Parity-time symmetry breaking physics of dissipative Mott insulators (arXiv:1510.08355)

Himadri Barman

Visiting Fellow
Tata Institute of Fundamental Research
Mumbai, India

DTP Colloquium
February 2, 2016

Plan

- Parity time-reversal ($\mathcal{PT}$) symmetric quantum mechanics.
- Mott metal-insulator transition.
- Effect of electric field on a Mott insulator (MI): Landau-Zener tunneling.
- Effect of electric field on a MI: $\mathcal{PT}$ symmetry breaking point of view.
- 1-dimension : Bethe ansatz.
- 2 and 3-dimension : Dynamical mean-field theory (DMFT).
- Vortex Mott transition.
- Summary and outlook.

$\mathcal{PT}$-symmetric quantum mechanics

Conventional quantum mechanics

- 'Reality' of *observables*: $\hat{x}^\dagger = \hat{x}$, $\hat{p}^\dagger = \hat{p}$, $\hat{H} = \hat{H}^\dagger$.
- Hermitian operators (eg. Hamiltonian) have real eigenvalues (eg. energies).

Generalized $\mathcal{PT}$-symmetric quantum mechanics

- Carl Bender (1998): $\mathcal{PT}$ symmetric $\hat{H}$ also has real E's.
- Eg. $\hat{H} = p^2 + ix^3$.
  $\mathcal{P}\hat{H} = p^2 - ix^3$ $[p \to -p,\ x \to -x]$;
  $\mathcal{T}\hat{H} = p^2 - ix^3$ $[p \to -p,\ i \to -i]$;
  $\mathcal{PT}\hat{H} = p^2 + ix^3 = \hat{H}$.

$\mathcal{PT}$-symmetric quantum mechanics

VOLUME 80, NUMBER 24 PHYSICAL REVIEW LETTERS 15 JUNE 1998

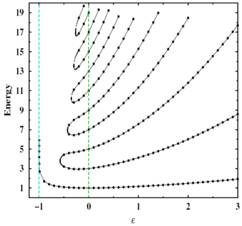
Real Spectra in Non-Hermitian Hamiltonians Having $\mathcal{PT}$ Symmetry

Carl M. Bender[1] and Stefan Boettcher[2,3]
[1]*Department of Physics, Washington University, St. Louis, Missouri 63130*
[2]*Center for Nonlinear Studies, Los Alamos National Laboratory, Los Alamos, New Mexico 87545*
[3]*CTSPS, Clark Atlanta University, Atlanta, Georgia 30314*
(Received 1 December 1997; revised manuscript received 9 April 1998)

The condition of self-adjointness ensures that the eigenvalues of a Hamiltonian are real and bounded below. Replacing this condition by the weaker condition of $\mathcal{PT}$ symmetry, one obtains new infinite classes of complex Hamiltonians whose spectra are also real and positive. These $\mathcal{PT}$ symmetric theories may be viewed as analytic continuations of conventional theories from real to complex phase space. This paper describes the unusual classical and quantum properties of these theories. [S0031-9007(98)06371-6]

Eg. $\hat{H} = \hat{p}^2 + \hat{x}^2 (i\hat{x})^{\varepsilon}$. [$\varepsilon = 0 \Rightarrow$ Harmonic oscillator.]

- For $\varepsilon \geq 0$, energy eigenvalues are always $+$ve and real.
- Near $\mathcal{PT}$-breaking (*exceptional points*) eigenvalues merge.



$\mathcal{PT}$-symmetric quantum mechanics

PRL 109, 150405 (2012) PHYSICAL REVIEW LETTERS week ending 12 OCTOBER 2012

Stimulation of the Fluctuation Superconductivity by $\mathcal{PT}$ Symmetry

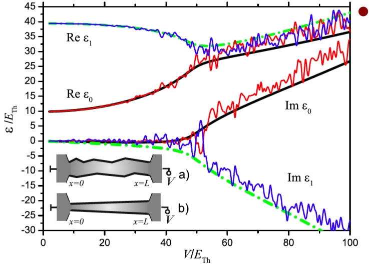
N. M. Chtchelkatchev,[1,2] A. A. Golubov,[3] T. I. Baturina,[4,5] and V. M. Vinokur[4]

[1]*Institute for High Pressure Physics, Russian Academy of Sciences, Troitsk 142190, Moscow region, Russia*
[2]*Department of Theoretical Physics, Moscow Institute of Physics and Technology, 141700 Moscow, Russia*
[3]*Faculty of Science and Technology and MESA+ Institute of Nanotechnology, University of Twente, Enschede, The Netherlands*
[4]*Materials Science Division, Argonne National Laboratory, Argonne, Illinois 60439, USA*
[5]*A. V. Rzhanov Institute of Semiconductor Physics SB RAS, Novosibirsk, 630090 Russia*

(Received 6 May 2012; published 9 October 2012)

We discuss fluctuations near the second-order phase transition where the free energy has an additional non-Hermitian term. The spectrum of the fluctuations changes when the odd-parity potential amplitude exceeds the critical value corresponding to the $\mathcal{PT}$-symmetry breakdown in the topological structure of the Hilbert space of the effective non-Hermitian Hamiltonian. We calculate the fluctuation contribution to the differential resistance of a superconducting weak link and find the manifestation of the $\mathcal{PT}$-symmetry breaking in its temperature evolution. We successfully validate our theory by carrying out measurements of far from equilibrium transport in mesoscale-patterned superconducting wires.

1D superconducting wire with varying thickness:



- Fluctuations smoothen at $\mathscr{E} < \mathscr{E}_c \Rightarrow \mathcal{PT}$-broken transition.

$\mathcal{PT}$-symmetric quantum mechanics

Other realizations

nature physics
LETTERS
PUBLISHED ONLINE: 24 JANUARY 2010 | DOI: 10.1038/NPHYS1515

Observation of parity–time symmetry in optics

Christian E. Rüter[1], Konstantinos G. Makris[2], Ramy El-Ganainy[2], Demetrios N. Christodoulides[2], Mordechai Segev[3] and Detlef Kip[1]*

PRL 108, 173901 (2012) PHYSICAL REVIEW LETTERS week ending 27 APRIL 2012

Pump-Induced Exceptional Points in Lasers

M. Liertzer,[1,*] Li Ge,[2] A. Cerjan,[3] A. D. Stone,[3] H. E. Türeci,[2,4] and S. Rotter[1,†]
[1]*Institute for Theoretical Physics, Vienna University of Technology, A-1040 Vienna, Austria, EU*
[2]*Department of Electrical Engineering, Princeton University, Princeton, New Jersey 08544, USA*
[3]*Department of Applied Physics, Yale University, New Haven, Connecticut 06520, USA*
[4]*Institute for Quantum Electronics, ETH-Zürich, CH-8093 Zürich, Switzerland*
(Received 2 September 2011; revised manuscript received 20 January 2012; published 24 April 2012)

We demonstrate that the above-threshold behavior of a laser can be strongly affected by exceptional points which are induced by pumping the laser nonuniformly. At these singularities, the eigenstates of the non-Hermitian operator which describes the lasing modes coalesce. In their vicinity, the laser may turn off even when the overall pump power deposited in the system is increased. Such signatures of a pump-induced exceptional point can be experimentally probed with coupled ridge or microdisk lasers.

RAPID COMMUNICATIONS
PHYSICAL REVIEW A **84**, 040101(R) (2011)

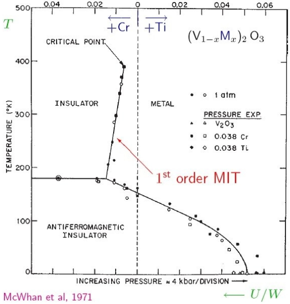
Experimental study of active *LRC* circuits with $\mathcal{PT}$ symmetries

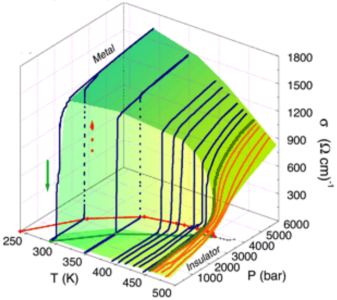
Joseph Schindler, Ang Li, Mei C. Zheng, F. M. Ellis, and Tsampikos Kottos
Department of Physics, Wesleyan University, Middletown, Connecticut 06459, USA
(Received 28 June 2011; revised manuscript received 31 August 2011; published 13 October 2011)

Mutually coupled modes of a pair of active *LRC* circuits, one with amplification and another with an equivalent amount of attenuation, provide an experimental realization of a wide class of systems where gain and loss mechanisms break the Hermiticity while preserving parity-time $\mathcal{PT}$ symmetry. For a value $\gamma_{\mathcal{PT}}$ of the gain and loss strength parameter the eigenfrequencies undergo a spontaneous phase transition from real to complex values, while the normal modes coalesce, acquiring a definite chirality. The consequences of the phase transition in the spatiotemporal energy evolution are also presented.

Mott transition (experiment)

Correlation driven metal-to-insulator transition (MIT)





McWhan *et al.* , PRL 27, 941 ('71)   Limelette *et al.* , Science 302, 89 ('03)

- High resistivity (low conductivity) $\Rightarrow$ insulator.
- Low resistivity (high conductivity) $\Rightarrow$ metal.

Mott metal-insulator transition (theory)

Model: Hubbard model

$$\hat{H} = -t\sum_{\langle ij\rangle} c_i^\dagger c_j - \mu\sum_i c_i^\dagger c_i + U\sum_i \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}\,. \tag{1}$$

$d = 1$ solution : Bethe ansatz [E. H. Lieb and F. Y. Wu, PRL 20, 1445 ('68)]

- Exact.
- Finds ground state energies of M $\uparrow$'s and M' $\downarrow$'s : $E(M,M';U)$.
- Finds chemical potentials $\mu_\pm \equiv \pm E(M\pm 1,M;U) \mp E(M,M;U)$.
- $\mu_+ \neq \mu_- \Rightarrow$ insulator.

$d > 1$ solution : Dynamical mean-field theory (DMFT)

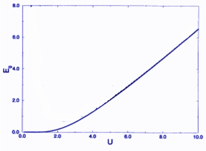
- Exact at $d = \infty$. [Georges *et al.* , RMP 68, 13 ('96)]
- Finds interacting DOS or spectral function : $A(\omega) = -\frac{1}{\pi}\mathrm{Im}G(\omega)$; G: single particle propagator or Green's function.
- Gap at Fermi level $(\omega = 0)$ signifies insulator.

Mott metal-insulator transition (theory)

Bethe ansatz on 1-D Hubbard model

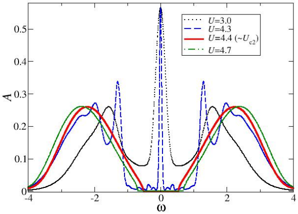
- No phase transition, always insulator at half-filling.

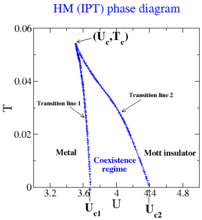
$$E_g = U - 4 + 8\int_0^\infty J_1(x)/(x(1+\exp(Ux/2))).$$



DMFT on Hubbard model for hypercubic lattice

- $A(\omega)$ shows metal-to-insulator transition : At $U > U_{c2}$, opens gap at $\omega = 0$.





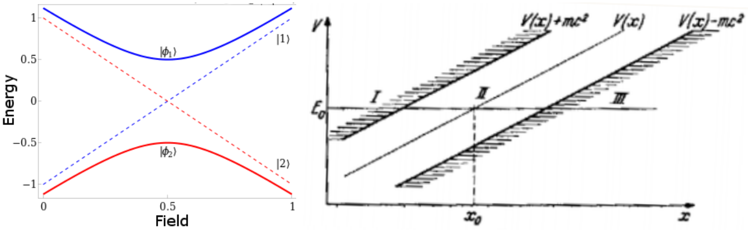
[H. Barman and N. S. Vidhyadhiraja, IJMPB 25, 2461 ('11)]

Effect of drive (electric field)

Dielectric breakdown: Landau Zener physics

- Eg. Two-level system: $\hat{H} = vFt\sigma^z + \Delta\sigma^x$.

[Zener, Proc. R. Soc. 145, 523 ('34)]



- Transition probability: $P_{1\to 2} = e^{-\gamma}$;
  $\gamma = \pi F_{\rm th}/F$; $F_{\rm th} = \Delta^2(U)/vF$; $F \equiv eE$.
- *Cf.* Pair production rate in QED: $p = e^{-\frac{\pi m^2}{|eE|}}$ [Schwinger '51].

Effect of drive (electric field)

Trending !

Access by Tata Institu

Dielectric Breakdown of the Insulating Charge-Ordered State in $La_{2-x}Sr_xNiO_4$

S. Yamanouchi, Y. Taguchi, and Y. Tokura
Phys. Rev. Lett. **83**, 5555 – Published 27 December 1999

Access by Tata Institute c

Dielectric breakdown of one-dimensional Mott insulators Sr_2CuO_3 and $SrCuO_2$

Y. Taguchi, T. Matsumoto, and Y. Tokura
Phys. Rev. B **62**, 7015 – Published 15 September 2000

Nonthermal and purely electronic resistive switching in a Mott memory

P. Stoliar, M. Rozenberg, E. Janod, B. Corraze, J. Tranchant, and L. Cario
Phys. Rev. B **90**, 045146 – Published 30 July 2014

Dielectric breakdown via emergent nonequilibrium steady states of the electric-field-driven Mott insulator

Woo-Ram Lee and Kwon Park
Phys. Rev. B **89**, 205126 – Published 27 May 2014

Effect of drive (electric field)

Hubbard model in a complex gauge field ψ:

$$\hat{H} = -t \sum_{\langle ij \rangle \sigma} [e^{i\Psi(t)} c^{\dagger}_{i\sigma} c_{j\sigma} + \text{h.c.}] + U \sum_{j} n_{i\uparrow} n_{i\downarrow} .$$

Landau-Zener-Schwinger (LZS) generalized: Landau-Dykhne formula

$$\gamma \sim \frac{1}{F} \mathrm{Re} \int_{\chi}^{\chi_C} d\chi' [E_1(\chi) - E_0(\chi')];$$

$\psi(t) = Ft + i\chi$. In non-dissipative case: get back the usual LZS

$$\gamma \sim \Delta^2/(vF) \equiv F_{\mathrm{th}}/F;\ v = |d\Delta/dt|.F\,.$$

Effect of dissipation : $\mathcal{PT}$-symmetric Hamiltonian

Hubbard model with only the dissipative term in the gauge field (imaginary)

$$
\begin{aligned}
H' &= -t \sum_{\langle ij \rangle, \sigma} [e^{\chi} c^{\dagger}_{i\sigma} c_{i\sigma} + e^{-\chi} c^{\dagger}_{j\sigma} c_{i\sigma}] + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} \\
&= -t(\cosh \chi) \sum_{\langle ij \rangle, \sigma} [c^{\dagger}_{i\sigma} c_{i\sigma} + c^{\dagger}_{j\sigma} c_{i\sigma}] + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} \\
&\quad - i(\sinh \chi) \hat{J}.
\end{aligned}
\tag{2}
$$

This has a generic form

$$
\hat{H}' = \hat{H} - i\lambda \hat{J} \tag{3}
$$

- For small λ, $\langle \hat{J} \rangle = 0 \Rightarrow$ real eigenvalues.
- For $\lambda > \lambda_c$, $\langle \hat{J} \rangle = I \Rightarrow$ complex eigenvalues ($\mathcal{PT}$ broken !!).

1D fermionic Hubbard model

Coupled Bethe ansatz equations:

$$\begin{aligned}
\rho(k) &= \frac{1}{2\pi} - \frac{\cos k}{2\pi}\int_{-\infty}^{\infty} d\lambda\, \theta'(\sin k - \lambda)\sigma(\lambda)\,, \\
\sigma(\lambda) &= -\frac{1}{2\pi}\int_{\mathcal{C}} dk\, \theta'(\sin k - \lambda)\rho(k) + \frac{1}{4\pi}\int_{-\infty}^{\infty} d\lambda'\theta'((\lambda-\lambda')/2)\sigma(\lambda')\,, \\
\chi(b) &= b - i\int_{-\infty}^{\infty} d\lambda\, \theta(\lambda + i\sinh b)\sigma(\lambda)\,.
\end{aligned} \tag{4}$$

$u \equiv U/(4t)$, $\theta(x) = -2\tanh^{-1}(x/u)$, b: parameter controlling contour $\mathcal{C}$ [Fukui and Kawakami, PRB 58, 16051 ('98)].

$$\Delta(b) = 4t\left[u - \cosh(b) + \int_{-\infty}^{\infty} \frac{d\omega}{2\pi}\frac{J_1(\omega)e^{\omega\sinh(b)}}{\omega(1+2^{2u|\omega|})}\right]\,; \tag{5}$$

- $\Delta(b_c) = 0$, $b_c = \sinh^{-1}(u)$.
- $\chi'(b) \simeq C(b-b_c) \Rightarrow \chi_c - \chi \simeq C_1(b-b_c)^2 \Rightarrow \Delta(\chi) \simeq C_2(\chi_c-\chi)^{\frac{1}{2}}$.
- $\Rightarrow \boxed{\Delta(F) \sim (F_c - F)^{\frac{1}{2}}} \Rightarrow \gamma \sim (F_c - F)^{3/2}$.

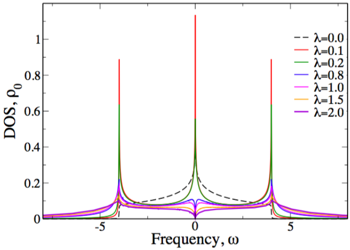
2D fermionic Hubbard model

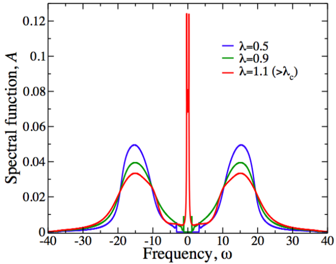
Numerics : DMFT

- Hamiltonian:

$$\hat{H} = \sum_{\mathbf{k},\sigma} [[-2t(\cos k_x + \cos k_y) - i\lambda \sin k_x - \mu] c^{\dagger}_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma}] + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} \, .$$

- Density of states :





$U = 0$ $\qquad$ $U = 30t_*$.

- Finite λ leads to 2D to 1D-like crossover at $U = 0$: splitting of van-Hove singularity.
- Finite λ renormalizes Mott gap, gap closes at $\lambda > \lambda_c \simeq 1.1$.

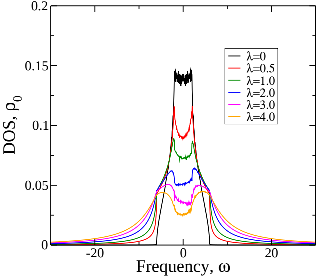
3D fermionic Hubbard model

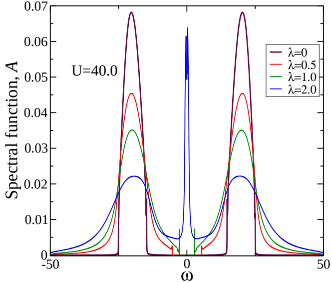
Numerics : DMFT

- Hamiltonian:

$$\hat{H} = \sum_{\mathbf{k},\sigma} [[-2t(\cos k_x + \cos k_y + \cos k_z) - i\lambda \sin k_x - \mu] c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma}] + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} \,.$$

- Density of states :



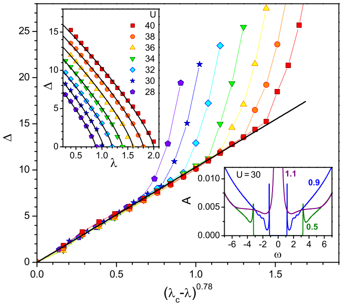


$U = 0$ $\qquad$ $U = 40t_*$.

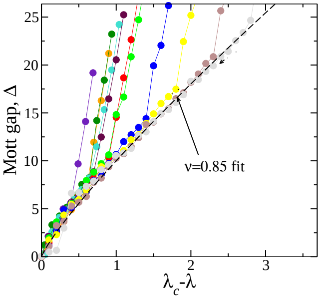
- Not exactly 3D-1D crossover at $U = 0$, two peaks arise near boundaries instead of singularities.
- Gap renormalization happens too, gap closes at $\lambda > \lambda_c \simeq 2.0$

Closing of gap : universality

Critical behaviors: 2D and 3D



$d = 2$

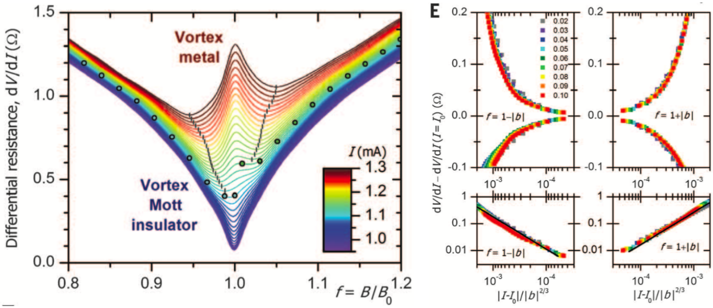


$d = 3.$

- Near the Mott transition, $\Delta \sim (\lambda_c - \lambda)^{\nu}\ \forall U$.
- 2D: $\nu = 0.78 \pm 0.03$, 3D: $\nu \simeq 0.85$. (Is $\nu = 1$ for mean-field $d > d_c$ limit?)

Vortex insulator-to-metal transition

Array of Nb superconducting islands on Si/SiO_2 substrate



[Poccia *et al.* , Science 349, 1202 ('15)]

- Increasing $I \Rightarrow$ Minimum (ins) to maximum (metal) flip in differential resistance (dV/dI).
- Critical scaling law:

$$\frac{dV(f,I)}{dI} - \frac{dV(f,I)}{dI}\Big|_{I=I_c} = \mathscr{F}\left(\frac{I - I_c^{\pm}}{|b|^{\varepsilon}}\right). \qquad (6)$$

- Scaling collapse $\Rightarrow \varepsilon = 2/3 \Rightarrow \gamma \sim (I_c - I)^{3/2}$

Vortex insulator-to-metal transition

- Landau-Ginzburg-Wilson Hamiltonian:

$$H = \int d^x \left[D|\nabla\Psi|^2 + m^2|\Psi|^2 + u|\Psi|^4\right] \tag{7}$$

ψ: vortex field, D: vortex stiffness, m: mass, u : interaction.

- Considering $\Psi(x,y,t) = e^{ik_y y - \lambda t}u(x)$ [Rubinstein, Sternberg, Ma, PRL 99, 167003 ('07)] :

$$Du_{xx} + i(I/\rho)xu = -(\lambda - m^2 - k_y^2)u \tag{8}$$

- $\Rightarrow \mathscr{H}_{\text{eff}} = -Du_{xx} - i(I/\rho)$
- $\mathcal{PT}$-symmetry limits: $I = 0 \Rightarrow E$'s real, $I \to \infty \Rightarrow E$'s imaginary.
- $\xi \equiv x/a$, $E \equiv (\lambda - m^2 - k_y^2)/E_T$, $E_T = D/a^2 \Rightarrow$

$$u_{\xi\xi} + i(Ia/E_T\rho)u = -Eu\,. \tag{9}$$

- $\Rightarrow (E_1 - E_0) \sim E_T(1 - I/I_c)^{\frac{1}{2}}$
- $\Rightarrow$ Same universality with 1D-fermions!.
- Landau-Dykhne $\Rightarrow \gamma \sim (I_c - I)^{3/2} \Rightarrow$ Supports experiment.

Summary and outlook

- Effect of electric field with dissipation on a Mott insulator can be modeled by a $\mathcal{PT}$-symmetric Hubbard model.
- The $\mathcal{PT}$-symmetry broken eigenstates signals onset of a insulator-to-metal transition (dielectric breakdown).
- 1D fermionic Mott insulator (Bethe ansatz) shows transition with critical exponent 0.5. Vortex Mott transition in superconducting islands reflects the same universality class.
- 2D and 3D fermionic Mott insulators (DMFT) show transitions with critical exponents $\nu \simeq 0.78$ and 0.85 (Does $d > d_c$ reproduces mean-field limit $\nu = 1$?)
- 1D LZW scheme on $\mathcal{PT}$-symmetric field equation explains critical behavior in vortex Mott transition.
- Microscopic theory could be developed for vortices (bosonic BA or B-DMFT ?).
- Benchmarking against results for dissipation treated through a coupled reservoir [eg. Aron, PRB 86, 085127 ('12)] .

Reference

- http://arxiv.org/abs/1510.08355 .

Collaborators

- Vikram Tripathi (TIFR, Mumbai, India),
- Valerie Vinokur (Argonne National Lab, USA),
- Alexy Galda (Argonne National Lab, USA).

Thanks for your kind attention !

Appendix A: More about $\mathcal{PT}$ symmetric QM

$\mathcal{PT}$ symmetric QM

Pseudo norm conservation

- $\langle \psi(t)|\mathcal{P}|\psi(t)\rangle = \langle \psi(0)|\mathcal{P}|\psi(0)\rangle$. [Miloslav Znojil, arXiv:math-ph/0104012]

Pseudo Hermiticity

- $\hat{A}^\dagger = \hat{\eta}\hat{A}\hat{\eta}$, $\hat{\eta}$: *intertwinning operator*.
- $\eta = \mathbf{1} \Rightarrow$ Hermitian QM.
- $\eta = \mathcal{P} \Rightarrow \mathcal{PT}$-symmetric QM.

Appendix B: DMFT

Classical Weiss mean-field theory

- Average magnetization at site 0:

$$m = \sum_{S_0=\pm 1} S_0 e^{\beta H^{\rm MF}} / \sum_{S_0=\pm 1} e^{\beta H^{\rm MF}}$$
$$= (e^{\beta h^{\rm MF}} - e^{-\beta h^{\rm MF}})/(e^{\beta h^{\rm MF}} + e^{-\beta h^{\rm MF}})$$
$$= \tanh(\beta h^{\rm MF})$$

- Now $h^{\rm MF} = h + \sum_{i \in \langle i0 \rangle} J_{i0} m_i = h + zJm$;

  $z=$ coordination number, $J_{ij} = J$ for nearest neighbor interaction, $m_i = m = \langle S_i \rangle$=average magnetization per site .

- Wrote $\langle S_i \rangle = m$ as well since S_0 is not spin of any special site, i.e. $\langle S_i \rangle = \langle S_0 \rangle$.

- Thus $\boxed{m = \tanh \beta (h + zJm)} \Rightarrow$ self-consistent MF equation.

Quantum version: Dynamical mean field theory (DMFT)

- No order parameter or extensive quantity, but a **Green's function** (probability amplitude of an electron moving from site i to site j starting at time τ and ending at τ'):

$$G_{ij,\sigma}(\tau-\tau') \equiv -\langle \hat{T} c_{i\sigma}(\tau) c^{\dagger}_{j\sigma}(\tau') \rangle$$

- No direct mean-field Hamiltonian, but an **effective or local action** for an interacting lattice model (e.g. Hubbard model):

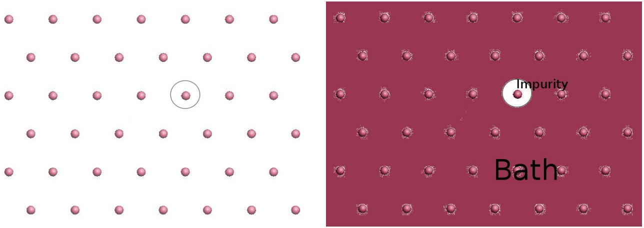
$$S_{\rm local} = -\int_0^{\beta} d\tau \int_0^{\beta} d\tau' \sum_{\sigma} c^{\dagger}_{0\sigma}(\tau) \mathscr{G}^{-1}(\tau-\tau') c_{0\sigma}(\tau') + U \int_0^{\beta} d\tau \, n_{0\uparrow}(\tau) n_{0\downarrow}(\tau)$$

- $\mathscr{G}$ represents Green's function of the *effective* conduction bath attached to an impurity atom. $\Rightarrow$ Single impurity Anderson model (SIAM).

Ref. *Georges and Kotliar, PRB 45, 6479 (1992)*

DMFT: Introduction

- A similar picture similar to the classical Weiss mean-field theory.



- Effective single-impurity Anderson model (SIAM) (e.g. a quantum dot attached to conducting leads)

$$
\begin{aligned}
H_{\text{SIAM}} &= H_{\text{bath}} + H_{\text{impurity}} + H_{\text{hybridization}} \\
&= \sum_{\mathbf{q}\sigma} \tilde{\varepsilon}_{\mathbf{q}} c^{\dagger}_{\mathbf{q}\sigma} c_{\mathbf{q}\sigma} + [(\varepsilon_0 - \mu) d^{\dagger}_{0\sigma} d_{0\sigma} + U n_{0\uparrow} n_{0\downarrow}] + \sum_{\mathbf{q}\sigma} (V_{\mathbf{q}} c^{\dagger}_{\mathbf{q}\sigma} d_{0\sigma} + \text{h.c.})
\end{aligned}
$$

- Host/bath/mean-field Green's function:

$$
\mathscr{G} = 1/(\omega^{+} + \mu - \Delta(\omega)); \quad \Delta(\omega) = \sum_{\mathbf{q}} |V_{\mathbf{q}}|^2 / (\omega^{+} - \tilde{\varepsilon}_l)
$$

DMFT: Introduction

- The impurity represents no special site. Mapping is true for each site in the lattice $\Rightarrow$ self-consistency

Impurity sector:

- Coulomb interaction at impurity site develops a *self-energy* for the host Green's function. Impurity Green's function obtained through Dyson's eq.: ${G_{\text{impurity}}}^{-1} = \mathscr{G}^{-1} - \Sigma_{\text{impurity}}$.

Lattice sector:

- **Further simplification:** $d \to \infty$. Only site-diagonal Green's function ($G_{ii\sigma}$) contribute and self-energy of the lattice become $\mathbf{k}$-independent.

$$G_{\text{local}} = \sum_{\mathbf{k}} G(\mathbf{k}, \omega) = \sum_{\mathbf{k}} \frac{1}{\omega^+ + \mu - \varepsilon_d + \varepsilon_{\mathbf{k}} - \Sigma_{\text{local}}(\omega)}$$

- Self-consistency $\Rightarrow$ $\boxed{G_{\text{impurity}} = G_{\text{local}};\ \Sigma_{\text{impurity}} = \Sigma_{\text{local}}}$
- No averaging out in the time domain, i.e. quantum *dynamics* intact.
- Hence the mean-field is *dynamical*.

DMFT: In practice

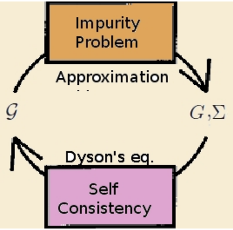
What can we do within DMFT framework?

- Green's function tells about the spectral density (DoS): $D(\omega) = -\frac{1}{\pi}\mathrm{Im}G(\omega)$; can be tested through ARPES experiment.
- Transport properties using Kubo formula (e.g. conductivity):

$$
\begin{aligned}
\sigma_1(\omega) &= \frac{1}{\hbar\omega}\int_0^\infty dt e^{i\omega t}\langle j(\mathbf{q},t)j(\mathbf{q},0)\rangle \\
&= \frac{\sigma_0 {t_*}^2}{2\pi^2}\mathrm{Re}\int d\omega' \frac{n_F(\omega')-n_F(\omega+\omega')}{\omega}\left[\frac{G^*(\omega')-G(\omega+\omega')}{\gamma(\omega+\omega')-\gamma^*(\omega')}\right. \\
&\qquad\left. - \frac{G(\omega')-G(\omega+\omega')}{\gamma(\omega+\omega')-\gamma(\omega')}\right]
\end{aligned}
$$

- And many more: Energy, specific heat, Hall coefficient, susceptibility.

DMFT: Numerical steps



1. Start with a guessed $\mathscr{G}$ or Σ.
2. Use and impurity solver (e.g. IPT, LMA, NRG, ED) to find Σ and $\mathscr{G}$.
3. Calculate the local Green's function for a given lattice DoS (D_0).

$$G(\omega) = \int d\varepsilon \, \frac{D_0(\varepsilon)}{\omega^+ - \varepsilon_d - \varepsilon - \Sigma(\omega)}$$

4. Use Dyson's eq. to update $\mathscr{G}$ or Σ:

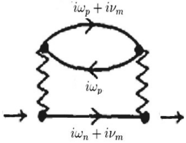
$$\mathscr{G}^{-1}(\omega) = G^{-1}(\omega) + \Sigma(\omega)$$

- The most difficult task is to find a suitable impurity solver

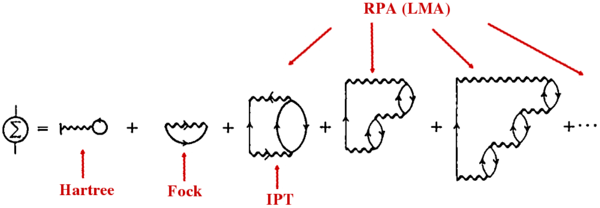
Semi-analytic impurity solver

Iterated perturbation theory (IPT)[Georges, Kotliar, Jarrell, Pruschke, Cox]

$$\Sigma_2(\omega) = \lim_{i\omega \to \omega^+} \frac{U^2}{\beta^2} \sum_{m,p} \mathscr{G}_0(i\omega + i\nu_m)\mathscr{G}_0(i\omega_p + i\nu_m)\mathscr{G}_0(i\omega_p)$$



Local moment approach (LMA) [Logan, Eastwood, Vidhyadhiraja]

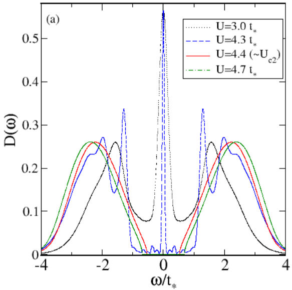


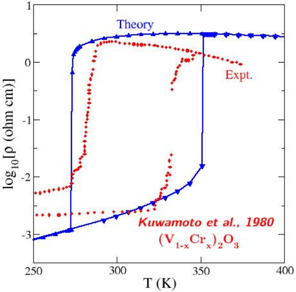
$$\Sigma_\sigma(\omega) = \frac{U^2}{2\pi i} \int_{-\infty}^{\infty} d\omega' \, \mathscr{G}_{\bar{\sigma}}(\omega - \omega') \Pi^{\sigma\bar{\sigma}}(\omega')$$

- Spin symmetry broken, but restored for Fermi liquid phase by satisfying: $\sum_\sigma \sigma\Sigma(0) = |\mu|U;\ \mu = \langle \hat{n}_{i\uparrow} - \hat{n}_{i\downarrow} \rangle$.

Results: Mott metal-insulator transition

DMFT+IPT: Spectral functions and resistivity





- Mott transition with thermal hysteresis observed.

[H. Barman and N. S. Vidhyadhiraja, IJMPB 25, 2461 (2011)]

Appendix C: Bethe Ansatz

Basic formalism

1. $f(x_1,\cdots,x_N)$: Amplitude of wavefunction with electrons ↓-spin residing in sites $x_1,\cdots,x_M$ and ↑-spin residing in sites $x_{M+1},\cdots,x_N$.
2. Ansatz: $f(x_1,\cdots,x_N)=\sum_P[Q,P]\exp(i\sum_{j=1}^N k_{P_j}x_{Q_j})$ where P, Q are set of N unequal real numbers.
3. Lieb-Wu equations:

$$\begin{aligned} Lk_j &= 2\pi I_j + \sum_{\beta=1}^{M}\theta(2\sin k_j - 2\Lambda_\beta), j=1,2,\ldots,N; \\ -\sum_{j=1}^{N}\theta(2\Lambda_\alpha - 2\sin k_j) &= 2\pi J_\alpha - \sum_{\beta=1}^{M}\theta(\Lambda_\alpha-\Lambda_\beta),\ \alpha=1,2,\ldots,M; \\ \theta(x) &= -2\tan^{-1}(2x/U),\ -\pi\le\theta<\pi, \end{aligned} \tag{10}$$

I_j:integers for M, J_α:integers for M'.