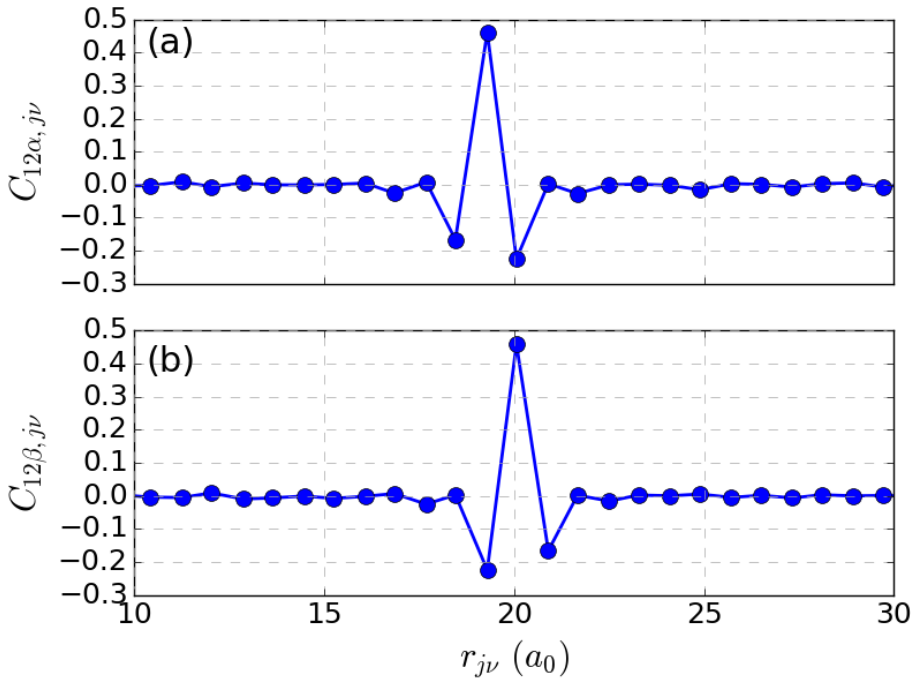
- charge gap closed at the MLC $\rightarrow$ ALC transition;
- further-than-nearest neighbor hoppings;
- chain exist in 3D (both single-particle wavefunctions and Coulomb potential are taken for $D = 3$);

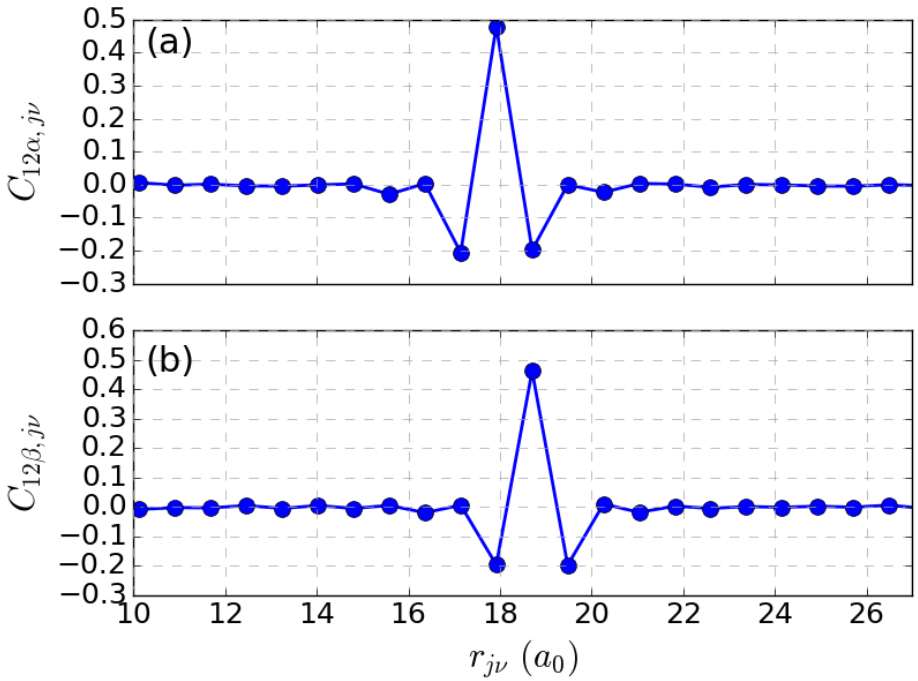
in agreement with L. Stella *et al.*, Phys. Rev. B **84**, 245117 (2011)

Density-density correlation

Density-density correlation

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



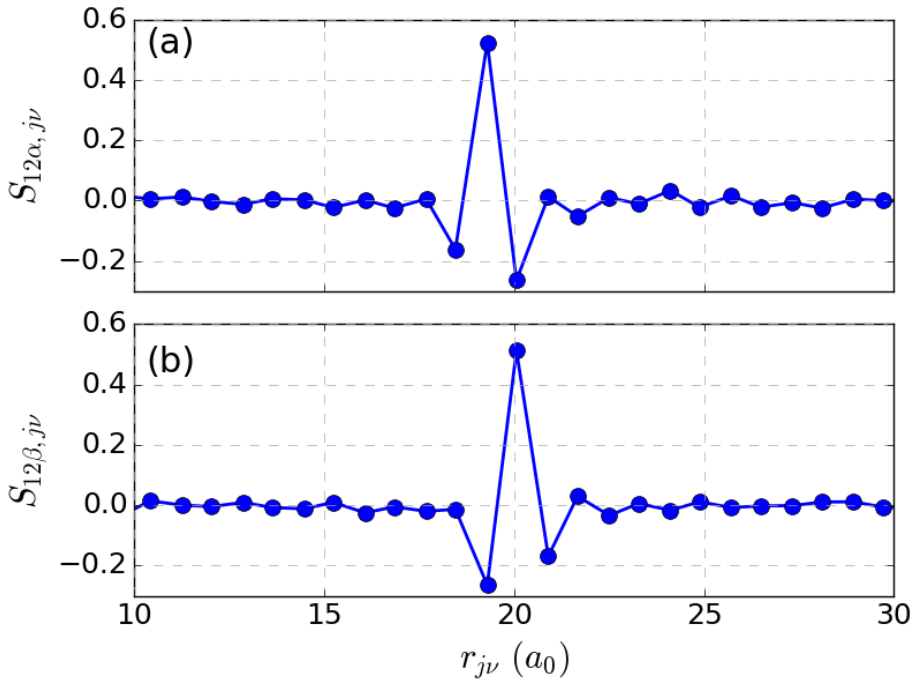


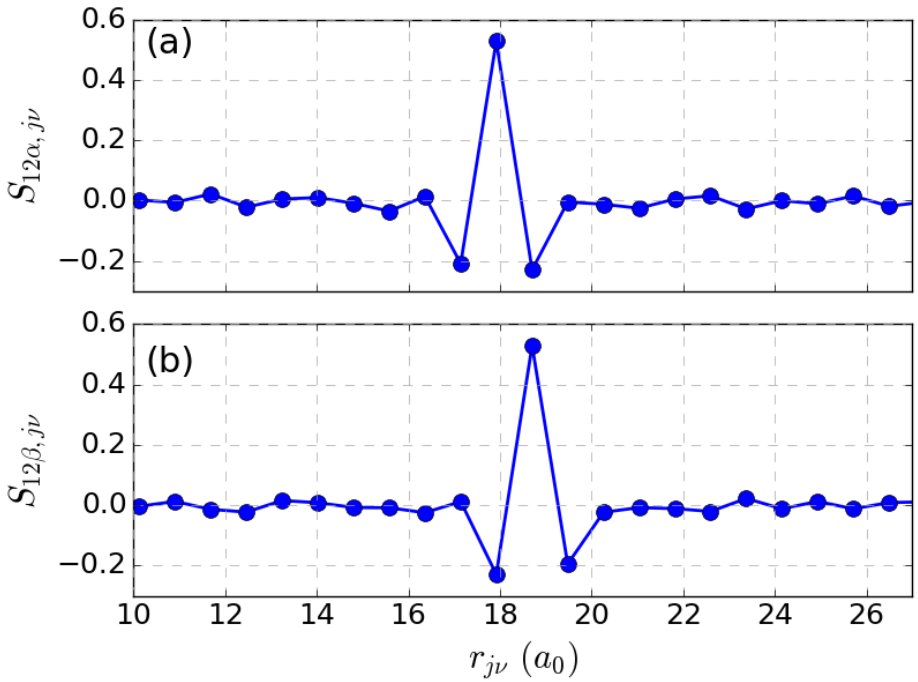
(LEFT) $f = 4.5$ Ry$/a_0$; (RIGHT) $f = 5.0$ Ry$/a_0$

Spin-spin correlation

Spin-spin correlation

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



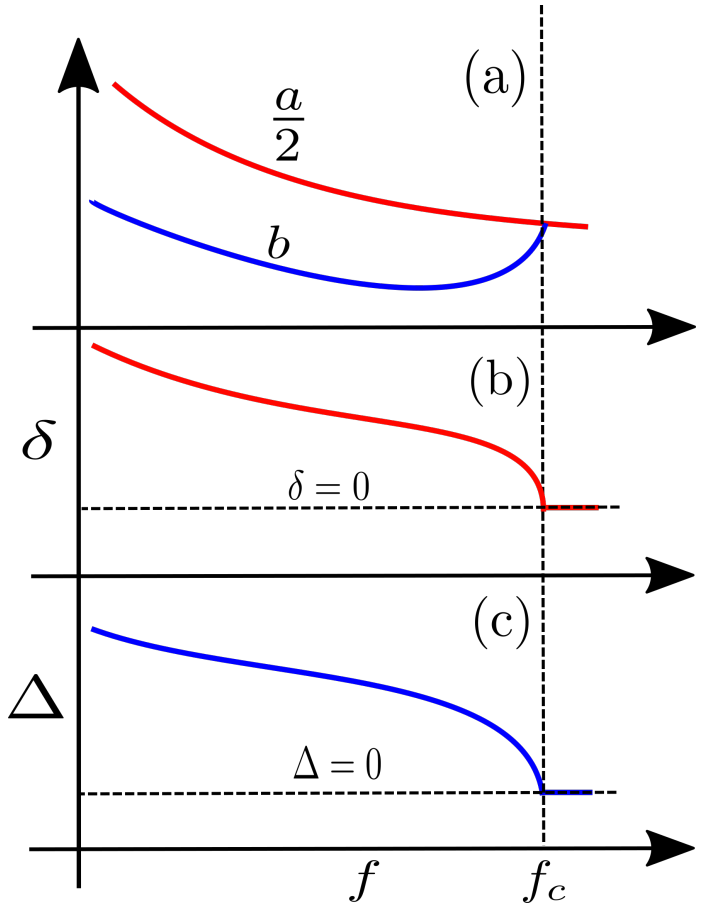


(LEFT) $f = 4.5$ Ry/a_0; (RIGHT) $f = 5.0$ Ry/a_0

Conclusions 1D

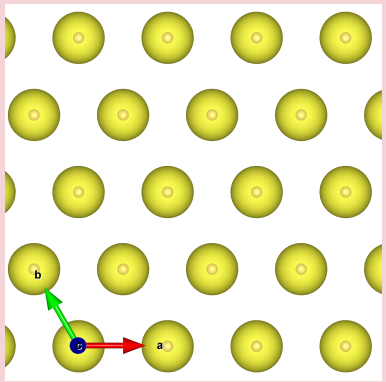
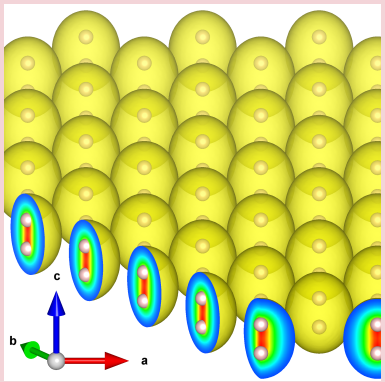
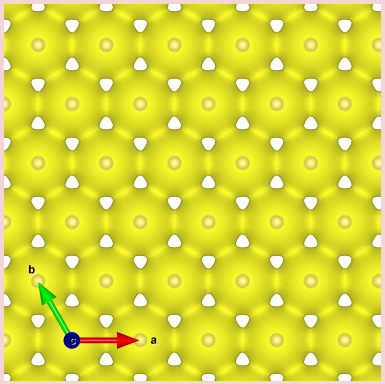
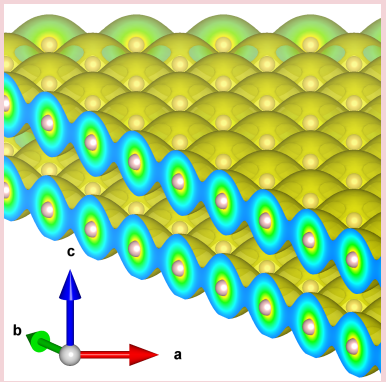
Hydrogen chain

- 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

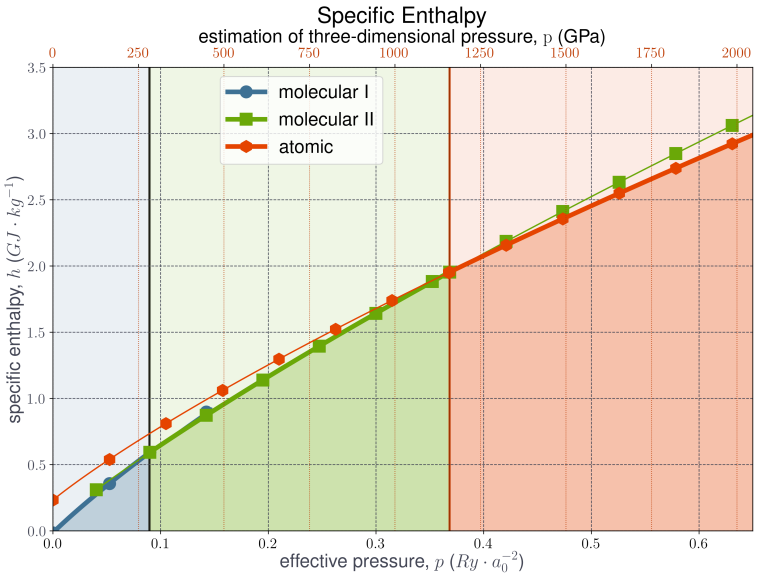





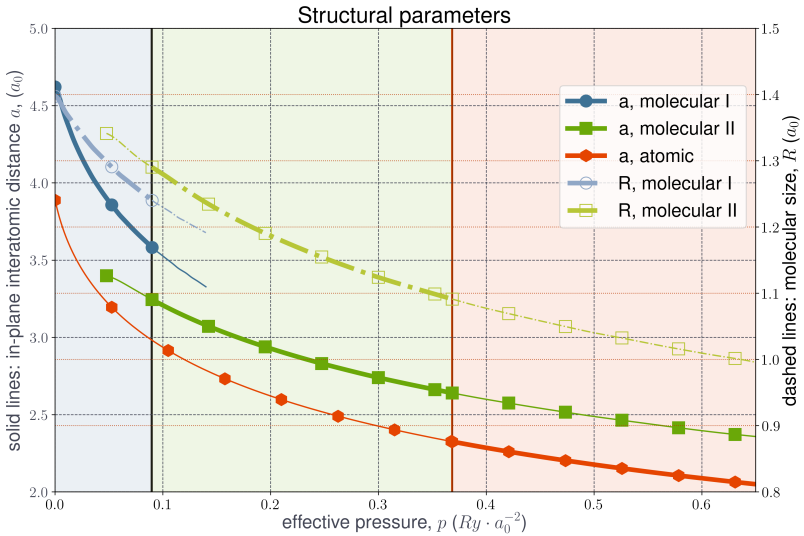
- periodic boundary conditions in xy plane;
- Lanczos algorithm for the diagonalization core of 6 and 8 atoms (to comply with proper Néel 120° and 90° phases);
- wavefunction constructed from 10 classes of nodes

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

$\hookrightarrow$ 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



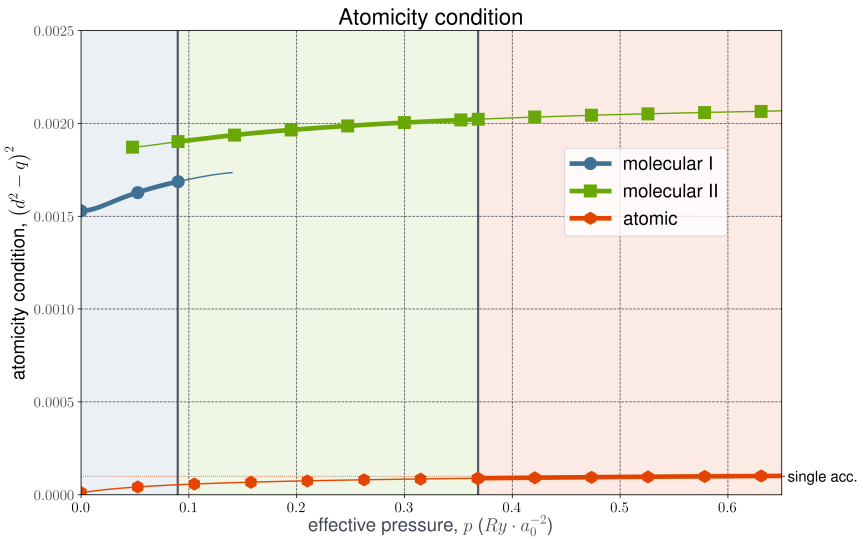


Question:

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

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

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



Magnetic order

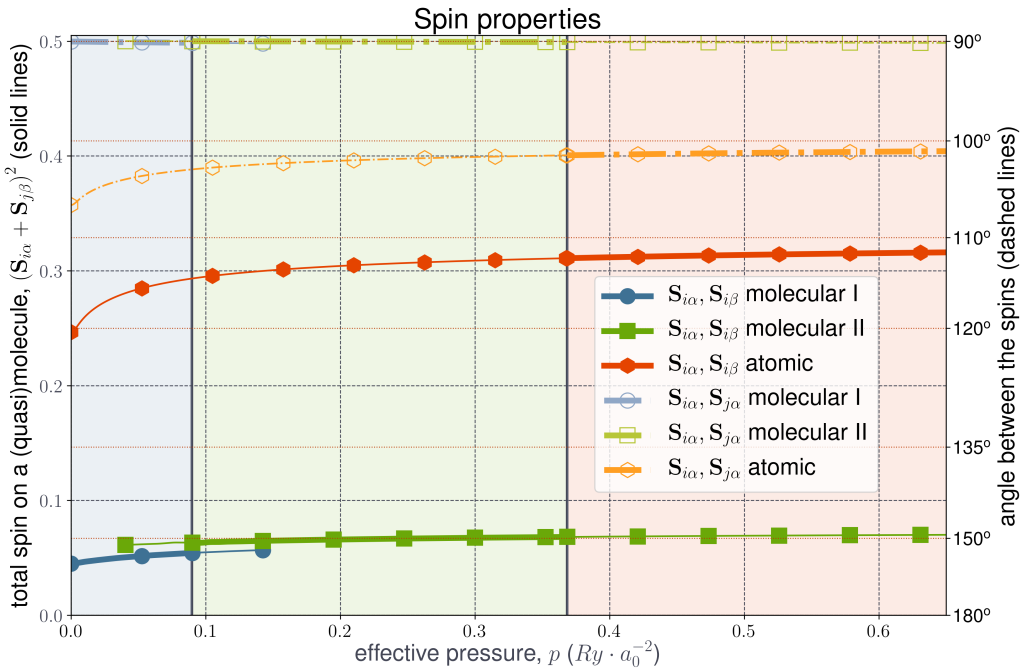
FM vs. AFM exchange

$J_{\text{FM, Hund-like}} \ll J_{\text{AFM, kinetic}}$

Required for the ambient pressure stability of the atomic phase!

Spin correlation

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



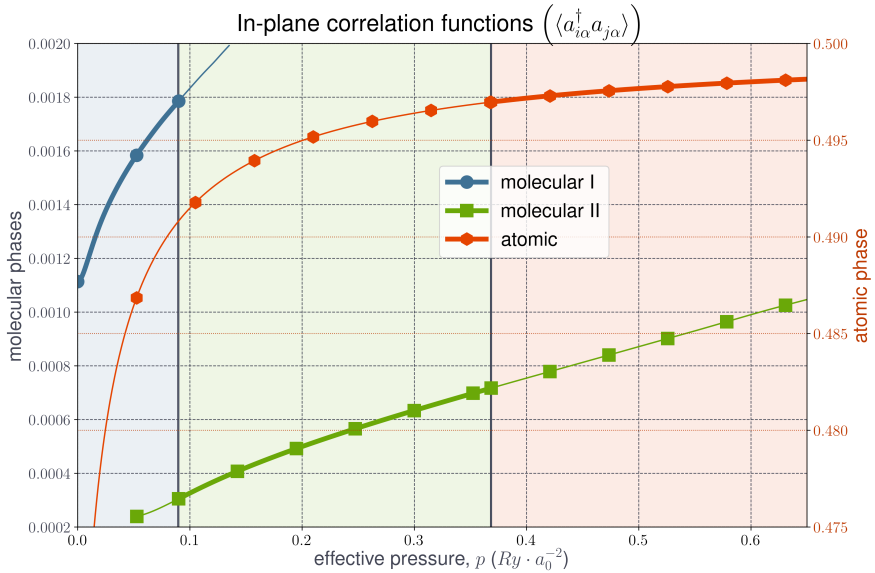
Total spin

	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

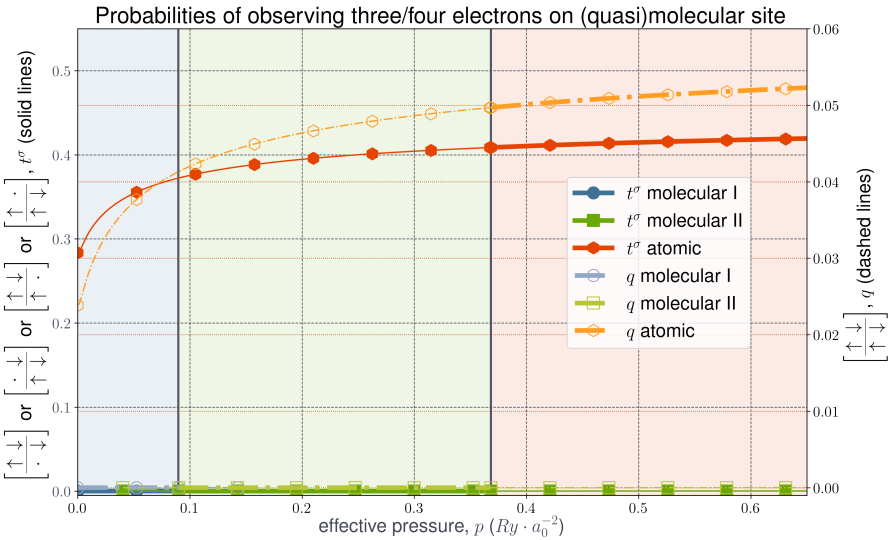
$$||\mathbf{S}||_{\mathbf{molecule}} \equiv ||\mathbf{S}(\mathbf{x}_{2D}, -\tfrac{R}{2}) + \mathbf{S}_2(\mathbf{x}_{2D}, \tfrac{R}{2})||$$

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

Metallization I: Correlation Functions



$$\mathcal{C}_{ij} \equiv \left\langle \hat{c}^\dagger_{i\sigma} \hat{c}_{i\sigma} \right\rangle = \left\langle \Phi_0 \middle| \hat{c}^\dagger_{i\sigma} \hat{c}_{i\sigma} \middle| \Phi_0 \right\rangle_G$$

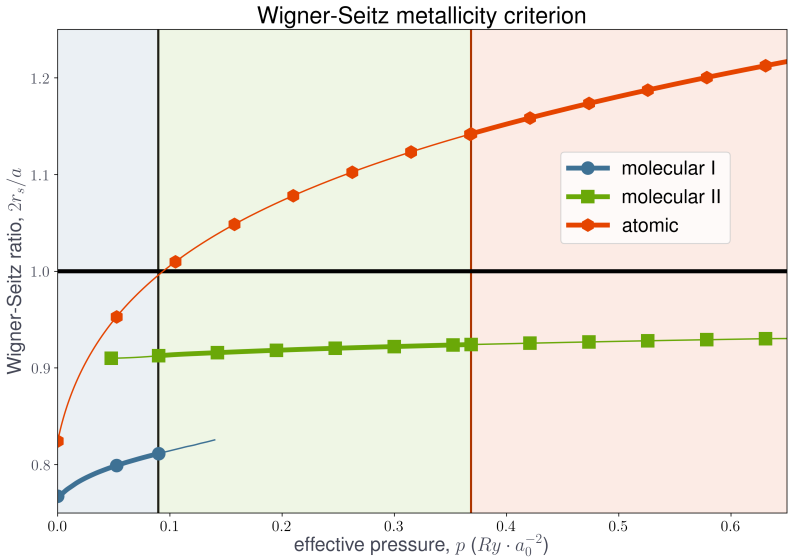


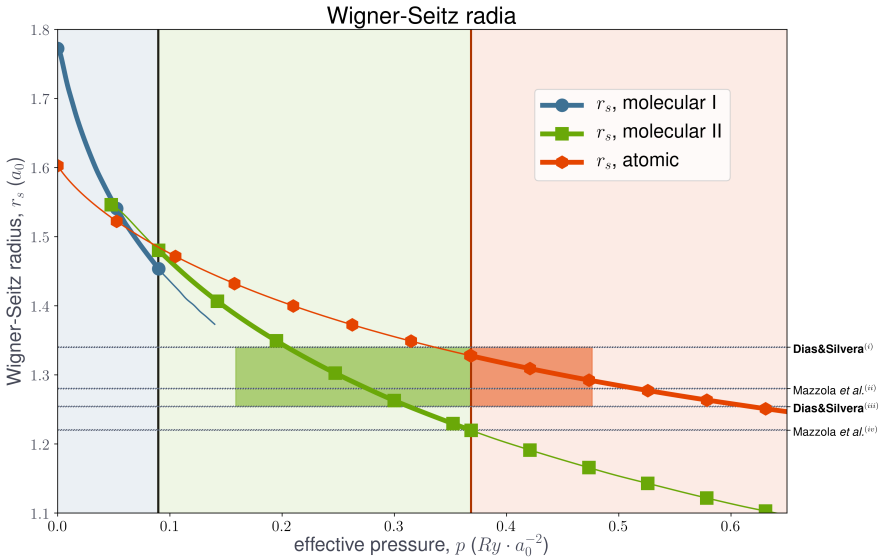
$$q \equiv P\left(\begin{array}{c}\uparrow\downarrow\\ \uparrow\downarrow\end{array}\right) \qquad d_0 \equiv P\left(\begin{array}{cc}\uparrow & \\ & \downarrow\end{array}\right)$$

$$t_\uparrow \equiv P\left(\begin{array}{c}\uparrow\\ \uparrow\downarrow\end{array}\right) \qquad d_\uparrow \equiv P\left(\begin{array}{c}\uparrow\\ \uparrow\end{array}\right)$$

$$t_\downarrow \equiv P\left(\begin{array}{c}\downarrow\\ \uparrow\downarrow\end{array}\right) \qquad d_\downarrow \equiv P\left(\begin{array}{c}\downarrow\\ \downarrow\end{array}\right)$$

Metallization II: Wigner-Seitz Criterion





$$r_S \equiv \left(\frac{3}{4\pi n}\right)^{1/3}$$

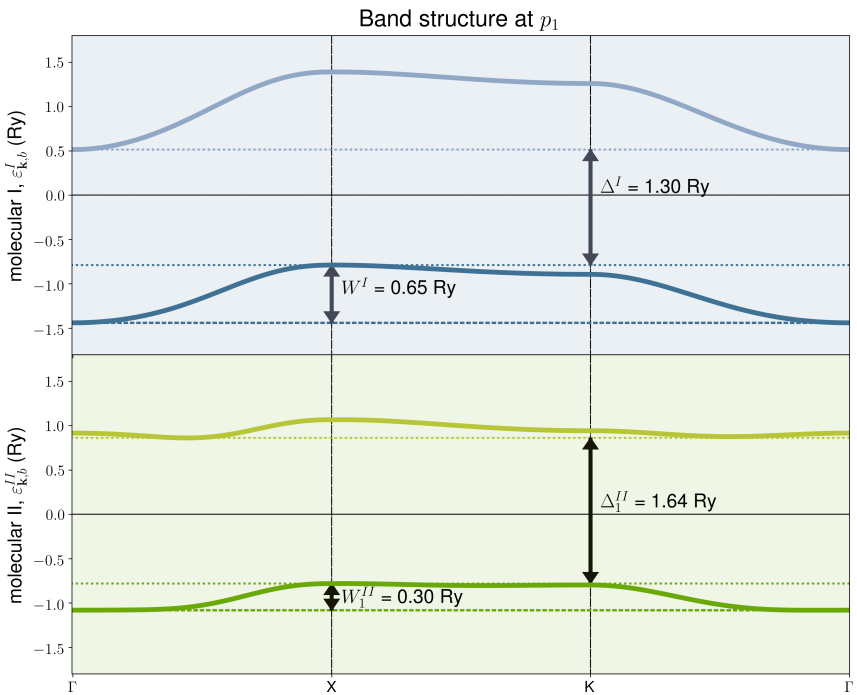
$$\text{metal} \Leftrightarrow 2r_s > d_{HH}$$

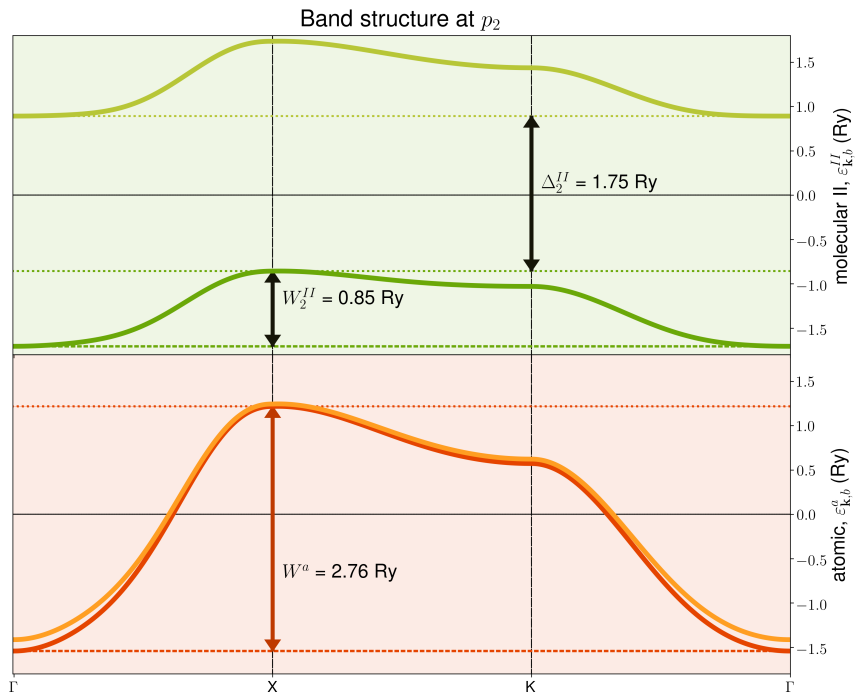
Can be found experimentally!

source	method	$r_s(a_0)$
Min et al., PRB **33**, 324 (1986)	LMTO	2.85
Pfrommer et al., PRB **58**, 12680 (1998)	GGA-PW91	2.50
Svane et al., SSC **76**, 851 (1990)	LSDA	2.45
Li et al. PRB **66**, 035102 (2002)	LSDA	2.78
Li et al. PRB **66**, 035102 (2002)	PBE	2.50
Mazzola et al., Nat.C. **5**, 3487 (2014)$^{(i)}$	DMC + MD	**1.28**$^{(ii)}$
McMinis et al., arXiv:1309.7051 (2013)	DMC	2.27
AB,APK,JS, PRB **96**, 085101 (2017)$^{(iii)}$	EDABI	**1.27**
molecular II	EDABI	$1.22^{+0.17}_{-0.06}$
atomic	EDABI	$1.33^{+0.10}_{-0.04}$
Dias & Silvera	experiment	**1.297(43)**

Metallization III: Band structure

Bare bands	Correlated bands	Bands + Correlator
■ easily calculable	■ full $\mathcal{H}$ dependence	■ calculable
■ depend only on $\mathcal{H}_{\text{free}}$	■ no generic method	∅ correlator physics





Possibility of superconducting state

Conventional Superconductivity

Atomic hydrogen is **metallic** $\Leftrightarrow$ **McMillan formula** for critical temperature

McMillan formula

$$T_C = \frac{\Theta_D}{1.45} \exp\left[-\frac{1.04(1+\lambda)}{\lambda + \mu^*(1+0.62\lambda)}\right]$$

- Θ_D - Debye temperature (from phonon DOS)
- λ - electron phonon coupling (from phononic and electronic dispersions)
- μ^* - Morel-Anderson pseudopotential - typically fitted to experimental data

We attempt to derive the ab-initio value of pseudopotential μ^*.

Morel-Anderson pseudopotential

$$\mu^* = \frac{\mu}{1 + \mu \log(\frac{\mathrm{T}_{\mathbf{phonons}}}{\mathrm{T}_{\mathbf{electrons}}})}$$

$$\mu^* = \frac{n(E_F)(U - K_1)}{1 + n(E_F)(U - K_1)\log(\frac{E_f}{k_B \Theta_D})}$$

Electron - phonon coupling

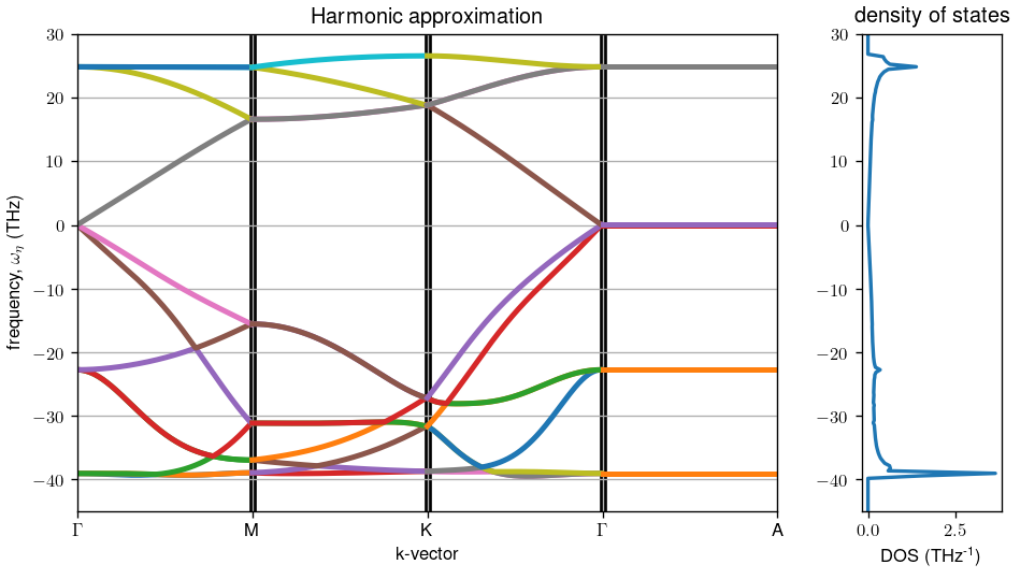
Eliashberg spectral function

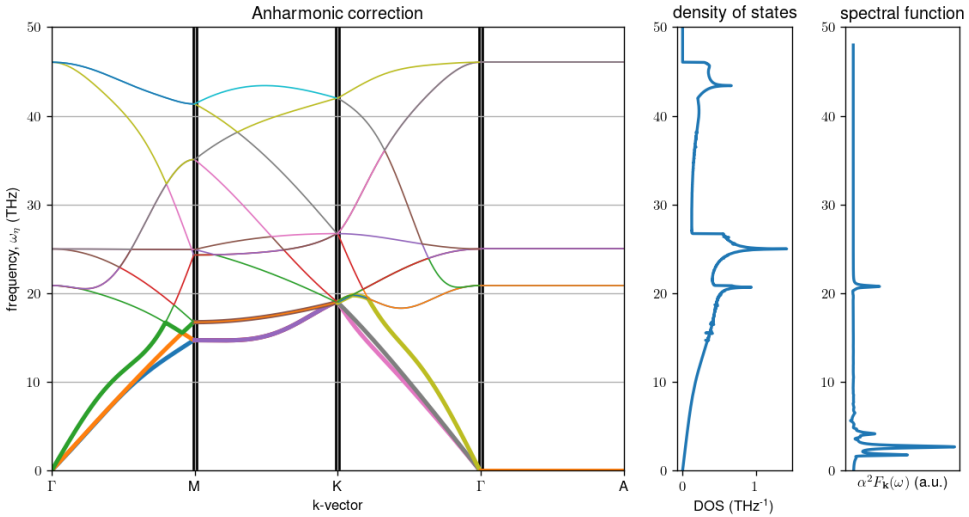
$$\alpha^2 F_{\mathbf{k}}(\omega) \sim \sum_\eta \int d\mathbf{q} M_\eta^2 \delta(\omega - \omega_\eta)\delta(\varepsilon(\mathbf{k}) - \varepsilon(\mathbf{k}+\mathbf{q}))$$

allows us to obtain electron-phonon coupling constant

$$\lambda = 2\int_0^\infty \frac{d\omega}{\omega} \alpha^2 F_{\mathbf{k_f}}(\omega)$$

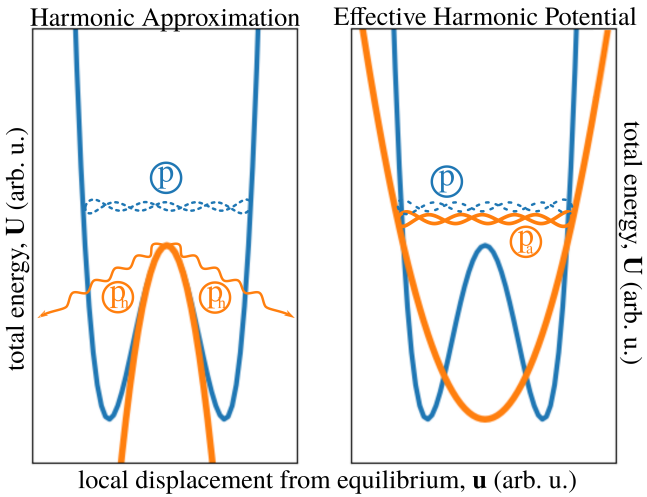
Electrons and Phonons: DFT calculations with EDABI constrains





We take the Mexican-hat potential:

$$U(\{u^i\}) = U_0 + \frac{1}{2}\Phi_{ij}u^{ij} + \frac{1}{4!}\Phi_{ijkl}u^{ijkl}$$



$$\mathrm{F}_i \to \mathrm{F}_i + \frac{1}{4!}\Phi_{i;j\langle kl\rangle}u^{ij\langle kl\rangle}.$$

At $p_{\mathrm{eff}} = 0.7Rya_0^{-2}$ $(\sim 1TPa)$

$U_{\mathrm{eff}} \equiv U - K_{pl}$ (Ry)	μ^*	λ
1.194	0.192	1.05
Θ_D (K)	T_C (K)	T_{AD} (K)
1300	164	**176**

DFT (VASP): SCAN meta-GGA + vdW corrections + charge from EDABI

Conclusions 2D

Physics of hydrogen planes

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

Hydrogen-induced superconductivity

- **medianly** correlated system;
- anharmonic correction to force constants necessary;
- superconductivity induced by electron-phonon coupling;
- Morel-Anderson pseudopotential **from First Principles**;
- high critical temperature $T_C = 176K$;
- extreme pressure (chemical?);

Thank you for your attention