

多体問題の計算科学

Computational Science for Many-Body Problems

#11 Krylov subspace methods and their
applications to quantum many-body problems

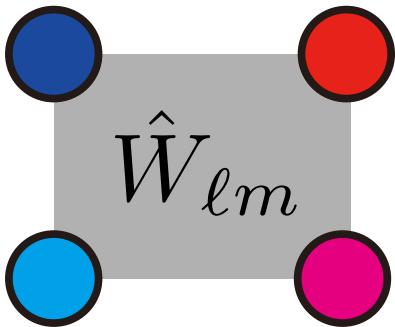
15:10-16:40 June 29, 2021

- 0. (Revisited) Negative sign problems in QMC
- 1. Numerical methods clarified emergent concepts
- 2. Excitation spectra
- 3. Conjugate gradient

Application of QMC

- Problems can be solved by QMC & the sign problem
- Dynamical mean-field theory
- Quantum chemistry

Negative Sign in Suzuki's Path Integral



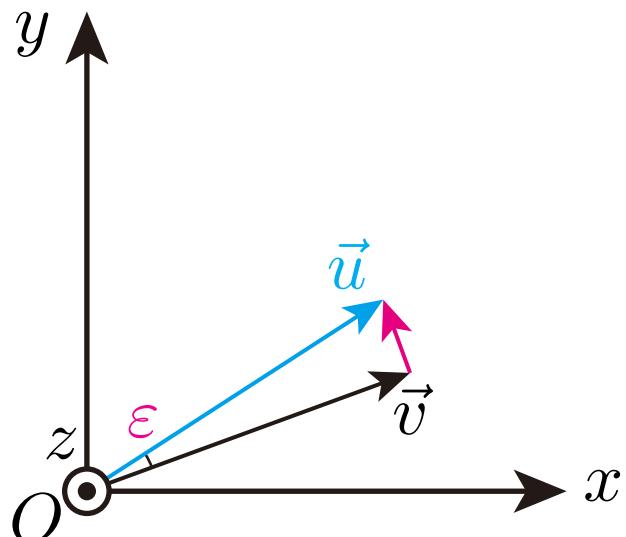
$$(\hat{W}_{\ell m})_{\sigma_\ell \sigma_m; \sigma_\ell \sigma_m} = \langle \sigma_\ell \sigma_m | e^{-\delta_\tau \hat{H}_{\ell m}} | \sigma_\ell \sigma_m \rangle$$

$$\begin{aligned} \hat{W}_{\ell m} &= \begin{pmatrix} \langle \downarrow\downarrow | e^{-\delta_\tau \hat{H}_{\ell m}} | \downarrow\downarrow \rangle & 0 & 0 & 0 \\ 0 & \langle \uparrow\downarrow | e^{-\delta_\tau \hat{H}_{\ell m}} | \uparrow\downarrow \rangle & \langle \uparrow\downarrow | e^{-\delta_\tau \hat{H}_{\ell m}} | \downarrow\uparrow \rangle & 0 \\ 0 & \langle \downarrow\uparrow | e^{-\delta_\tau \hat{H}_{\ell m}} | \uparrow\downarrow \rangle & \langle \downarrow\uparrow | e^{-\delta_\tau \hat{H}_{\ell m}} | \downarrow\uparrow \rangle & 0 \\ 0 & 0 & 0 & \langle \uparrow\uparrow | e^{-\delta_\tau \hat{H}_{\ell m}} | \uparrow\uparrow \rangle \end{pmatrix} \\ &= \begin{pmatrix} e^{-\delta_\tau J_z/4} & 0 & 0 & 0 \\ 0 & e^{+\delta_\tau J_z/4} \cosh(\delta_\tau J_x/2) & -e^{+\delta_\tau J_z/4} \sinh(\delta_\tau J_x/2) & 0 \\ 0 & -e^{+\delta_\tau J_z/4} \sinh(\delta_\tau J_x/2) & e^{+\delta_\tau J_z/4} \cosh(\delta_\tau J_x/2) & 0 \\ 0 & 0 & 0 & e^{-\delta_\tau J_z/4} \end{pmatrix} \end{aligned}$$

Rotation of Vector

Infinitesimal rotation ε :

$$\begin{pmatrix} u_1 \\ u_2 \\ u_3 \end{pmatrix} = \begin{pmatrix} 1 & -\varepsilon & 0 \\ +\varepsilon & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \\ v_3 \end{pmatrix}$$



$$\begin{pmatrix} 1 & -\varepsilon & 0 \\ +\varepsilon & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} - i\varepsilon \begin{pmatrix} 0 & -i & 0 \\ +i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

$$\simeq e^{-i\varepsilon \ell_z}$$

$$\ell_z \equiv \begin{pmatrix} 0 & -i & 0 \\ +i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

$$\ell_x \equiv \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & +i & 0 \end{pmatrix}$$

$$\ell_y \equiv \begin{pmatrix} 0 & 0 & +i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{pmatrix}$$

Finite Angle Rotation

Finite rotation

$$\vec{u} = e^{-i\theta \vec{n} \cdot \vec{\ell}} \vec{v}$$

$$\lim_{N \rightarrow +\infty} \left(1 - i \frac{\theta}{N} \vec{n} \cdot \vec{\ell} \right)^N = e^{-i\theta \vec{n} \cdot \vec{\ell}}$$

Rotations are not commutable:

$$e^{-i\theta_1 \ell_z} = \begin{pmatrix} +\cos \theta_1 & -\sin \theta_1 & 0 \\ +\sin \theta_1 & +\cos \theta_1 & 0 \\ 0 & 0 & +1 \end{pmatrix}$$

$$e^{-i\theta_2 \ell_x} = \begin{pmatrix} +1 & 0 & 0 \\ 0 & +\cos \theta_2 & -\sin \theta_2 \\ 0 & +\sin \theta_2 & +\cos \theta_2 \end{pmatrix}$$

$$e^{-i\theta_1 \ell_z} e^{-i\theta_2 \ell_x} \neq e^{-i\theta_2 \ell_x} e^{-i\theta_1 \ell_z}$$

Infinitesimal Rotation: An Example of Lie Algebra

$$\text{SU}(2) \quad [\ell_\alpha, \ell_\beta] = i\epsilon_{\alpha\beta\gamma}\ell_\gamma$$

$$[\ell_\alpha, \ell_\beta] \equiv \ell_\alpha \ell_\beta - \ell_\beta \ell_\alpha \quad \alpha, \beta, \gamma = x, y, z$$

Antisymmetric tensor: $\epsilon_{\alpha\beta\gamma} = \begin{cases} +1 & \text{for } (\alpha, \beta, \gamma) = (x, y, z), (y, z, x), (z, x, y) \\ -1 & \text{for } (\alpha, \beta, \gamma) = (x, z, y), (y, x, z), (z, y, x) \\ 0 & \text{others} \end{cases}$

3D representation:

$$\ell_z \equiv \begin{pmatrix} 0 & -i & 0 \\ +i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

$$\ell_x \equiv \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & +i & 0 \end{pmatrix}$$

$$\ell_y \equiv \begin{pmatrix} 0 & 0 & +i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{pmatrix}$$

2D representation:

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

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

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

有限回転はSO(3)と呼ばれるリー群

$$e^{-i\theta \vec{n} \cdot \vec{\ell}}$$

2D Rep. to 3D Rep.

Wave function to spin components

$$\vec{u} = \begin{pmatrix} u_1 \\ u_2 \end{pmatrix}$$

$$\langle s_z \rangle \equiv \vec{u}^\dagger s_z \vec{u}$$

$$\langle s_x \rangle \equiv \vec{u}^\dagger s_x \vec{u}$$

$$\langle s_y \rangle \equiv \vec{u}^\dagger s_y \vec{u}$$

$$\vec{s} = \begin{pmatrix} \langle s_x \rangle \\ \langle s_y \rangle \\ \langle s_z \rangle \end{pmatrix}$$

Rep. & Basis of Rotation Group

	“Wave function”	Double rep.
$e^{-i\phi s_z} e^{-i\theta s_y} \begin{pmatrix} 1 \\ 0 \end{pmatrix}$		$\vec{u} = \begin{pmatrix} \cos \frac{\theta}{2} e^{-i\frac{\phi}{2}} \\ \sin \frac{\theta}{2} e^{+i\frac{\phi}{2}} \end{pmatrix}$
	Spin	
$e^{-i\phi \ell_z} e^{-i\theta \ell_y} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$		$\vec{s} = \frac{1}{2} \begin{pmatrix} \sin \theta \cos \phi \\ \sin \theta \sin \phi \\ \cos \theta \end{pmatrix}$

Rotation of Local Spin Coordinate

M. Suzuki, S. Miyashita, & A. Kuroda, PTP 58, 1377 (1977).
As a review, H. G. Evertz, Adv. Phys. 52, 1 (2003).

An example: 1D XXZ model

$$\hat{H} = J_x \sum_i (\hat{S}_i^x \hat{S}_{i+1}^x + \hat{S}_i^y \hat{S}_{i+1}^y) + J_z \sum_i \hat{S}_i^z \hat{S}_{i+1}^z$$



$$\tilde{S}_{2\ell}^x = e^{-i\pi \hat{S}_{2\ell}^z} \hat{S}_{2\ell}^x e^{+i\pi \hat{S}_{2\ell}^z} = -\hat{S}_{2\ell}^x$$

$$\tilde{S}_{2\ell}^y = e^{-i\pi \hat{S}_{2\ell}^z} \hat{S}_{2\ell}^y e^{+i\pi \hat{S}_{2\ell}^z} = -\hat{S}_{2\ell}^y$$

$$\tilde{S}_{2\ell+1}^x = \hat{S}_{2\ell+1}^x$$

$$\tilde{S}_{2\ell+1}^y = \hat{S}_{2\ell+1}^y$$

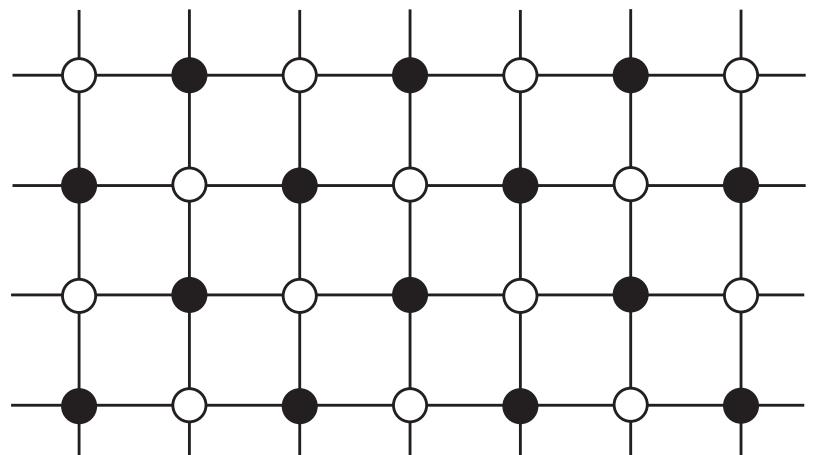
$$\tilde{H} = -J_x \sum_i (\tilde{S}_i^x \tilde{S}_{i+1}^x + \tilde{S}_i^y \tilde{S}_{i+1}^y) + J_z \sum_i \hat{S}_i^z \hat{S}_{i+1}^z$$

Removal of Negative Weight

$$\tilde{H} = -J_x \sum_i (\tilde{S}_i^x \tilde{S}_{i+1}^x + \tilde{S}_i^y \tilde{S}_{i+1}^y) + J_z \sum_i \hat{S}_i^z \hat{S}_{i+1}^z$$

$$\begin{aligned} \widetilde{W}_{\ell m} &= \begin{pmatrix} \langle \downarrow \downarrow | e^{-\delta_\tau \tilde{H}_{\ell m}} | \downarrow \downarrow \rangle & 0 & 0 & 0 \\ 0 & \langle \uparrow \downarrow | e^{-\delta_\tau \tilde{H}_{\ell m}} | \uparrow \downarrow \rangle & \langle \uparrow \downarrow | e^{-\delta_\tau \tilde{H}_{\ell m}} | \downarrow \uparrow \rangle & 0 \\ 0 & \langle \downarrow \uparrow | e^{-\delta_\tau \tilde{H}_{\ell m}} | \uparrow \downarrow \rangle & \langle \downarrow \uparrow | e^{-\delta_\tau \tilde{H}_{\ell m}} | \downarrow \uparrow \rangle & 0 \\ 0 & 0 & 0 & \langle \uparrow \uparrow | e^{-\delta_\tau \tilde{H}_{\ell m}} | \uparrow \uparrow \rangle \end{pmatrix} \\ &= \begin{pmatrix} e^{-\delta_\tau J_z/4} & 0 & 0 & 0 \\ 0 & e^{+\delta_\tau J_z/4} \cosh(\delta_\tau J_x/2) & +e^{+\delta_\tau J_z/4} \sinh(\delta_\tau J_x/2) & 0 \\ 0 & +e^{+\delta_\tau J_z/4} \sinh(\delta_\tau J_x/2) & e^{+\delta_\tau J_z/4} \cosh(\delta_\tau J_x/2) & 0 \\ 0 & 0 & 0 & e^{-\delta_\tau J_z/4} \end{pmatrix} \end{aligned}$$

Applicable to bipartite lattice

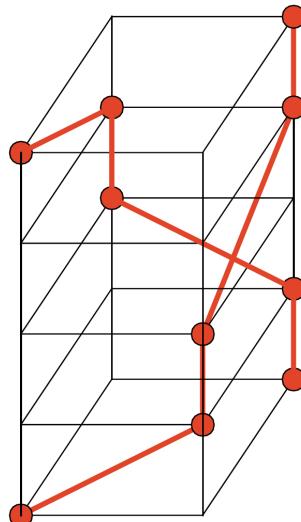


Negative Sign in Fermions

M. Troyer and U.-J. Wiese, Phys. Rev. Lett. 94, 170201 (2005).

Another formulation of path integral

$$Z = \text{tr}[e^{-\beta \hat{H}}] = \sum_{n=0}^{\infty} \frac{(-\beta)^n}{n!} \text{tr}[\hat{H}^n]$$
$$= \sum_{n=0}^{\infty} \sum_{\nu_1, \nu_2, \dots, \nu_n} \frac{(-\beta)^n}{n!} \langle \nu_1 | \hat{H} | \nu_2 \rangle \langle \nu_2 | \hat{H} | \nu_3 \rangle \cdots \langle \nu_n | \hat{H} | \nu_1 \rangle$$



Negative Sign in Fermions

M. Troyer and U.-J. Wiese, Phys. Rev. Lett. 94, 170201 (2005).

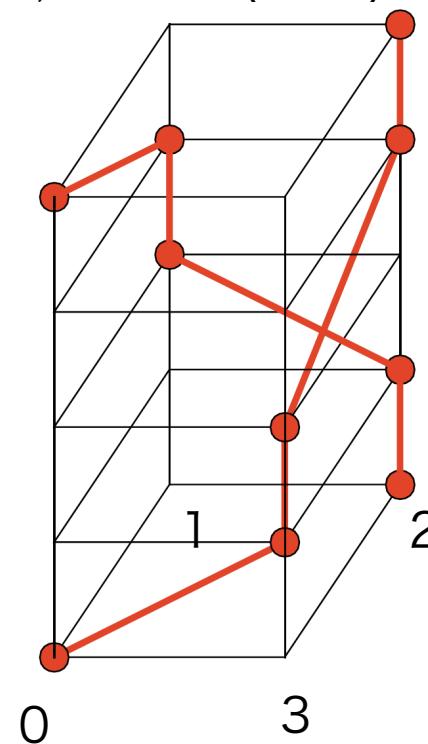
$$|\nu_1\rangle = \hat{c}_2^\dagger \hat{c}_0^\dagger |0\rangle$$

$$|\nu_4\rangle = \hat{c}_2^\dagger \hat{c}_1^\dagger |0\rangle$$

$$|\nu_3\rangle = \hat{c}_3^\dagger \hat{c}_1^\dagger |0\rangle$$

$$|\nu_2\rangle = \hat{c}_3^\dagger \hat{c}_2^\dagger |0\rangle$$

$$|\nu_1\rangle = \hat{c}_2^\dagger \hat{c}_0^\dagger |0\rangle$$



$$\hat{H} = \sum_{\langle i,j \rangle} (\hat{c}_i^\dagger \hat{c}_j + \hat{c}_j^\dagger \hat{c}_i) \quad \text{nearest-neighbor hopping}$$

$$\langle \nu_1 | \hat{H} | \nu_2 \rangle \langle \nu_2 | \hat{H} | \nu_3 \rangle \langle \nu_3 | \hat{H} | \nu_4 \rangle \langle \nu_4 | \hat{H} | \nu_1 \rangle = -1$$

Definition of Averaged Sign

$$\begin{aligned} Z &= \text{tr}[e^{-\beta \hat{H}}] = \sum_{n=0}^{\infty} \frac{(-\beta)^n}{n!} \text{tr}[\hat{H}^n] \\ &= \sum_{n=0}^{\infty} \sum_{\nu_1, \nu_2, \dots, \nu_n} \frac{(-\beta)^n}{n!} \langle \nu_1 | \hat{H} | \nu_2 \rangle \langle \nu_2 | \hat{H} | \nu_3 \rangle \cdots \langle \nu_n | \hat{H} | \nu_1 \rangle \\ &= \sum_{n=0}^{\infty} \sum_{\nu_1, \nu_2, \dots, \nu_n} p(\nu_1, \nu_2, \dots, \nu_n) = \sum_c p(c) \end{aligned}$$

M. Troyer and U.-J. Wiese, Phys. Rev. Lett. 94, 170201 (2005).

$$\langle \text{sign} \rangle = \frac{\sum_c p(c)}{\sum_c |p(c)|} = \frac{Z_f}{Z_b} = e^{-V\beta(f_f - f_b)}$$

-Basis dependent

For example, H. Shinaoka *et al.*, Phys. Rev. B 92, 195126 (2015).

Symmetry Removes Negative Sign

BSS QMC for Hubbard model

$$\hat{H} = \sum_{\langle i,j \rangle, \sigma} (\hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + \hat{c}_{j\sigma}^\dagger \hat{c}_{i\sigma}) + U \sum_i \hat{c}_{i\uparrow}^\dagger \hat{c}_{i\uparrow} \hat{c}_{i\downarrow}^\dagger \hat{c}_{i\downarrow}$$

Weight for each Ising configuration: $Z = Z_\uparrow Z_\downarrow$

$$Z_\sigma = \det [I + B_M^\sigma B_{M-1}^\sigma \cdots B_1^\sigma]$$

Attractive Hubbard model $U < 0$

-Ising variables are spin independent $Z_\uparrow = Z_\downarrow$

Repulsive Hubbard model $U > 0$

-Particle-hole symmetry $Z_\uparrow = c Z_\downarrow$ ($c > 0$)

J. E. Hirsch, Phys. Rev. B 28, 4059 (1983).

cf.) symmetry of Kane-Mele-Hubbard model

Numerical Methods Clarified Emergent Concepts in Many-Body Problems

Important Applications of Lanczos Method and Exact Wave Functions

Emergent concepts in many-body physics has been verified by using Lanczos and exact wf

Fractional quantum Hall effect

Experiment: D. C. Tsui, *et al.*, Phys. Rev. Lett. 48, 1559 (1982).

Theory: R. B. Laughlin, Phys. Rev. Lett. 50, 1395 (1983).

F. D. M. Haldane, Phys. Rev. Lett. 55, 2095 (1985).

-Verification of Laughlin-Jastrow wave function

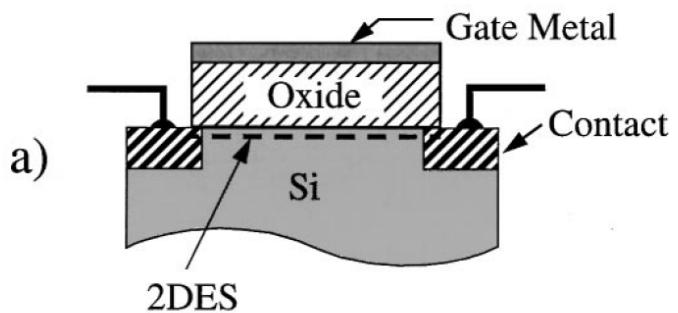
Thermalization of isolated quantum systems

M. Rigol, V. Dunjko, and M. Olshanii, Nature 452, 854 (2008).

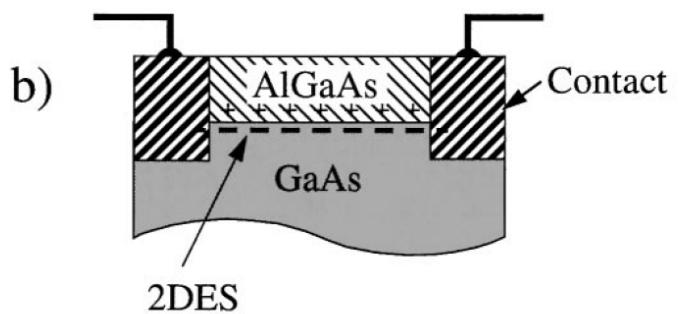
- Linear responses of strongly correlated electrons
- Frustrated magnetism
- Haldane gap

FQHE

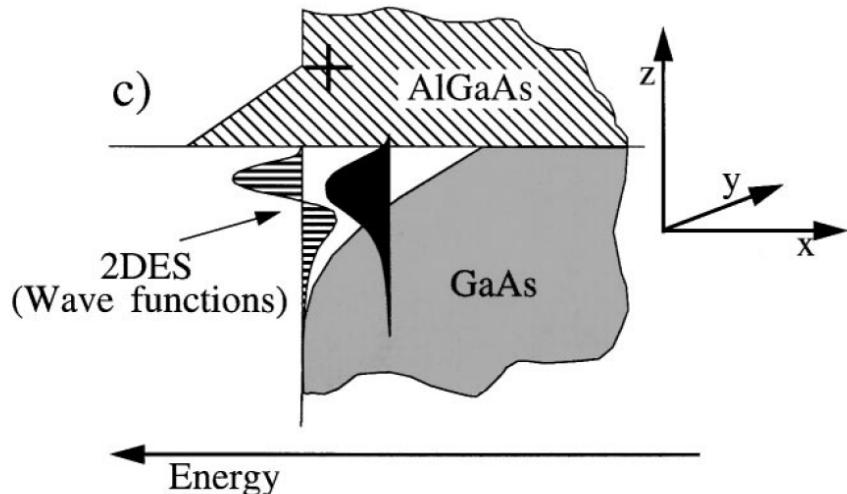
Two Dimensional Electron Gas



MOSFET
(metal-oxide-semiconductor field-effect transistor)



HEMT
(high electron mobility transistor)



H. L. Stormer,
Rev. Mod. Phys. 71, 875 (1999).

Discovery of FQHE

Hall resistance of HEMT

D. C. Tsui, *et al.*,

Phys. Rev. Lett. 48, 1559 (1982).

A. M. Chang, *et al.*,

Phys. Rev. Lett. 53, 997 (1984).

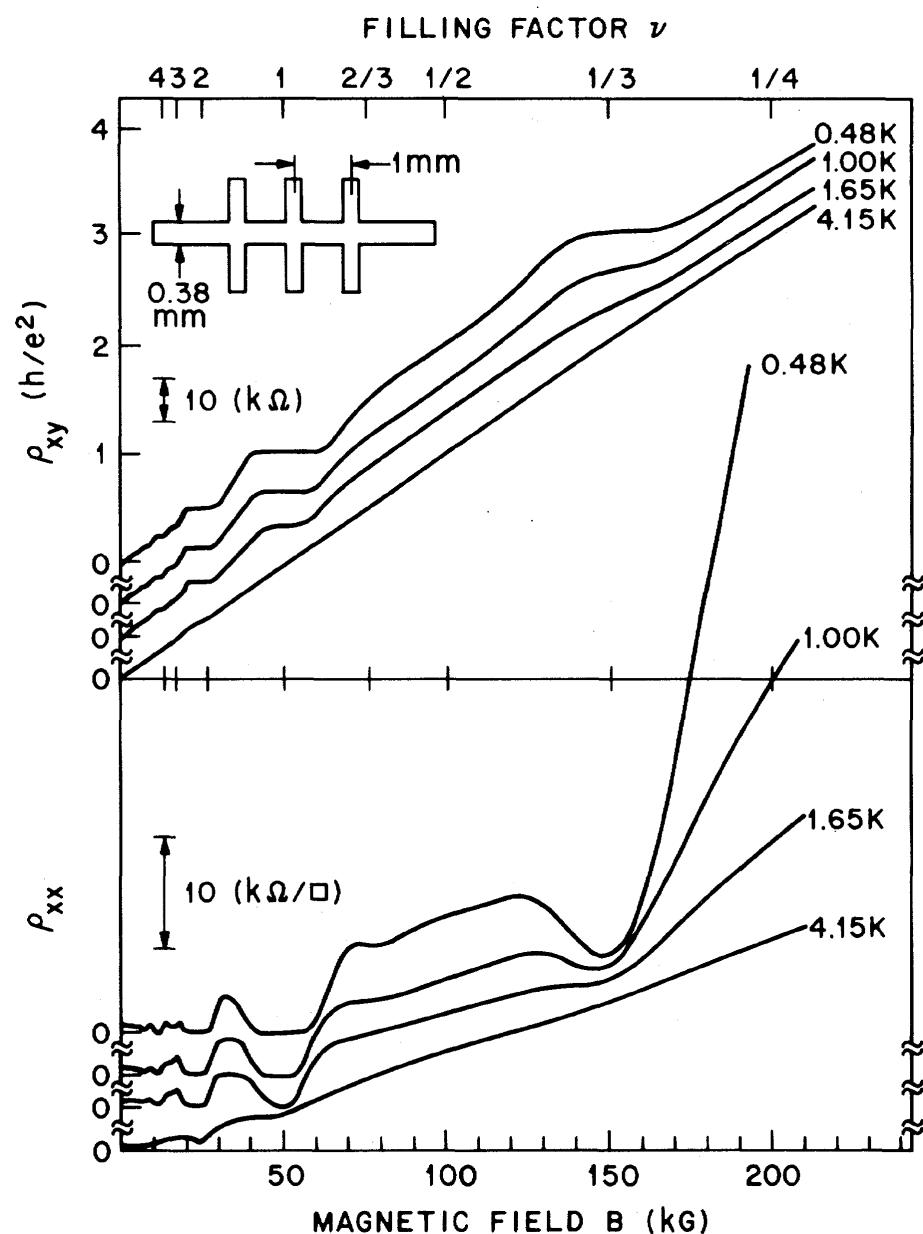
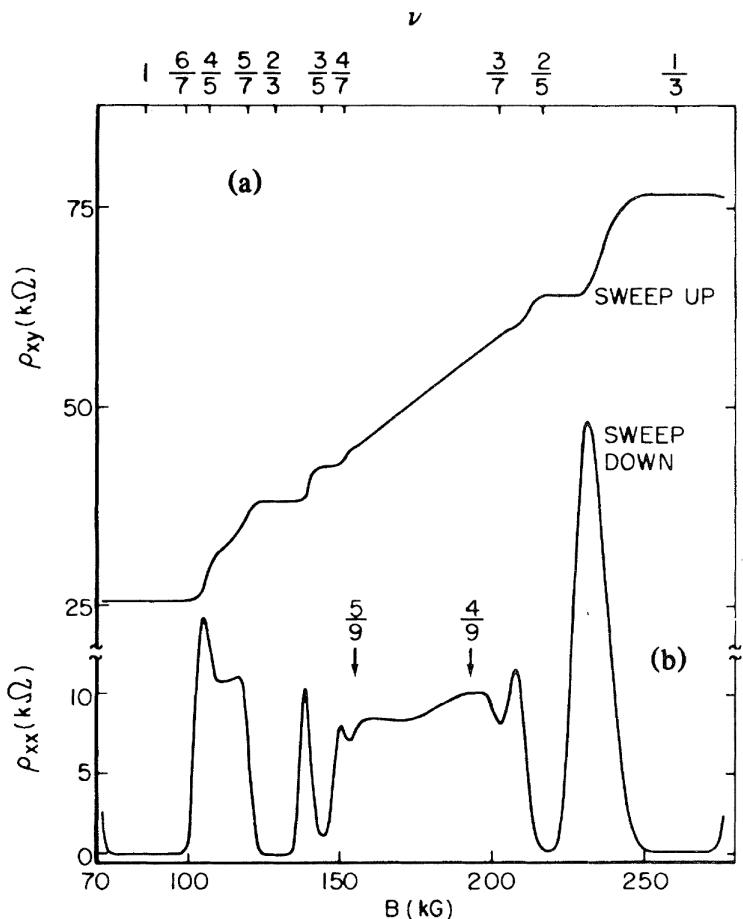


FIG. 1. ρ_{xy} and ρ_{xx} vs B , taken from a GaAs-Al_{0.3}-Ga_{0.7}As sample with $n = 1.23 \times 10^{11}/\text{cm}^2$, $\mu = 90\,000 \text{ cm}^2/\text{V sec}$, using $I = 1 \mu\text{A}$. The Landau level filling factor is defined by $\nu = nh/eB$.

Laughlin-Jastrow Trial Wave Function

R. B. Laughlin, Phys. Rev. Lett. 50, 1395 (1983).

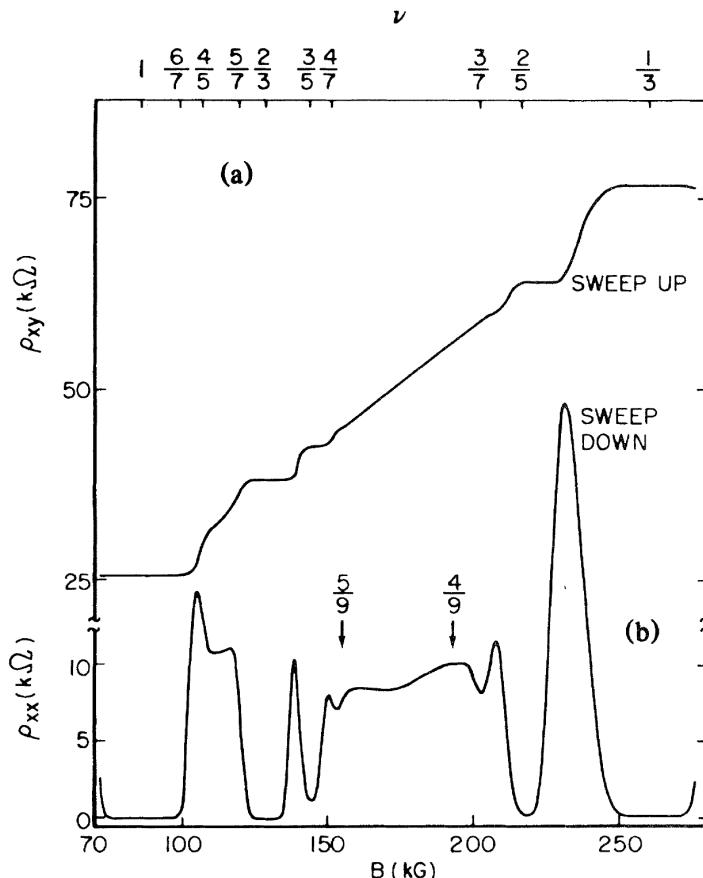
$$\psi_m(z_1, z_2, \dots, z_N) = \left[\prod_{i < j} (z_i - z_j)^m \right] \exp \left(-\frac{1}{4} \sum_k |z_k|^2 \right)$$

$$z_j = x_j - iy_j$$

$$m = 1/\nu$$

F. D. M. Haldane,
Phys. Rev. Lett. 55, 2095 (1985).

Exact wave function for
6 electrons in 18 states ($\nu = 1/3$)
-98.81% overlap with the LJ trial w.f.



Haldane Gap

Background: Topological Phase

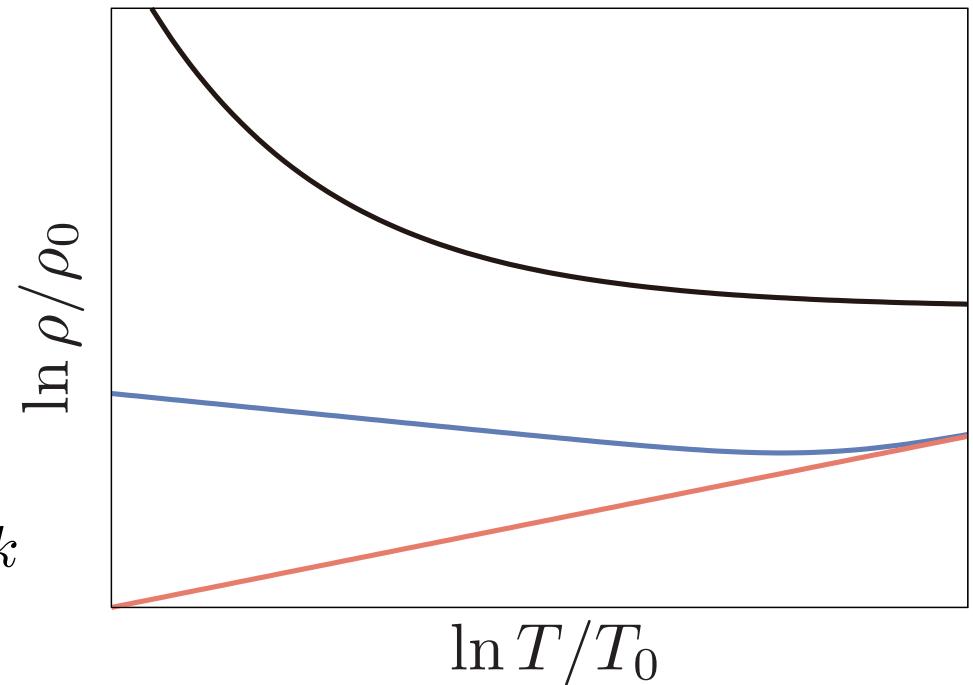
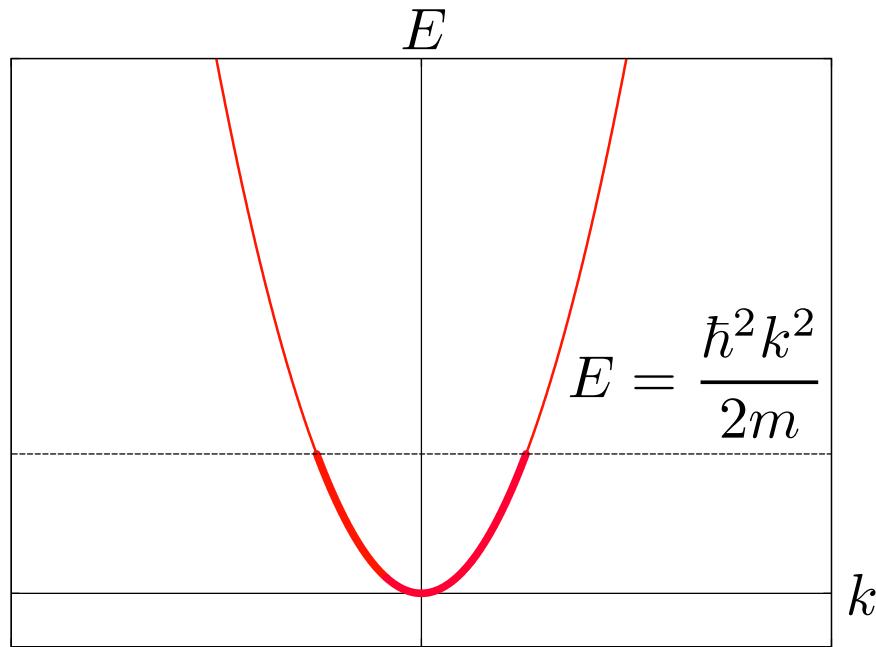
Classification of gapped quantum phases

Nobel Prize in 2016

“Topological phase transitions and
topological phases of matter”

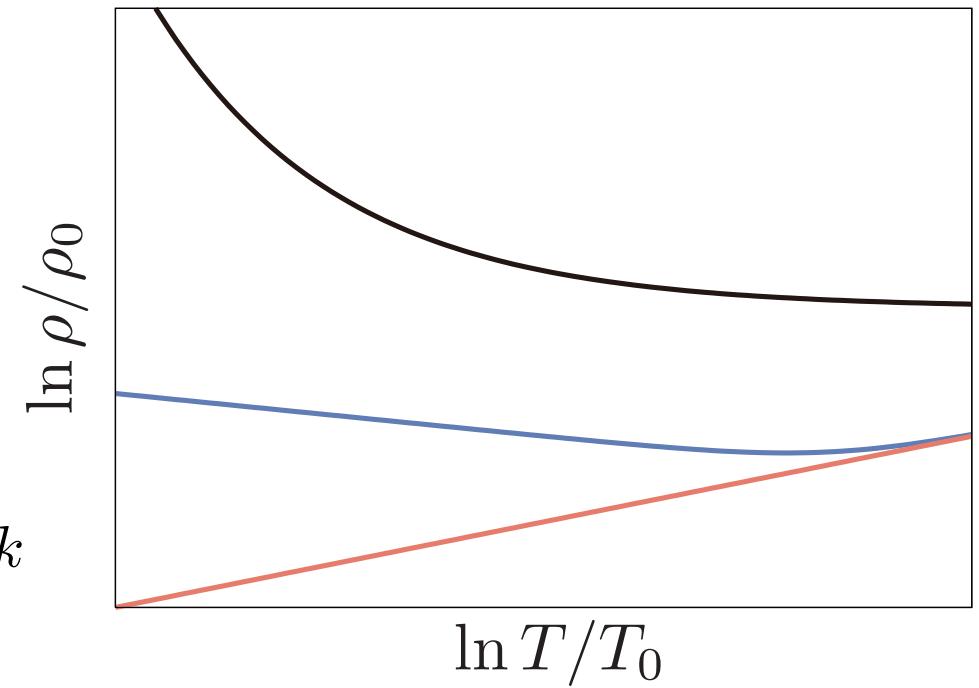
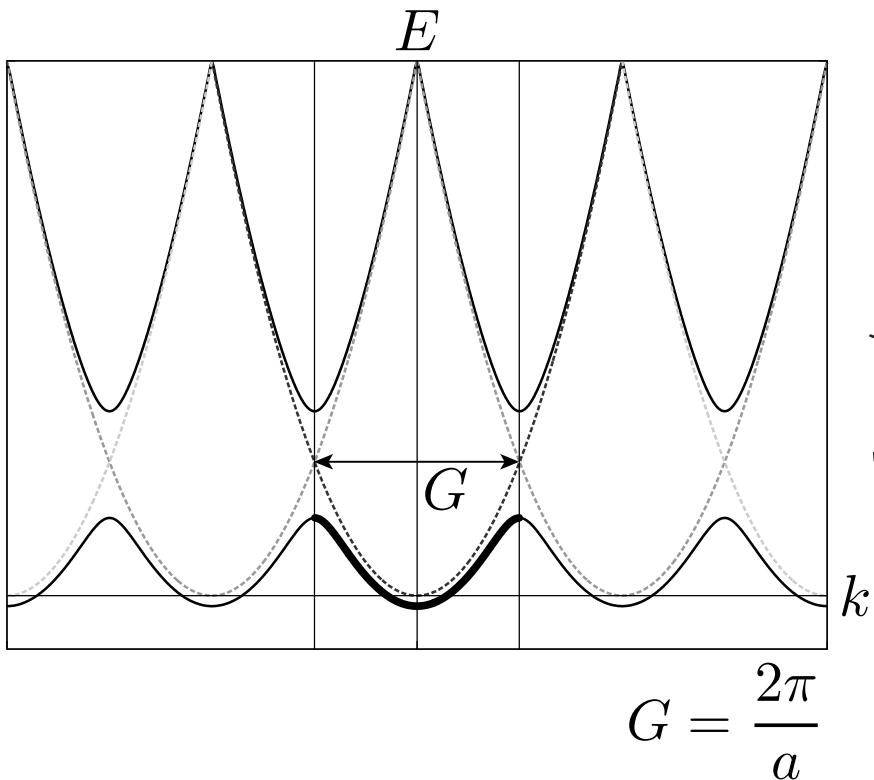
Classification of Crystalline Solids from Electric Transport

- Metal
- Zero gap semiconductor
- Semiconductor • Band insulator
- Mott insulator



Classification of Crystalline Solids from Electric Transport

- Metal
- Zero gap semiconductor
- Semiconductor • Band insulator
- Mott insulator

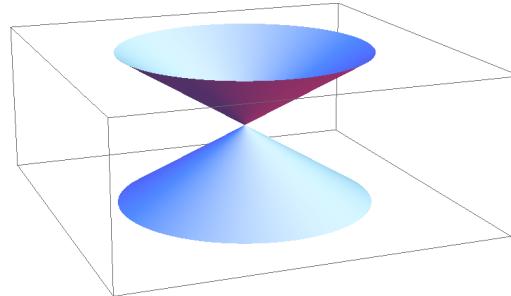
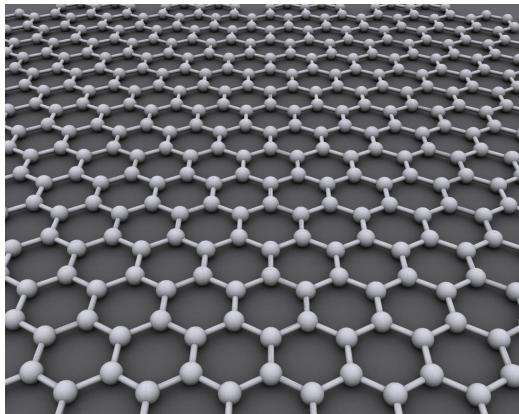


Classification of Crystalline Solids from Electric Transport

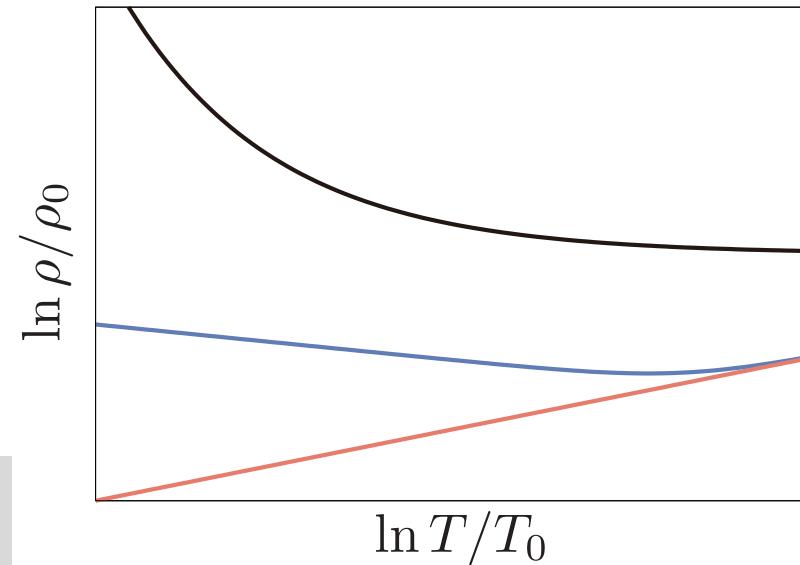
- Metal
- Zero gap semiconductor
- Band insulator
- Mott insulator

Example of zero gap semi.

2 D Dirac: Graphene

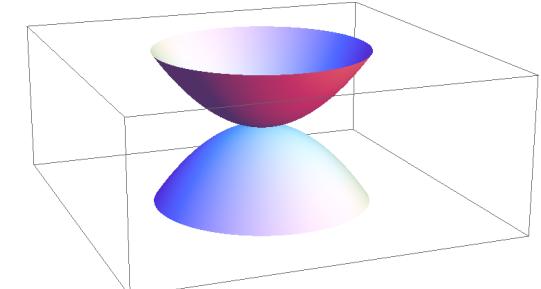


Castro Neto, Guinea, Peres, Novoselov, & Geim,
Rev. Mod. Phys. 81, 109 (2009)



3 D Dirac:
 Cd_3As_2 , Na_3Bi

HgTe, α -Sn (gray tin)



Classification of Crystalline Solids from Electric Transport

- Metal
- Zero gap semiconductor
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- Mott insulator

Trivial insulator

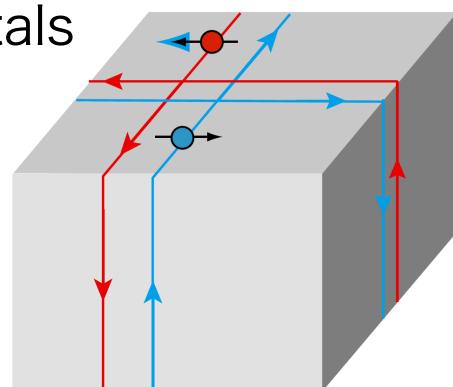
Si

Topological insulator

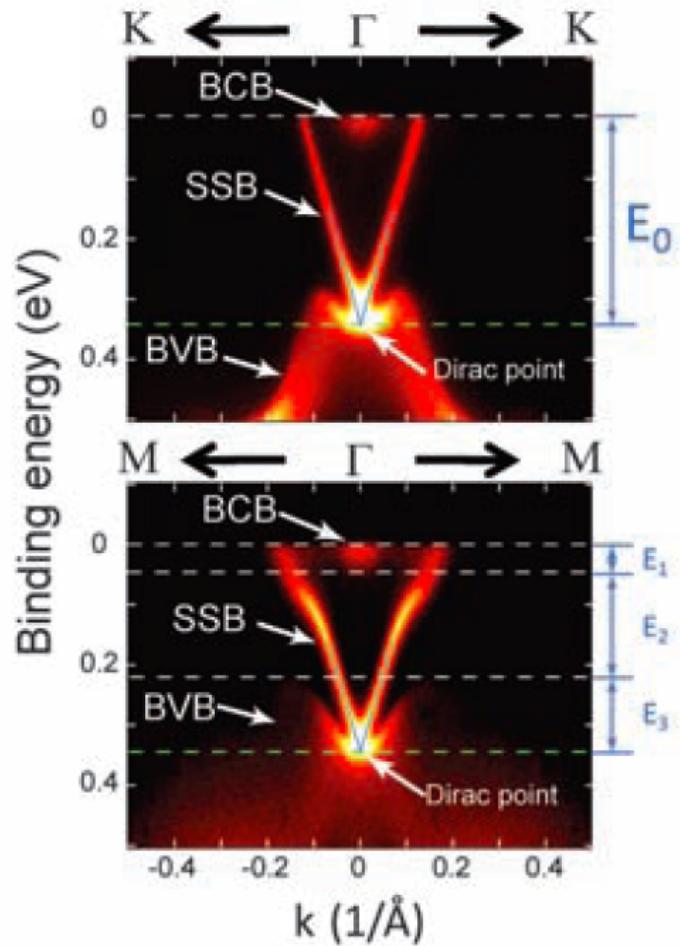
Bi_2Te_3

Thermoelectric

Surface metals

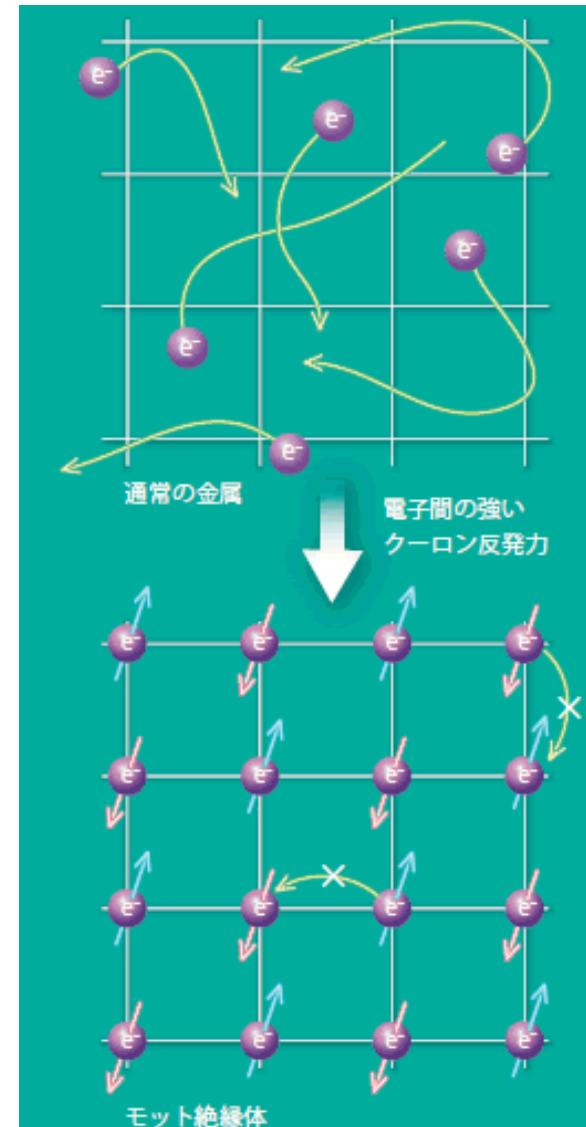


Y. L. Chen, *et al.*, Science 325, 178 (2009)



Classification of Crystalline Solids from Electric Transport

- Metal
- Zero gap semiconductor
- Band insulator
- Mott insulator



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Spin Angular Momentum Coupling

- An electron has $S=1/2$ ((spin angular momentum) = $\hbar/4\pi$)
- Origin of magnetism due to total angular momentum of many electrons in solids
- Example of spin angular momentum coupling:
Rare earth gadolinium Gd^{+3} $S=7/2$
- Classical Heisenberg spins obtained in $S \rightarrow +\infty$ limit

$S=1$ consists of two $S=1/2$

$$|m_z = +1; S = 1\rangle = | \uparrow\uparrow \rangle$$

$$|m_z = 0; S = 1\rangle = \frac{1}{\sqrt{2}} (| \uparrow\downarrow \rangle + | \downarrow\uparrow \rangle)$$

$$|m_z = -1; S = 1\rangle = | \downarrow\downarrow \rangle$$

Spin Operators for $S=1$ Quantum Spins

Matrix representation for $S=1$

$$\hat{S}^x \doteq \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & +1 & 0 \\ +1 & 0 & +1 \\ 0 & +1 & 0 \end{pmatrix}$$

$$\hat{S}^y \doteq \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & -i & 0 \\ +i & 0 & -i \\ 0 & +i & 0 \end{pmatrix}$$

$$\hat{S}^z \doteq \begin{pmatrix} +1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

\hat{S}^x	+1	0	-1
+1	0	$+1/\sqrt{2}$	0
0	$+1/\sqrt{2}$	0	$+1/\sqrt{2}$
-1	0	$+1/\sqrt{2}$	0

\hat{S}^y	+1	0	-1
+1	0	$-i/\sqrt{2}$	0
0	$+i/\sqrt{2}$	0	$-i/\sqrt{2}$
-1	0	$+i/\sqrt{2}$	0

\hat{S}^z	+1	0	-1
+1	+1	0	0
0	0	0	0
-1	0	0	-1

$S=1$ Heisenberg Model

Haldane gap

F. D. M. Haldane, Phys. Rev. Lett. 50, 1153 (1983); Phys. Lett. 93A, 464 (1983).

-Theoretical prediction on excitation gap:

Gapless: $S=1/2, 3/2, 5/2, \dots$

Gapful: $S=1, 2, 3, \dots$

cf.) AKLT I. Affleck, T. Kennedy, E. H. Lieb, and H. Tasaki,
Commun. Math. Phys. 115, 477 (1988).

$$\Delta(S) = \begin{cases} 0.41048(6) & \text{for } S = 1 \\ 0.08917(4) & \text{for } S = 2 \\ 0.01002(3) & \text{for } S = 3 \end{cases}$$

S. Todo and K. Kato, Phys. Rev. Lett. 87, 047203 (2001).

→ Symmetry Protected Topological (SPT) state

$S=1$ Heisenberg Model

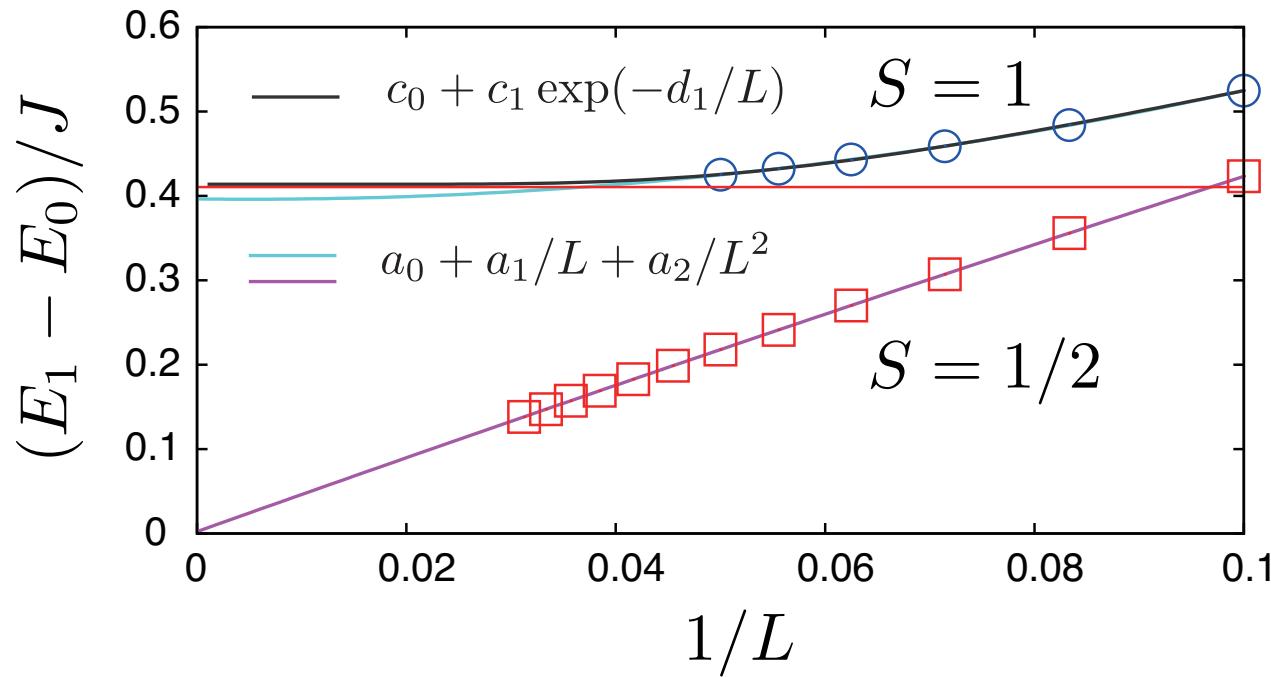
Edge states

Please see the lecture slide of Haldane

https://www.nobelprize.org/nobel_prizes/physics/laureates/2016/haldane-lecture.html

$S=1$ Heisenberg Model

Haldane gap



ED: $S=1$ up to 22 sites

O. Golinelli, Th. Jolicoeur, and R. Lacaze, Phys. Rev. B 50, 3037 (1994).

QMC: S. Todo and K. Kato, Phys. Rev. Lett. 87, 047203 (2001).

Excited States: Linear Responses or Dynamical Correlations in Many-body Electrons

An Example: Dynamical Spin Structure Factor

$$S(\vec{Q}, \omega) = \sum_{\alpha=x,y,z} \sum_m |\langle m | \hat{S}_{+\vec{Q}}^\alpha | 0 \rangle|^2 \delta(\omega - E_m + E_0)$$

$$\hat{S}_{\vec{Q}}^\alpha = \frac{1}{N} \sum_{j=0}^{N-1} \hat{S}_j^\alpha e^{+i\vec{Q} \cdot \vec{r}_j}$$

Fermi's golden rule gives probability of transition (per unit time) from the ground state to excited states with energy $\omega = E_m - E_0$

Representation by using Green's function

$$\begin{aligned} S(\vec{Q}, \omega) &= - \lim_{\delta \rightarrow 0+} \frac{1}{\pi} \text{Im} \sum_{\alpha=x,y,z} \sum_m \frac{\langle 0 | \hat{S}_{-\vec{Q}}^\alpha | m \rangle \langle m | \hat{S}_{+\vec{Q}}^\alpha | 0 \rangle}{\omega + i\delta - E_m + E_0} \\ &= - \lim_{\delta \rightarrow 0+} \frac{1}{\pi} \text{Im} \sum_{\alpha=x,y,z} \sum_m \langle 0 | \hat{S}_{-\vec{Q}}^\alpha \frac{1}{\omega + i\delta - \hat{H} + E_0} \hat{S}_{+\vec{Q}}^\alpha | 0 \rangle \end{aligned}$$

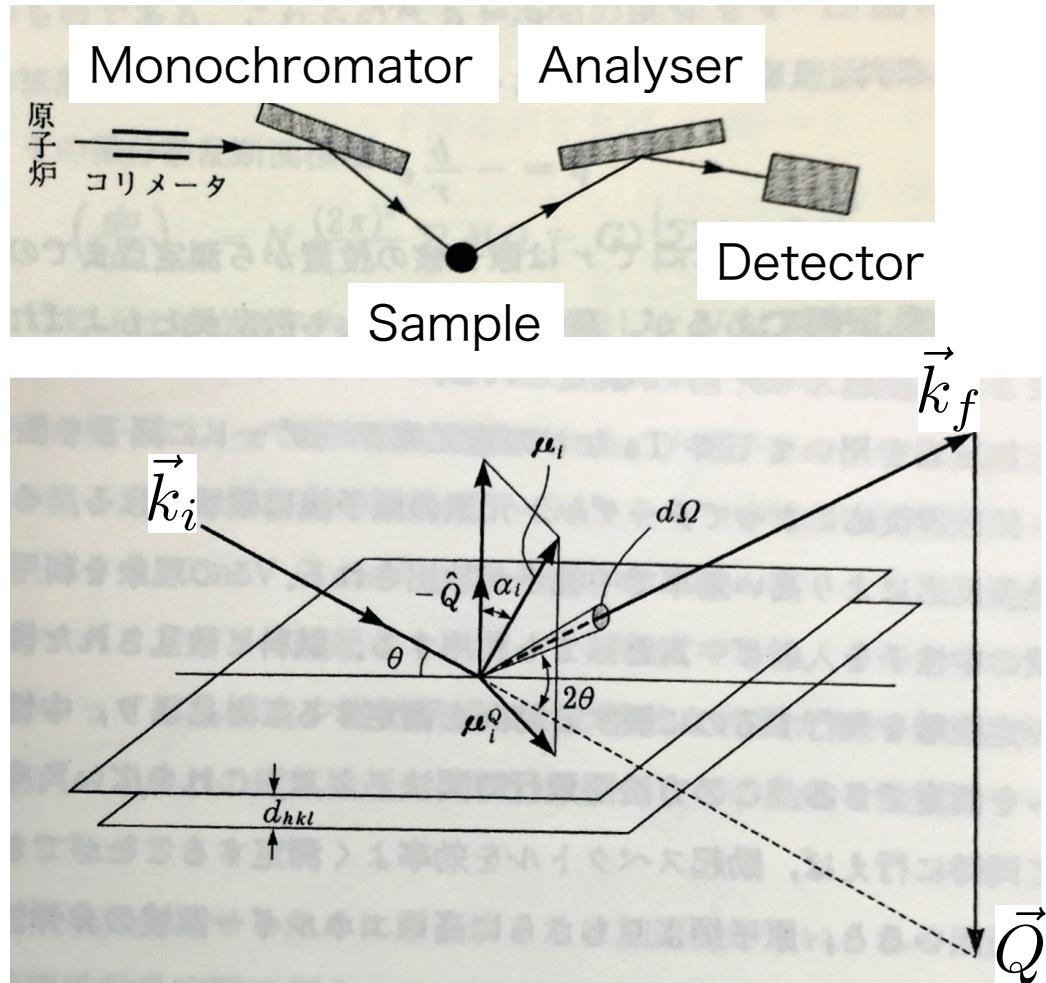
Corresponding Experiment: Neutron Scattering

$$S(\vec{Q}, \omega) = \sum_{\alpha=x,y,z} \sum_m |\langle m | \hat{S}_{+\vec{Q}}^\alpha | 0 \rangle|^2 \delta(\omega - E_m + E_0)$$

Nuclear reactor

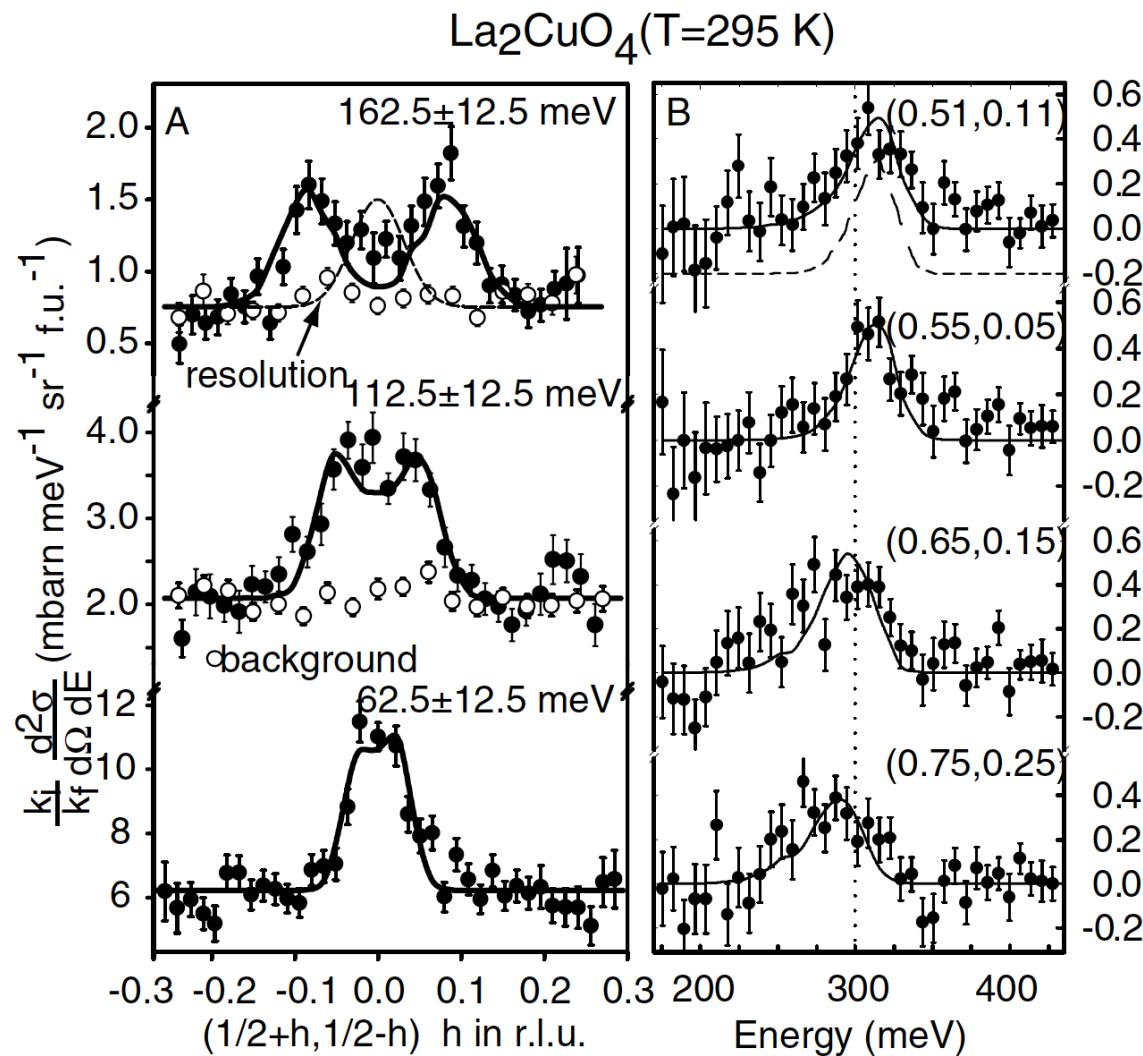
$$\vec{k}_i - \vec{k}_f = \vec{Q}$$

$$E_i - E_f = \omega$$



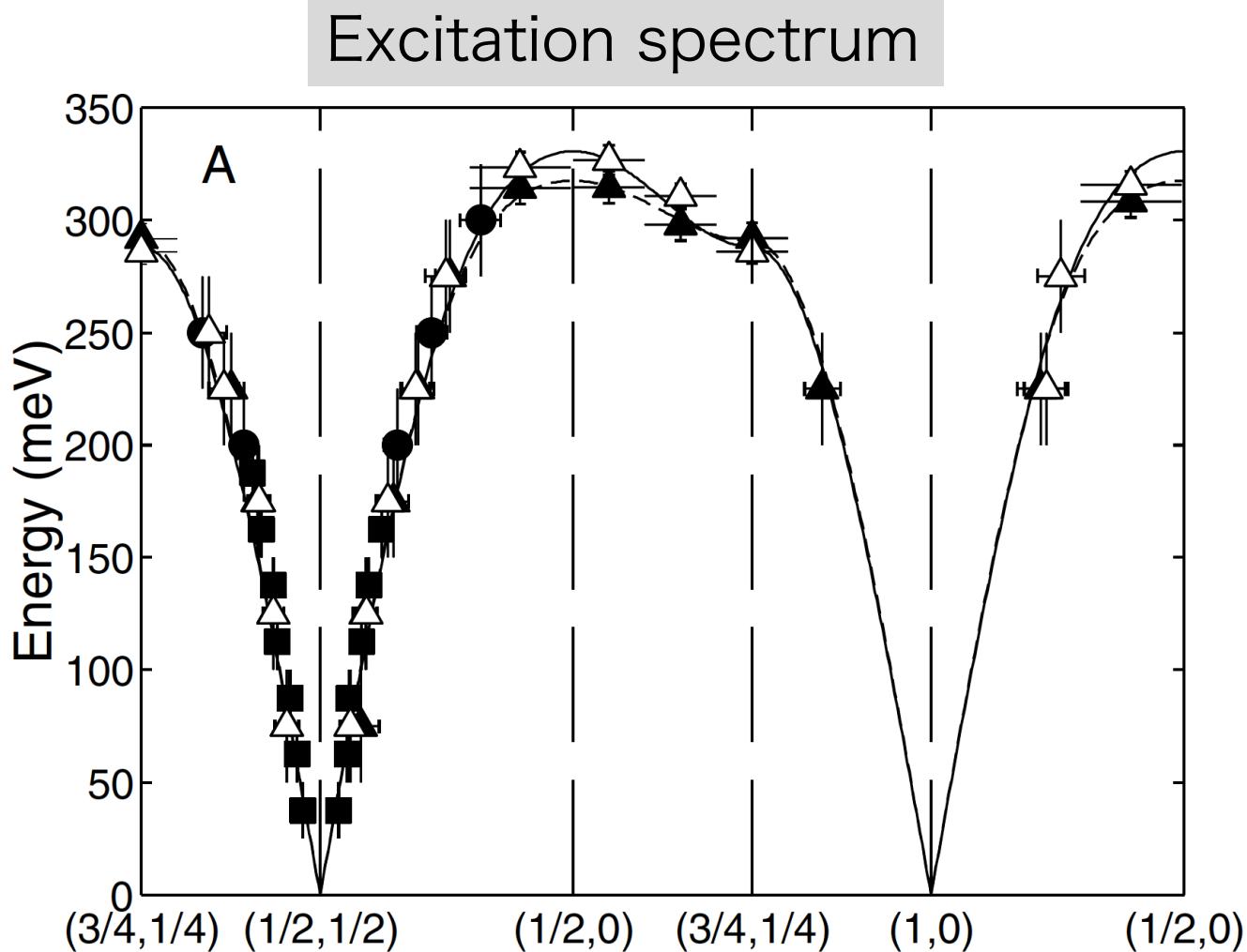
Inelastic Neutron Scattering Measurement of La_2CuO_4

R. Coldea, *et al.*,
Phys. Rev. Lett. 86, 5377 (2001).



Inelastic Neutron Scattering Measurement of La_2CuO_4

R. Coldea, *et al.*,
Phys. Rev. Lett. 86, 5377 (2001).



Simulating Spectroscopy Measurements

Linear response of ground state $|\psi\rangle$

Green's function

$$G_{\hat{O}}(z) = \langle \psi | \hat{O}^\dagger (z \mathbf{1} - \hat{H})^{-1} \hat{O} | \psi \rangle$$
$$z \rightarrow \omega \quad (z \in \mathbb{C}, \omega \in \mathbb{R})$$

Excitation spectrum $-\frac{1}{\pi} \text{Im} G_{\hat{O}}(\omega + i\delta)$

Example of **perturbation** & **response**:
Magnetization of spins under **magnetic fields**

$$\hat{H}_{\text{ex}} = e^{i\omega t} B_z \left(\frac{1}{N} \sum_{j=0}^{N-1} \hat{S}_j^z \right)$$
$$\hat{O} = \frac{1}{N} \sum_{j=0}^{N-1} \hat{S}_j^z$$

Excitation Spectra

Lanczos steps with initial vector defined as

$$|\phi_0\rangle = \hat{O}|\psi\rangle / \sqrt{\langle\psi|\hat{O}^\dagger\hat{O}|\psi\rangle} \quad (\text{multiplying excitation operator to g.s.})$$

Lanczos' tridiagonal matrix

$$z\mathbf{1} - H \doteq z\mathbf{1} - H_{\text{td}} = \begin{bmatrix} z - \alpha_0 & -\beta_1 & 0 & 0 & \cdots \\ -\beta_1 & z - \alpha_1 & -\beta_2 & 0 & \cdots \\ 0 & -\beta_2 & z - \alpha_2 & -\beta_3 & \\ 0 & 0 & -\beta_3 & z - \alpha_3 & \\ \vdots & \vdots & & & \ddots \end{bmatrix}$$

→ Excitation Spectrum

$$\begin{aligned} \langle\psi|\hat{O}^\dagger(z\mathbf{1} - \hat{H})^{-1}\hat{O}|\psi\rangle &= \sqrt{\langle\psi|\hat{O}^\dagger\hat{O}|\psi\rangle} \{(z\mathbf{1} - H)^{-1}\}_{00} \\ &= \frac{\sqrt{\langle\psi|\hat{O}^\dagger\hat{O}|\psi\rangle}}{z - \alpha_0 - \frac{\beta_1^2}{z - \alpha_1 - \frac{\beta_2^2}{z - \alpha_2 - \cdots}}} \end{aligned}$$

Continued Fraction

Representation for inverse of a matrix
by Grassmann number

$$\frac{\int \psi_\ell \bar{\psi}_m e^{-\bar{\psi} M \psi} [d\bar{\psi} d\psi]}{\int e^{-\bar{\psi} M \psi} [d\bar{\psi} d\psi]} = (M^{-1})_{\ell m}$$

Continued Fraction

Representation for inverse of a matrix
by Grassmann number

$$\frac{\int \psi_1 \bar{\psi}_1 e^{-\bar{\psi} M \psi} [d\bar{\psi} d\psi]}{\int e^{-\bar{\psi} M \psi} [d\bar{\psi} d\psi]} = (M^{-1})_{11}$$

An example for 2x2 matrix

$$\begin{aligned} & \int e^{-\bar{\psi}_1 M_{11} \psi_1 - \bar{\psi}_1 M_{12} \psi_2 - \bar{\psi}_2 M_{21} \psi_1 - \bar{\psi}_2 M_{22} \psi_2} d\bar{\psi}_2 d\psi_2 d\bar{\psi}_1 d\psi_1 \\ &= \int M_{22} e^{-\bar{\psi}_1 \left[M_{11} - \frac{M_{12} M_{21}}{M_{22}} \right] \psi_1} d\bar{\psi}_1 d\psi_1 \end{aligned}$$

$$(M^{-1})_{11} = \frac{1}{M_{11} - \frac{M_{12} M_{21}}{M_{22}}}$$

Continued Fraction

General matrices: Schur complement

$$M = \begin{bmatrix} M_{11} & M_{12} & 0 & \cdots & 0 & 0 & 0 \\ M_{21} & M_{22} & M_{23} & \cdots & 0 & 0 & 0 \\ 0 & M_{32} & M_{33} & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & M_{m-2,m-2} & M_{m-2,m-1} & 0 \\ 0 & 0 & 0 & \cdots & M_{m-1,m-2} & M_{m-1,m-1} & M_{m-1,m} \\ 0 & 0 & 0 & \cdots & 0 & M_{m,m-1} & M_{m,m} \end{bmatrix}$$

Continued Fraction

General matrices: Schur complement

Integrating m th component

$$M/M_{m,m} = \begin{bmatrix} M_{11} & M_{12} & 0 & \cdots & 0 & 0 \\ M_{21} & M_{22} & M_{23} & \cdots & 0 & 0 \\ 0 & M_{32} & M_{33} & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & M_{m-2,m-2} & M_{m-2,m-1} \\ 0 & 0 & 0 & \cdots & M_{m-1,m-2} & M'_{m-1,m-1} \end{bmatrix}$$

$$M'_{m-1,m-1} = M_{m-1,m-1} - \frac{M_{m-1,m} M_{m,m-1}}{M_{m,m}}$$

Continued Fraction

General matrices: Schur complement

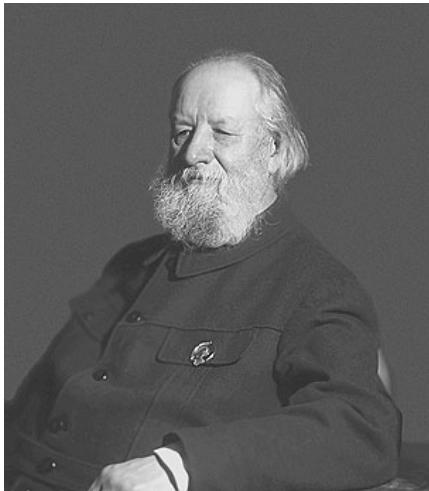
Integrating m th and $(m-1)$ th components

$$(M/M_{m,m})/M_{m-1,m-1} = \begin{bmatrix} M_{11} & M_{12} & 0 & \cdots & 0 \\ M_{21} & M_{22} & M_{23} & \cdots & 0 \\ 0 & M_{32} & M_{33} & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & M'_{m-2,m-2} \end{bmatrix}$$

$$\begin{aligned} M'_{m-2,m-2} &= M_{m-2,m-2} - \frac{M_{m-2,m-1}M_{m-1,m-2}}{M'_{m-1,m-1}} \\ &= M_{m-2,m-2} - \frac{M_{m-2,m-1}M_{m-1,m-2}}{M_{m-1,m-1} - \frac{M_{m-1,m}M_{m,m-1}}{M_{m,m}}} \end{aligned}$$

→ Iteratively, continued fraction form is obtained

Krylov Subspace Method



Alexey Krylov

Aleksey Nikolaevich Krylov

1863-1945

Russian naval engineer and applied mathematician

Krylov subspace

$$\mathcal{K}_n(\zeta - \hat{H}, |\rho\rangle) = \text{span}\{|\rho\rangle, (\zeta - \hat{H})|\rho\rangle, \dots, (\zeta - \hat{H})^{n-1}|\rho\rangle\}$$

Shift invariance

$$\mathcal{K}_n(\zeta - \hat{H}, |\rho\rangle) = \mathcal{K}_n(\zeta' - \hat{H}, |\rho\rangle)$$

Green's Function by Solving Linear Equations

Green's function

$$G^{AB}(\zeta) = \langle 0 | \hat{A}^\dagger (\zeta - \hat{H})^{-1} \hat{B} | 0 \rangle$$

-Lanczos/Arnoldi methods

$$\begin{aligned} |\lambda\rangle &= \hat{A}|0\rangle \\ |\rho\rangle &= \hat{B}|0\rangle \\ |\chi(\zeta)\rangle &= (\zeta - \hat{H})^{-1}|\rho\rangle \end{aligned}$$

$$\rightarrow G^{AB}(\zeta) = \langle \lambda | \chi(\zeta) \rangle$$

→ Linear equations

$$(\zeta - \hat{H})|\chi(\zeta)\rangle = |\rho\rangle$$

-CG-type methods, ...

Green's Function by Krylov Subspace Method

Searching solutions in Krylov subspaces

$\mathcal{K}_n(\zeta - \hat{H}, |\rho\rangle) = \text{span}\{|\rho\rangle, (\zeta - \hat{H})|\rho\rangle, \dots, (\zeta - \hat{H})^{n-1}|\rho\rangle\}$
-Lanczos/Arnoldi methods, **CG-type methods**, ...

Initial: $|\chi_0(\zeta)\rangle = |\rho\rangle$

For $n=1, 2, \dots, m$

Find $|\chi_n(\zeta)\rangle$ in $\mathcal{K}_n(\zeta - \hat{H}, |\rho\rangle)$
 $|\rho_n(\zeta)\rangle = (\zeta - \hat{H})|\chi_n(\zeta)\rangle - |\rho\rangle$

CG-type method

A. Frommer, Computing 70, 87 (2003).

Collinear residuals $|\rho_n(\zeta)\rangle \propto |\rho_n(\zeta')\rangle$

$$\mathcal{K}_n(\zeta - \hat{H}, |\rho\rangle) = \mathcal{K}_n(\zeta' - \hat{H}, |\rho\rangle)$$

→ **Seed switch**

S. Yamamoto, T. Sogabe, T. Hoshi, S.-L. Zhang, & T. Fujiwara,
J. Phys. Soc. Jpn. 77, 114713 (2008).

Library Kw (released) by Dr. Kawamura (ISSP)

Conjugate Gradient Method

Linear Equations

Algorithm for linear equations
instead of eigenvalue problems

$$A\vec{x} = \vec{b}$$

A simple method: Gradient descent/steepest descent

Solving a linear equation is mapped onto
finding a minimum of a cost function

For symmetric matrix A

$$f(\vec{x}) = \frac{1}{2}\vec{x}^T A \vec{x} - \vec{b}^T \vec{x}$$

$$\vec{\nabla}_x f(\vec{x}) = A\vec{x} - \vec{b}$$

$$\vec{x}_{k+1} = \vec{x}_k - \alpha \vec{\nabla}_x f(\vec{x})|_{\vec{x}=\vec{x}_k}$$

-Only local information is utilized,
and thus often captured by local minima

Conjugate Gradient Method

M. R. Hestenes & E. Stiefel, J. Res. Natl. Bur. Stand. 49, 409 (1952).

Find an approximate solution in a Krylov subspace

$$\vec{x}_k = \sum_{j=0}^{k-1} a_j \vec{p}_j$$

Conjugate basis set $\{\vec{p}_k\}$ $\vec{p}_i^T A \vec{p}_j = 0 \quad (i \neq j)$

Additional constraint: Find orthogonal residual vectors

$$\vec{r}_k = \vec{b} - A \vec{x}_k$$

Orthogonal basis set $\{\vec{r}_k\}$ $\vec{r}_i^T \vec{r}_j = 0 \quad (i \neq j)$

Conjugate Gradient Method: Algorithm

Linear equations $A\vec{x} = \vec{b}$

For symmetric matrix A

$$\vec{p}_0 = \vec{r}_0 = \vec{b} - A\vec{x}_0$$

For $k = 0, 1, \dots, m$

$$\alpha_k = \frac{\vec{r}_k^T \vec{r}_k}{\vec{p}_k^T A \vec{p}_k}$$

$$\vec{x}_{k+1} = \vec{x}_k + \alpha_k \vec{p}_k$$

$$\vec{r}_{k+1} = \vec{r}_k - \alpha_k A \vec{p}_k$$

$$\beta_k = \frac{\vec{r}_{k+1}^T \vec{r}_{k+1}}{\vec{r}_k^T \vec{r}_k}$$

$$\vec{p}_{k+1} = \vec{r}_{k+1} + \beta_k \vec{p}_k$$

M. R. Hestenes & E. Stiefel,
J. Res. Natl. Bur. Stand. 49, 409 (1952).

The algorithm generates
-Conjugate basis set $\{\vec{p}_k\}$
-Orthogonal basis set $\{\vec{r}_k\}$
 \leftarrow A Krylov subspace

CG method finds an approximate solution
of the linear equation in a Krylov subspace

Sketch of Proof for CG Method 0.

Induction

Assume $\{\vec{r}_0, \vec{r}_1, \dots, \vec{r}_k\}$ is orthogonal basis set

$$\vec{r}_i^T \vec{r}_j = 0 \quad (i \neq j, i \leq k, j \leq k)$$

Assume $\{\vec{p}_0, \vec{p}_1, \dots, \vec{p}_k\}$ is conjugate basis set

$$\vec{p}_i^T A \vec{p}_j = 0 \quad (i \neq j, i \leq k, j \leq k)$$

Prove \vec{r}_{k+1} satisfies $\vec{r}_j^T \vec{r}_{k+1} = 0 \quad (j \leq k)$

Prove \vec{p}_{k+1} satisfies $\vec{p}_j^T A \vec{p}_{k+1} = 0 \quad (j \leq k)$

Sketch of Proof for CG Method 1.

Ansatz

$$\begin{aligned}\vec{x}_{k+1} &= \vec{x}_k + \alpha_k \vec{p}_k \\ \rightarrow \vec{r}_{k+1} &= \vec{b} - A\vec{x}_{k+1} \\ &= \vec{r}_k - \alpha_k A\vec{p}_k\end{aligned}$$

Requirement

$$\begin{aligned}\vec{r}_k^T \vec{r}_{k+1} &= 0 \\ \rightarrow \vec{r}_k^T \vec{r}_{k+1} &= \vec{r}_k^T \vec{r}_k - \vec{r}_k^T \alpha_k A\vec{x}_{k+1} = 0 \\ \rightarrow \alpha_k &= \frac{\vec{r}_k^T \vec{r}_k}{\vec{r}_k^T A\vec{p}_k} \\ \left\{ \begin{array}{l} \vec{p}_k = \vec{r}_k + \beta_{k-1} \vec{p}_{k-1} \\ \vec{p}_{k-1}^T A\vec{p}_k = 0 \end{array} \right. &\quad \text{← assumption} \\ \rightarrow \alpha_k &= \frac{\vec{r}_k^T \vec{r}_k}{\vec{r}_k^T A\vec{p}_k} = \frac{\vec{r}_k^T \vec{r}_k}{\vec{p}_k^T A\vec{p}_k}\end{aligned}$$

$$\begin{aligned}\vec{r}_j^T \vec{r}_{k+1} &= \vec{r}_j^T \vec{r}_{k+1} - \alpha_k \vec{r}_j^T A\vec{p}_{k+1} \\ &= -\alpha_k \vec{p}_j^T A\vec{p}_{k+1} \quad (\vec{p}_j = \vec{r}_j + \beta_{j-1} \vec{p}_{j-1}, \vec{r}_j^T \vec{r}_{k+1} = 0) \\ &= 0 \quad (j < k)\end{aligned}$$

Sketch of Proof for CG Method 2.

Ansatz &
Requirement

$$\left\{ \begin{array}{l} \vec{p}_{k+1} = \vec{r}_{k+1} + \beta_k \vec{p}_k \\ (\vec{p}_k^T A) \vec{p}_{k+1} = 0 \\ \rightarrow (\vec{p}_k^T A) \vec{p}_{k+1} = (\vec{p}_k^T A) \vec{r}_{k+1} + \beta_k (\vec{p}_k^T A) \vec{p}_k = 0 \\ \rightarrow \beta_k = -\frac{\vec{p}_k^T A \vec{r}_{k+1}}{\vec{p}_k^T A \vec{p}_k} \\ \vec{r}_{k+1} = \vec{r}_k - \alpha_k A \vec{p}_k \\ \rightarrow A \vec{p}_k = \frac{\vec{r}_k - \vec{r}_{k+1}}{\alpha_k} \\ \beta_k = -\frac{\vec{p}_k^T A \vec{r}_{k+1}}{\vec{p}_k^T A \vec{p}_k} = -\frac{(\vec{r}_k - \vec{r}_{k+1})^T \vec{r}_{k+1}}{\alpha_k \vec{p}_k^T A \vec{p}_k} \\ = \frac{\vec{r}_{k+1}^T \vec{r}_{k+1}}{\vec{r}_k^T \vec{r}_k} = \frac{\vec{r}_{k+1}^T \vec{r}_{k+1}}{\vec{r}_k^T \vec{r}_k} \\ \vec{p}_j^T A \vec{p}_{k+1} = 0 \quad (j < k) \end{array} \right.$$

Variation of CG Method

Variation of CG method:

- A : symmetric \rightarrow Conjugate Gradient
- A : hermitian \rightarrow Conjugate Gradient ($T \rightarrow +$)
- $A + \sigma I$: symmetric A and complex σ
 \rightarrow Conjugate Orthogonal Conjugate Gradient (COCG)
- $A + \sigma I$: hermitian A and complex σ
 \rightarrow Bi-Conjugate Gradient (BiCG)

An important application:

- Calculation of eigenvectors after the Lanczos method

Inverse iteration: $(\hat{H} - E_m)\vec{v}_{k+1} = \vec{v}_k$
 $\vec{v}_k \rightarrow |m\rangle$

SD vs CG

Numerical Algorithm Is Not Originally for Modern Computers

- Gauss-Seidel & Jacobi method for linear equations
(19th century)
- Krylov's original work
 - "On the numerical solution of the equation by which, in technical matters, frequencies of small oscillations of material systems are determined"*
(1931)
- ZND detonation model calculated by hand
for designing nuclear bomb @LANL
(1940's)

Many modern numerical algorithm is based on algorithm before the invention of modern computers

One of the Simplest Example of Linear Equations

$$A\vec{x} = \vec{b}$$

$$A = \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix}$$

$$\vec{b} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

Analytical solution

$$\vec{x} = A^{-1}\vec{b}$$

$$\begin{aligned}\vec{x} &= A^{-1}\vec{b} \\ &= \frac{1}{3} \begin{pmatrix} 2 & -1 \\ -1 & 2 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \\ &= \begin{pmatrix} 2/3 \\ -1/3 \end{pmatrix}\end{aligned}$$

Steepest Descent

$$A\vec{x} = \vec{b}$$

$$\vec{\nabla}_x f(\vec{x}) = A\vec{x} - \vec{b} \quad \vec{x}_{k+1} = \vec{x}_k - \alpha \vec{\nabla}_x f(\vec{x})|_{\vec{x}=\vec{x}_k}$$

Formal solution

$$\begin{aligned}\vec{x}_{k+1} &= \vec{x}_k + \alpha(\vec{b} - A\vec{x}_k) \\&= (1 - \alpha A)\vec{x}_k + \alpha\vec{b} \\&= (1 - \alpha A)^2\vec{x}_{k-1} + \alpha\vec{b} + \alpha(1 - \alpha A)\vec{b} \\&= \dots \\&= (1 - \alpha A)^{k+1}\vec{x}_0 + \alpha\vec{b} + \alpha(1 - \alpha A)\vec{b} + \dots + \alpha(1 - \alpha A)^k\vec{b} \\&= \alpha \frac{1 - (1 - \alpha A)^{k+1}}{1 - (1 - \alpha A)} \vec{b} \\&= A^{-1}[1 - (1 - \alpha A)^{k+1}]\vec{b}\end{aligned}$$

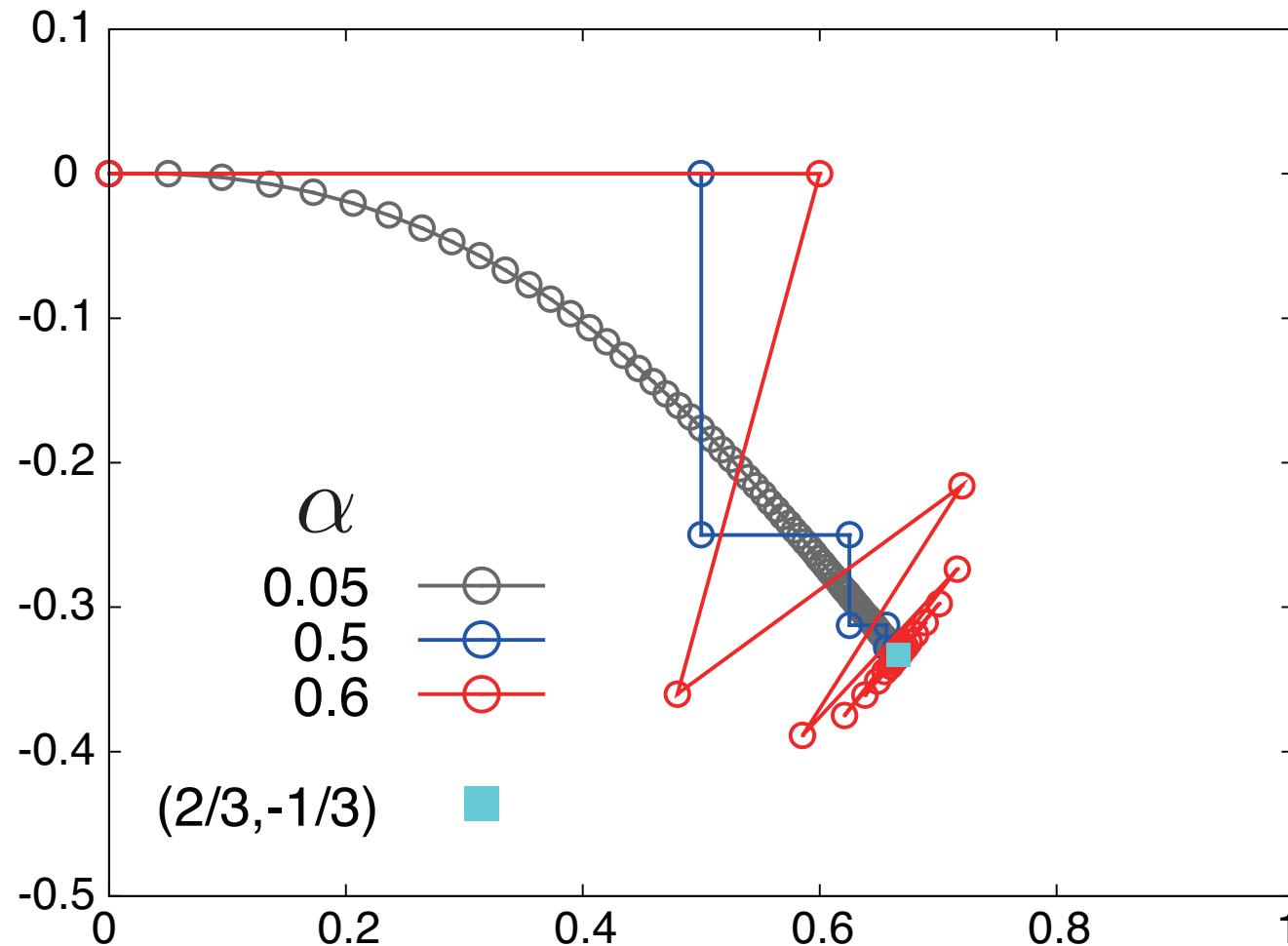
SD finds the exact solution only when $(1 - \alpha A)^{k+1}\vec{b} = \vec{0}$

Slow Convergence of Steepest Descent

$$A\vec{x} = \vec{b}$$

$$\vec{\nabla}_x f(\vec{x}) = A\vec{x} - \vec{b}$$

$$\vec{x}_{k+1} = \vec{x}_k - \alpha \vec{\nabla}_x f(\vec{x})|_{\vec{x}=\vec{x}_k}$$



Conjugate Gradient

$$A\vec{x} = \vec{b}$$

$$\vec{p}_0 = \vec{r}_0 = \vec{b} - A\vec{x}_0$$

For $k = 0, 1, \dots, m$

$$\alpha_k = \frac{\vec{r}_k^T \vec{r}_k}{\vec{p}_k^T A \vec{p}_k}$$

$$\vec{x}_{k+1} = \vec{x}_k + \alpha_k \vec{p}_k$$

$$\vec{r}_{k+1} = \vec{r}_k - \alpha_k A \vec{p}_k$$

$$\beta_k = \frac{\vec{r}_{k+1}^T \vec{r}_{k+1}}{\vec{r}_k^T \vec{r}_k}$$

$$\vec{p}_{k+1} = \vec{r}_{k+1} + \beta_k \vec{p}_k$$

1st Step of CG

$$A\vec{x} = \vec{b}$$

$$\vec{p}_0 = \vec{r}_0 = \vec{b} - A\vec{x}_0$$

For $k = 0, 1, \dots, m$

$$\alpha_k = \frac{\vec{r}_k^T \vec{r}_k}{\vec{p}_k^T A \vec{p}_k}$$

$$\vec{x}_{k+1} = \vec{x}_k + \alpha_k \vec{p}_k$$

$$\vec{r}_{k+1} = \vec{r}_k - \alpha_k A \vec{p}_k$$

$$\beta_k = \frac{\vec{r}_{k+1}^T \vec{r}_{k+1}}{\vec{r}_k^T \vec{r}_k}$$

$$\vec{p}_{k+1} = \vec{r}_{k+1} + \beta_k \vec{p}_k$$

$$\vec{x}_0 = \vec{0}$$

$$\vec{p}_0 = \vec{r}_0 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$\alpha_0 = \frac{1}{(1, 0) \begin{pmatrix} 2 \\ 1 \end{pmatrix}} = \frac{1}{2}$$

$$\vec{x}_1 = \vec{0} + \frac{1}{2} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1/2 \\ 0 \end{pmatrix}$$

$$\vec{r}_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix} - \frac{1}{2} \begin{pmatrix} 2 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ -1/2 \end{pmatrix}$$

$$\beta_0 = \frac{\vec{r}_1^T \vec{r}_1}{\vec{r}_0^T \vec{r}_0} = \frac{1/4}{1} = \frac{1}{4}$$

$$\vec{p}_1 = \begin{pmatrix} 0 \\ -1/2 \end{pmatrix} + \frac{1}{4} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1/4 \\ -1/2 \end{pmatrix}$$

2nd Step of CG

$$A\vec{x} = \vec{b}$$

$$\vec{p}_0 = \vec{r}_0 = \vec{b} - A\vec{x}_0$$

For $k = 0, 1, \dots, m$

$$\alpha_k = \frac{\vec{r}_k^T \vec{r}_k}{\vec{p}_k^T A \vec{p}_k}$$

$$\vec{x}_{k+1} = \vec{x}_k + \alpha_k \vec{p}_k$$

$$\vec{r}_{k+1} = \vec{r}_k - \alpha_k A \vec{p}_k$$

$$\beta_k = \frac{\vec{r}_{k+1}^T \vec{r}_{k+1}}{\vec{r}_k^T \vec{r}_k}$$

$$\vec{p}_{k+1} = \vec{r}_{k+1} + \beta_k \vec{p}_k$$

$$\vec{x}_1 = \vec{0} + \frac{1}{2} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1/2 \\ 0 \end{pmatrix}$$

$$\vec{r}_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix} - \frac{1}{2} \begin{pmatrix} 2 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ -1/2 \end{pmatrix}$$

$$\vec{p}_1 = \begin{pmatrix} 0 \\ -1/2 \end{pmatrix} + \frac{1}{4} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1/4 \\ -1/2 \end{pmatrix}$$

$$\alpha_1 = \frac{1/4}{(1/4, -1/2) \begin{pmatrix} 0 \\ -3/4 \end{pmatrix}} = \frac{2}{3}$$

$$\vec{x}_2 = \begin{pmatrix} 1/2 \\ 0 \end{pmatrix} + \frac{2}{3} \begin{pmatrix} 1/4 \\ -1/2 \end{pmatrix} = \begin{pmatrix} 2/3 \\ -1/3 \end{pmatrix}$$

$$\vec{r}_2 = \begin{pmatrix} 0 \\ -1/2 \end{pmatrix} - \frac{2}{3} \begin{pmatrix} 0 \\ -3/4 \end{pmatrix} = \vec{0}$$

CG finds the exact solution at the 2nd step!

Shifted Krylov Subspace Method

Collinear Residual

A. Frommer, Computing 70, 87 (2003).

$$A\vec{x} = \vec{b}$$

$$\vec{r}_0 = \vec{b} \text{ if } \vec{x}_0 = \vec{0}$$

$$(A + \sigma \mathbf{1})\vec{x}^\sigma = \vec{b}$$

$$\vec{r}_0^\sigma = \vec{b} \text{ if } \vec{x}_0^\sigma = \vec{0}$$

Shift invariance of Krylov subspace

$$\text{span}\{\vec{r}_0, \vec{r}_1, \dots, \vec{r}_k\} = \text{span}\{\vec{r}_0^\sigma, \vec{r}_1^\sigma, \dots, \vec{r}_k^\sigma\}$$

CG-type methods find a new residual vector

$$\vec{r}_{k+1} \perp \text{span}\{\vec{r}_0, \vec{r}_1, \dots, \vec{r}_k\}$$

$$\vec{r}_{k+1}^\sigma \perp \text{span}\{\vec{r}_0^\sigma, \vec{r}_1^\sigma, \dots, \vec{r}_k^\sigma\}$$

Shift invariance of Krylov subspace

$$\text{span}\{\vec{r}_0, \vec{r}_1, \dots, \vec{r}_k, \vec{r}_{k+1}\} = \text{span}\{\vec{r}_0^\sigma, \vec{r}_1^\sigma, \dots, \vec{r}_k^\sigma, \vec{r}_{k+1}^\sigma\}$$

$$\vec{r}_{k+1} \propto \vec{r}_{k+1}^\sigma$$

Details of Collinear Residual 1.

Coefficient

A. Frommer, Computing 70, 87 (2003).

$$\vec{r}_k^\sigma = (1/\pi_k^\sigma) \vec{r}_k$$

$$\vec{x}_k = q_{k-1}(A) \vec{b}$$

$$\vec{r}_k = p_k(A) \vec{b} \quad (= \vec{b} - Aq_{k-1}(A) \vec{b} = \vec{b} - A\vec{x}_k)$$

$$p_k(t) = 1 - tq_{k-1}(t)$$

$$q_{k-1}(t) = \sum_{m=0}^{k-1} d_m t^m$$

$$\vec{r}_k^\sigma = p_k^\sigma(A + \sigma \mathbf{1}) \vec{b}$$

$$p_k^\sigma(A + \sigma \mathbf{1}) \vec{b} = (1/\pi_k^\sigma) p_k(A) \vec{b}$$

$$\rightarrow p_k^\sigma(t + \sigma) = (1/\pi_k^\sigma) p_k(t)$$

$$\pi_k^\sigma = p_k(-\sigma) \quad (\text{since } p_k^\sigma(0) = 1)$$

Details of Collinear Residual 2.

A. Frommer, Computing 70, 87 (2003).

Recurrence formula for residual vectors

$$\vec{p}_{k-1} = \frac{1}{\beta_k}(\vec{r}_k - \vec{p}_k), \quad A\vec{p}_k = \frac{1}{\alpha_k}(\vec{r}_k - \vec{r}_{k+1})$$

$$\begin{aligned}\rightarrow \vec{r}_k &= \vec{r}_{k-1} - \alpha_{k-1}A\vec{p}_{k-1} = \vec{r}_{k-1} - \frac{\alpha_{k-1}}{\beta_k}A(\vec{r}_k - \vec{p}_k) \\ &= \vec{r}_{k-1} - \frac{\alpha_{k-1}}{\beta_k}A\vec{r}_k + \frac{\alpha_{k-1}}{\alpha_k\beta_k}(\vec{r}_k - \vec{r}_{k+1})\end{aligned}$$

$$\rightarrow \vec{r}_{k+1} = -\alpha_k A\vec{r}_k + \left(1 - \frac{\alpha_k\beta_k}{\alpha_{k-1}}\right)\vec{r}_k + \frac{\alpha_k\beta_k}{\alpha_{k-1}}\vec{r}_{k-1}$$

$$\rightarrow p_{k+1}(t) = -\alpha_k t \cdot p_k(t) + \left(1 - \frac{\alpha_k\beta_k}{\alpha_{k-1}}\right)p_k(t) + \frac{\alpha_k\beta_k}{\alpha_{k-1}}p_{k-1}(t)$$

$$\rightarrow \pi_{k+1}^\sigma = \left(1 + \alpha_k\sigma - \frac{\alpha_k\beta_k}{\alpha_{k-1}}\right)\pi_k^\sigma + \frac{\alpha_k\beta_k}{\alpha_{k-1}}\pi_{k-1}^\sigma$$

Shifted CG: Algorithm

Initial $\vec{r}_0 = \vec{b}$, $\alpha_{-1} = 1$, $\rho_{-1} = +\infty$,
 $\pi_0^\sigma = \pi_{-1}^\sigma = 1$, $\vec{p}_{-1}^\sigma = \vec{x}_{-1}^\sigma = \vec{0}$

For $k = 0, 1, \dots, m$

-Seed equations

$$\rho_k = \vec{r}_k^T \vec{r}_k$$

$$\beta_{k-1} = \frac{\rho_k}{\rho_{k-1}}$$

$$\alpha_k = \frac{\rho_k}{\vec{r}_k^T A \vec{r}_k - \beta_{k-1} \frac{\rho_k}{\alpha_{k-1}}}$$

$$\vec{r}_{k+1} = \left(1 + \frac{\alpha_k \beta_{k-1}}{\alpha_{k-1}}\right) \vec{r}_k - \alpha_k A \vec{r}_k - \frac{\alpha_k \beta_{k-1}}{\alpha_{k-1}} \vec{r}_{k-1}$$

-Shifted equations

$$\pi_{k+1}^\sigma = (1 + \alpha_k \sigma) \pi_k^\sigma - \frac{\alpha_k \beta_{k-1}}{\alpha_{k-1}} (\pi_{k-1}^\sigma - \pi_k^\sigma)$$

$$\vec{p}_k^\sigma = \frac{1}{\pi_k^\sigma} \vec{r}_k + \beta_{k-1} \left(\frac{\pi_{k-1}^\sigma}{\pi_k^\sigma} \right)^2 \vec{p}_{k-1}^\sigma$$

$$\vec{x}_k^\sigma = \vec{x}_{k-1}^\sigma + \frac{\pi_k^\sigma}{\pi_{k+1}^\sigma} \alpha_k \vec{p}_k^\sigma$$

Shifted CG: The Simplest Example

$$(A + \sigma \mathbf{1})\vec{x}^\sigma = \vec{b} \quad A = \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix} \quad \vec{b} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

Seed equations Shifted equations

Oth step

$$\begin{aligned} \rho_0 &= 1 \\ \beta_{-1} &= 0 \\ \alpha_0 &= 1/2 \\ \vec{r}_1 &= \begin{pmatrix} 0 \\ -1/2 \end{pmatrix} \end{aligned}$$

$$\begin{aligned} \pi_1^\sigma &= (1 + \sigma/2) \\ \vec{p}_0^\sigma &= \begin{pmatrix} 1 \\ 0 \end{pmatrix} \\ \vec{x}_0^\sigma &= \frac{1}{2 + \sigma} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \end{aligned}$$

1st step

$$\begin{aligned} \rho_1 &= 1/4 \\ \beta_0 &= 1/4 \\ \alpha_1 &= 2/3 \\ \vec{r}_2 &= \vec{0} \end{aligned}$$

$$\begin{aligned} \pi_2^\sigma &= 1 + 4\sigma/3 + \sigma^2/3 \\ \vec{p}_1^\sigma &= \begin{pmatrix} 1/\{2 + \sigma\}^2 \\ -1/\{2 + \sigma\} \end{pmatrix} \\ \vec{x}_1^\sigma &= \begin{pmatrix} \{2 + \sigma\}/\{3 + 4\sigma + \sigma^2\} \\ -1/\{3 + 4\sigma + \sigma^2\} \end{pmatrix} \end{aligned}$$

$$(A + \sigma \mathbf{1}) \vec{x}^\sigma = \vec{b}$$

$$A = \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix}$$

$$\vec{b} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

Analytical solution

$$\begin{pmatrix} 2 + \sigma & 1 \\ 1 & 2 + \sigma \end{pmatrix}^{-1} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{1}{(2 + \sigma)^2 - 1} \begin{pmatrix} 2 + \sigma \\ -1 \end{pmatrix}$$

Numerical solution

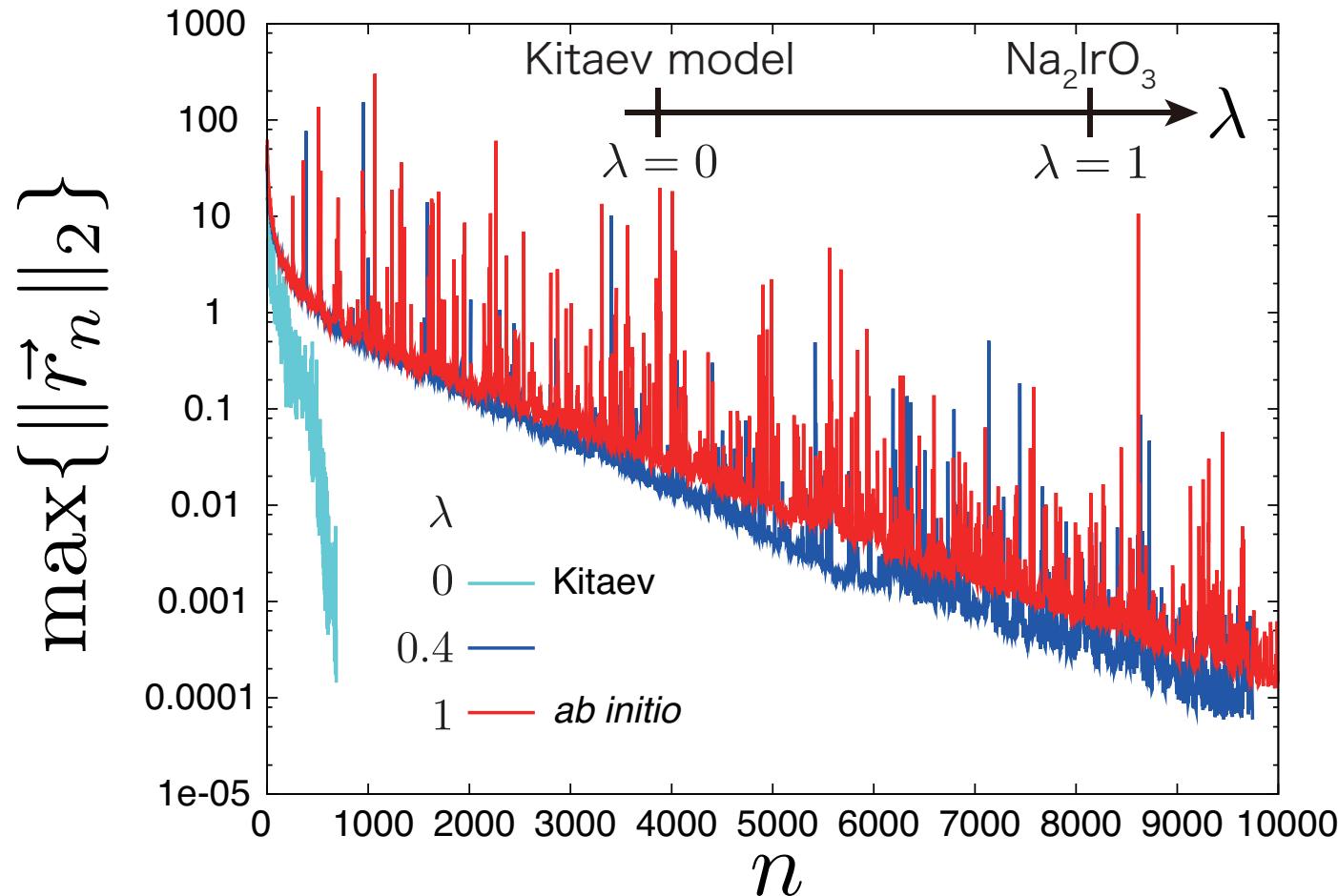
$$\vec{x}_1^\sigma = \begin{pmatrix} \frac{2 + \sigma}{3 + 4\sigma + \sigma^2} \\ -\frac{1}{3 + 4\sigma + \sigma^2} \end{pmatrix}$$

Shifted CG finds
the set of solution!

Convergence of Krylov Subspace Method

Krylov subspace method
finds a solution within N_H steps

An example of shifted BiCG for $N_H=16,777,216$



Important Notice 1

Lanczos method

Pros

- Simple to implement
- Cheap memory cost

Cons

- Eigenvectors are not directly obtained

Important Notice 2

CG method

$$A\vec{x} = E\vec{x}$$

-Eigenvalues and eigenvectors

Locally optimal block CG (LOBCG):

A. V. Knyazev,

SIAM journal on scientific computing 23, 517 (2001).

LOB(P)CG

Algorithm of LOBCG

Initial condition: m orthogonal initial vectors $\mathbf{x}_0^{(i)}$
 $\mathbf{p}_0^{(i)} = \mathbf{0}$ ($i = 1, \dots, m$)

for ($k = 0; k < k_{\max}; k++$)

$$\mu_k^{(i)} = \frac{(\mathbf{x}_k^{(i)} A \mathbf{x}_k^{(i)})}{(\mathbf{x}_k^{(i)}, \mathbf{x}_k^{(i)})} \quad \leftarrow \text{approximation of } i\text{th smallest eigenvalue}$$

$$\mathbf{w}_k^{(i)} = A \mathbf{x}_k^{(i)} - \mu_k^{(i)} \mathbf{x}_k^{(i)}$$

$$S_A = \{\mathbf{w}_k^{(1)}, \dots, \mathbf{w}_k^{(m)}, \mathbf{x}_k^{(1)}, \dots, \mathbf{x}_k^{(m)}, \mathbf{p}_k^{(1)}, \dots, \mathbf{p}_k^{(m)}\}^T A \{\mathbf{w}_k^{(1)}, \dots, \mathbf{w}_k^{(m)}, \mathbf{x}_k^{(1)}, \dots, \mathbf{x}_k^{(m)}, \mathbf{p}_k^{(1)}, \dots, \mathbf{p}_k^{(m)}\}$$

$$S_B = \{\mathbf{w}_k^{(1)}, \dots, \mathbf{w}_k^{(m)}, \mathbf{x}_k^{(1)}, \dots, \mathbf{x}_k^{(m)}, \mathbf{p}_k^{(1)}, \dots, \mathbf{p}_k^{(m)}\}^T \{\mathbf{w}_k^{(1)}, \dots, \mathbf{w}_k^{(m)}, \mathbf{x}_k^{(1)}, \dots, \mathbf{x}_k^{(m)}, \mathbf{p}_k^{(1)}, \dots, \mathbf{p}_k^{(m)}\}$$

Obtain i th smallest eigenstate of $S_A \mathbf{v}^{(i)} = \mu^{(i)} S_B \mathbf{v}^{(i)}$, $\mathbf{v}^{(i)} = (\alpha_1^{(i)}, \dots, \alpha_m^{(i)}, \beta_1^{(i)}, \dots, \beta_m^{(i)}, \gamma_1^{(i)}, \dots, \gamma_m^{(i)})^T$
 $(i = 1, \dots, m)$

$\leftarrow m$ smallest eigenstates are chosen from $3m$ states

$$\mathbf{x}_{k+1}^{(i)} = \sum_{j=1}^m \left(\alpha_j^{(i)} \mathbf{w}_k^{(j)} + \beta_j^{(i)} \mathbf{x}_k^{(j)} + \gamma_j^{(i)} \mathbf{p}_k^{(j)} \right)$$

$$\mathbf{p}_{k+1}^{(i)} = \sum_{j=1}^m \left(\alpha_j^{(i)} \mathbf{w}_k^{(j)} + \gamma_j^{(i)} \mathbf{p}_k^{(j)} \right)$$

Until convergence

Target of Tuning: LOB(P)CG

Algorithm for implementation

Initial condition: m orthogonal initial vectors $\mathbf{x}_0^{(i)}$
 $\mathbf{p}_0^{(i)} = \mathbf{0}$ ($i = 1, \dots, m$) $\mathbf{X}_0^{(i)} = A\mathbf{x}_0^{(i)}$ ← matrix-vector product

for ($k = 0; k < k_{\max}; k++$)

$$\mu_k^{(i)} = \frac{(\mathbf{x}_k^{(i)}, \mathbf{X}_k^{(i)})}{(\mathbf{x}_k^{(i)}, \mathbf{x}_k^{(i)})}$$

$$\mathbf{w}_k^{(i)} = \mathbf{X}_k^{(i)} - \mu_k^{(i)} \mathbf{x}_k^{(i)}$$

$$\mathbf{W}_k^{(i)} = A\mathbf{w}_k^{(i)} \quad \leftarrow \text{matrix-vector product}$$

$$S_A = \{\mathbf{w}_k^{(1)}, \dots, \mathbf{w}_k^{(m)}, \mathbf{x}_k^{(1)}, \dots, \mathbf{x}_k^{(m)}, \mathbf{p}_k^{(1)}, \dots, \mathbf{p}_k^{(m)}\}^T \{\mathbf{W}_k^{(1)}, \dots, \mathbf{W}_k^{(m)}, \mathbf{X}_k^{(1)}, \dots, \mathbf{X}_k^{(m)}, \mathbf{P}_k^{(1)}, \dots, \mathbf{P}_k^{(m)}\}$$

$$S_B = \{\mathbf{w}_k^{(1)}, \dots, \mathbf{w}_k^{(m)}, \mathbf{x}_k^{(1)}, \dots, \mathbf{x}_k^{(m)}, \mathbf{p}_k^{(1)}, \dots, \mathbf{p}_k^{(m)}\}^T \{\mathbf{w}_k^{(1)}, \dots, \mathbf{w}_k^{(m)}, \mathbf{x}_k^{(1)}, \dots, \mathbf{x}_k^{(m)}, \mathbf{p}_k^{(1)}, \dots, \mathbf{p}_k^{(m)}\}$$

Obtain i th smallest eigenstate of $S_A \mathbf{v}^{(i)} = \mu^{(i)} S_B \mathbf{v}^{(i)}$, $\mathbf{v}^{(i)} = (\alpha_1^{(i)}, \dots, \alpha_m^{(i)}, \beta_1^{(i)}, \dots, \beta_m^{(i)}, \gamma_1^{(i)}, \dots, \gamma_m^{(i)})^T$

$$\mathbf{x}_{k+1}^{(i)} = \sum_{j=1}^m \left(\alpha_j^{(i)} \mathbf{w}_k^{(j)} + \beta_j^{(i)} \mathbf{x}_k^{(j)} + \gamma_j^{(i)} \mathbf{p}_k^{(j)} \right)$$

$$\mathbf{X}_{k+1}^{(i)} = \sum_{j=1}^m \left(\alpha_j^{(i)} \mathbf{W}_k^{(j)} + \beta_j^{(i)} \mathbf{X}_k^{(j)} + \gamma_j^{(i)} \mathbf{P}_k^{(j)} \right) = \sum_{j=1}^m \left(\alpha_j^{(i)} A\mathbf{w}_k^{(j)} + \beta_j^{(i)} A\mathbf{x}_k^{(j)} + \gamma_j^{(i)} A\mathbf{p}_k^{(j)} \right)$$

$$\mathbf{p}_{k+1}^{(i)} = \sum_{j=1}^m \left(\alpha_j^{(i)} \mathbf{w}_k^{(j)} + \gamma_j^{(i)} \mathbf{p}_k^{(j)} \right)$$

$$\mathbf{P}_{k+1}^{(i)} = \sum_{j=1}^m \left(\alpha_j^{(i)} \mathbf{W}_k^{(j)} + \gamma_j^{(i)} \mathbf{P}_k^{(j)} \right) = \sum_{j=1}^m \left(\alpha_j^{(i)} A\mathbf{w}_k^{(j)} + \gamma_j^{(i)} A\mathbf{p}_k^{(j)} \right)$$

Until convergence

Important Notice 3

Shifted Krylov subspace method

- Same accuracy as CG obtain for same # of steps
- Solve many shifted equations with
nearly same costs for a single equation

Lecture Schedule

Classical

Quantum

- #1 Many-body problems in physics
- #2 Why many-body problem is hard to solve
- #3 Classical statistical model and numerical simulation
- #4 Classical Monte Carlo method and its applications
- #5 Molecular dynamics and its application
- #6 Extended ensemble method for Monte Carlo methods
- #7 Quantum lattice models and numerical approaches
- #8 Quantum Monte Carlo methods
- #9 Applications of quantum Monte Carlo methods
 - Path integral & applications
- #10 Linear algebra of large and sparse matrices for quantum many-body problems
- #11 Krylov subspace methods and their applications to quantum many-body problems
- #12 Large sparse matrices and quantum statistical mechanics
- #13 Parallelization for many-body problems