Continuous-time QMC Solvers for Electronic Systems in Fermionic and Bosonic Baths

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Goal: Detailed overview of CT-INT and CT-AUX (CT-HYB → See notes)

Outline

- Weak coupling CT-QMC – Basics.
  – Add ons: Retarded interactions: phonon degrees of freedom.
- Selected applications. Topological insulators, electron-phonon interaction.
- Conclusions.

I. Weak coupling CT-QMC (CT-INT).

Consider:

$$H = H_0 + U \underbrace{d_\uparrow^\dagger d_\uparrow}_{n_\uparrow} \underbrace{d_\downarrow^\dagger d_\downarrow}_{n_\uparrow}$$

H_0 is a single body Hamiltonian

We would like to compute for example:

$$G^\sigma(\tau_2,\tau_1) = \left\langle T\, d_\sigma^\dagger(\tau_2) d_\sigma(\tau_1) \right\rangle$$

Prior knowledge:

$$G_0^\sigma(\tau_2,\tau_1) = \left\langle T\, d_\sigma^\dagger(\tau_2) d_\sigma(\tau_1) \right\rangle_0$$

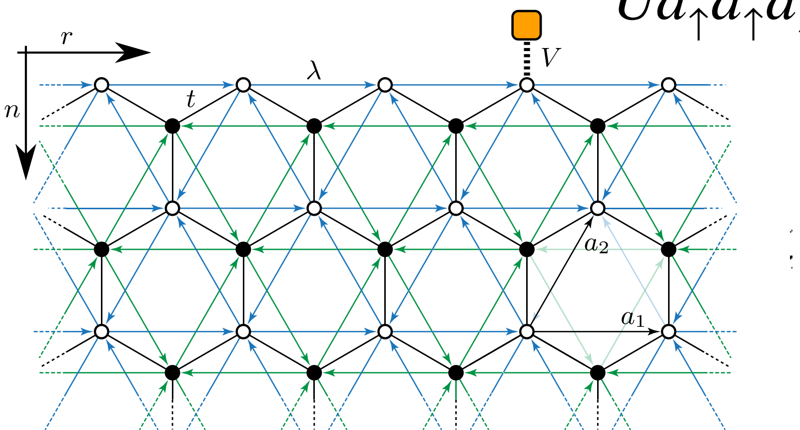
We will assume time reversal symmetry such that G_0 is diagonal in *spin* degrees of freedom.

Examples: Single impurity Anderson model (→ DMFT)

Magnetic impurity on the edge of a topological insulator (Important for understanding spin transport)

$$U d_\uparrow^\dagger d_\uparrow d_\downarrow^\dagger d_\downarrow$$

H_0



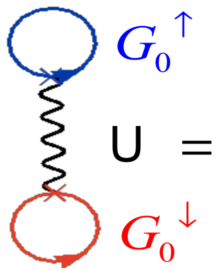
F. Goth et al. Phys. Rev. B (2013)

I. Weak coupling CT-QMC (CT-INT).

Dyson. Expansion around U=0. (Notes → Path integral formulation
Here → More pedestrian second quantized formulation)

$$\frac{\mathrm{Tr}\left[e^{-\beta H}\right]}{\mathrm{Tr}\left[e^{-\beta H_0}\right]} = \sum_n \int_0^{\beta} d\tau_1 \cdots \int_0^{\tau_{n-1}} d\tau_n \, (-U)^n \left\langle n_\uparrow(\tau_1) n_\downarrow(\tau_1) \cdots n_\uparrow(\tau_n) n_\downarrow(\tau_n) \right\rangle_0$$

Wick

n=1 

U $= -U \det \begin{pmatrix} G_0^{\uparrow}(\tau_1,\tau_1) & 0 \\ 0 & G_0^{\downarrow}(\tau_1,\tau_1) \end{pmatrix} \equiv -U \det\left[M_1(\tau_1) \right]$

$$G_0^{\sigma}(\tau_2,\tau_1) = \left\langle T \, \hat{d}_\sigma^{+}(\tau_2) \hat{d}_\sigma(\tau_1) \right\rangle_0$$

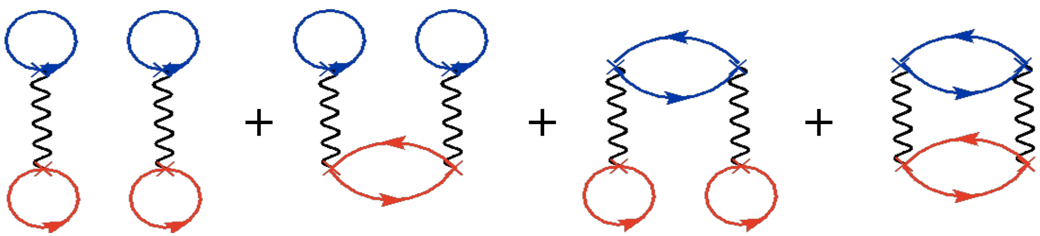
I. Weak coupling CT-QMC (CT-INT).

Dyson. Expansion around U=0.

$$\frac{\mathrm{Tr}\left[e^{-\beta H}\right]}{\mathrm{Tr}\left[e^{-\beta H_0}\right]} = \sum_n \int_0^\beta d\tau_1 \cdots \int_0^{\tau_{n-1}} d\tau_n \, (-U)^n \left\langle n_\uparrow(\tau_1) n_\downarrow(\tau_1) \cdots n_\uparrow(\tau_n) n_\downarrow(\tau_n) \right\rangle_0$$

Wick

n=2



$$= U^2 \det\left[M_2\left(\tau_1, \tau_2\right)\right]$$

$$\det\left[M_2\left(\tau_1,\tau_2\right)\right] = \prod_\sigma \det \begin{pmatrix} G_0^\sigma(\tau_1,\tau_1) & G_0^\sigma(\tau_1,\tau_2) \\ G_0^\sigma(\tau_2,\tau_1) & G_0^\sigma(\tau_2,\tau_2) \end{pmatrix}$$

Sum of connected & disconnected diagrams

$$\frac{\mathrm{Tr}\left[e^{-\beta H}\right]}{\mathrm{Tr}\left[e^{-\beta H_0}\right]} = \underbrace{\sum_n \int_0^\beta d\tau_1 \cdots \int_0^{\tau_{n-1}} d\tau_n}_{\textit{Sum}\text{ with Monte Carlo}} \underbrace{(-U)^n \det\left[M_n\left(\tau_1,\cdots,\tau_n\right)\right]}_{\text{Weight}}$$

with

$$\det\left[M_n\left(\tau_1,\tau_2,\cdots,\tau_n\right)\right] = \prod_\sigma \det\begin{pmatrix} G_0^\sigma(\tau_1,\tau_1) & \cdots & G_0^\sigma(\tau_1,\tau_n) \\ \vdots & \ddots & \vdots \\ G_0^\sigma(\tau_n,\tau_1) & \ldots & G_0^\sigma(\tau_n,\tau_n) \end{pmatrix}$$

= Sum over all connected and disconnected diagrams at order n.

We can now see how to define the configuration space

let C=:{τ_1, τ_2,…, τ_n}, and we will carry out the sum over C with Monte Carlo importance sampling.

$$\frac{\mathrm{Tr}\left[e^{-\beta H}\right]}{\mathrm{Tr}\left[e^{-\beta H_0}\right]} = \underbrace{\sum_n \int_0^\beta d\tau_1 \cdots \int_0^{\tau_{n-1}} d\tau_n}_{\textit{Sum}\text{ with Monte Carlo}} \underbrace{(-U)^n \det\left[M_n\left(\tau_1, \cdots, \tau_n\right)\right]}_{\text{Weight}}$$

Weight / Sign.

- $H_U \rightarrow \frac{U}{2} \sum_{s=\pm 1} \left(n_\uparrow{}^d - [1/2 - s\delta]\right)\left(n_\downarrow{}^d - [1/2 + s\delta]\right) = -\frac{K}{2\beta} \sum_s e^{s\alpha\left(n_\uparrow{}^d - n_\downarrow{}^d\right)}$

$$K = U\beta(\delta^2 - 1/4), \ \cosh(\alpha) - 1 = \frac{1}{2(\delta^2 - 1/4)}, \qquad \delta > 1/2$$

→ New dynamical variable s. Exact mapping onto CT-AUX (K. Mikelsons et al. PRE 09)
(Rombouts et al. PRL 99, Gull et. al EPL 08)

→Sign problem behaves as in Hirsch-Fye, and auxiliary field methods
(Absent for one-dimensional chains, particle-hole symmetry, impurity models)

$$\frac{\mathrm{Tr}\left[e^{-\beta H}\right]}{\mathrm{Tr}\left[e^{-\beta H_0}\right]} = \underbrace{\sum_n \int_0^\beta d\tau_1 \cdots \int_0^{\tau_{n-1}} d\tau_n}_{\textit{Sum}\text{ with Monte Carlo}} \underbrace{(-U)^n \det\left[M_n\left(\tau_1,\cdots,\tau_n\right)\right]}_{\text{Weight}}$$

Weight / Sign.

- $$H_U \rightarrow \frac{U}{2}\sum_{s=\pm 1}\left(n_\uparrow{}^d - \left[1/2 - s\delta\right]\right)\left(n_\downarrow{}^d - \left[1/2 + s\delta\right]\right) = -\frac{K}{2\beta}\sum_s e^{s\alpha\left(n_\uparrow{}^d - n_\downarrow{}^d\right)}$$

$$K = U\beta(\delta^2 - 1/4),\ \cosh(\alpha) - 1 = \frac{1}{2(\delta^2 - 1/4)}\ , \qquad \delta > 1/2$$

- $$H_U = U\left(n_\uparrow{}^d - [1/2 - \delta]\right)\left(n_\downarrow{}^d - [1/2 + \delta]\right) \underbrace{+\,U\delta(n_\uparrow{}^d - n_\downarrow{}^d)}_{\text{Absorb in } H_0}$$

- Particle-Hole symmetry $\delta = 0$ and only even powers of n occur in expansion.

$$\frac{\mathrm{Tr}\left[e^{-\beta H}\right]}{\mathrm{Tr}\left[e^{-\beta H_0}\right]} = \underbrace{\sum_n \int_0^\beta d\tau_1 \sum_{s_1} \cdots \int_0^{\tau_{n-1}} d\tau_n \sum_{s_n}}_{\textit{Sum}\text{ with Monte Carlo}} \underbrace{\left(-\frac{U}{2}\right)^n \det\left[M_n\left(\tau_1, s_1 \cdots, \tau_n, s_n\right)\right]}_{\text{Weight}}$$

$$\det\left[M_n\left(\tau_1, s_1, \cdots, \tau_n, s_n\right)\right] =$$

$$\left\langle T \ \left[n_\uparrow(\tau_1) - \alpha_\uparrow(s_1)\right]\left[n_\downarrow(\tau_1) - \alpha_\downarrow(s_1)\right] \cdots \left[n_\uparrow(\tau_n) - \alpha_\uparrow(s_n)\right]\left[n_\downarrow(\tau_n) - \alpha_\downarrow(s_n)\right]\right\rangle_0 =$$

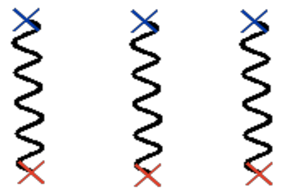
$$\prod_\sigma \det\begin{pmatrix} G_0^\sigma(\tau_1, \tau_1) - \alpha_\sigma(s_1) & \cdots & G_0^\sigma(\tau_1, \tau_n) \\ \vdots & \ddots & \vdots \\ G_0^\sigma(\tau_n, \tau_1) & \cdots & G_0^\sigma(\tau_n, \tau_n) - \alpha_\sigma(s_n) \end{pmatrix}$$

Note: $\alpha_\sigma(s) = \left[1/2 - \sigma s \delta\right]$

$$\frac{\mathrm{Tr}\left[e^{-\beta H}\right]}{\mathrm{Tr}\left[e^{-\beta H_0}\right]} = \underbrace{\sum_n \int_0^\beta d\tau_1 \sum_{s_1} \cdots \int_0^{\tau_{n-1}} d\tau_n \sum_{s_n}}_{\textit{Sum} \text{ with Monte Carlo}} \underbrace{\left(-\frac{U}{2}\right)^n \det\left[M_n\left(\tau_1, s_1 \cdots, \tau_n, s_n\right)\right]}_{\text{Weight}}$$

Importance sampling (See notes Appendix A)

Configuration C: set of n-vertices at imaginary times $\left[\tau_1,s_1\right]\left[\tau_2,s_2\right]\cdots,\left[\tau_n,s_n\right]$



$\left[\tau_1,s_1\right]\left[\tau_2,s_2\right]\left[\tau_3,s_3\right]$

$$\frac{\mathrm{Tr}\left[e^{-\beta H}\right]}{\mathrm{Tr}\left[e^{-\beta H_0}\right]} = \underbrace{\sum_n \int_0^\beta d\tau_1 \sum_{s_1} \cdots \int_0^{\tau_{n-1}} d\tau_n \sum_{s_n}}_{\textit{Sum}\text{ with Monte Carlo}} \underbrace{\left(-\frac{U}{2}\right)^n \det\left[M_n\left(\tau_1, s_1 \cdots, \tau_n, s_n\right)\right]}_{\text{Weight}}$$

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Configuration C: set of n-vertices at imaginary times $[\tau_1, s_1][\tau_2, s_2]\cdots,[\tau_n, s_n]$

Importance sampling produces a (Monte Carlo) time series of configurations.

Transition Prob. $P_{C\to C'} = \min\left(\frac{T^0_{C'\to C} W(C')}{T^0_{C\to C'} W(C)}, 1\right)$ → C_N, C_{N-1}, ……, C_2, C_1

In this time series, the configuration C occurs with probability: $P(C) = \frac{W(C)}{\sum_C W(C)}$

$$\langle O \rangle = \frac{\sum_C W(C) O(C)}{\sum_C W(C)} = \frac{1}{N}\sum_{n=1}^{N} O(C_n) \pm \sqrt{\frac{\left\langle \left(O - \langle O \rangle\right)^2 \right\rangle}{N}}$$

Assumptions

1) The moves are ergodic
2) The configurations C_i are statistically independent
3) The variance exits

→ Irrespective on the dimension of the configuration space the precision scales as $1/\sqrt{\mathrm{CPU}}$

See notes, Appendix A

$$\frac{\mathrm{Tr}\left[e^{-\beta H}\right]}{\mathrm{Tr}\left[e^{-\beta H_0}\right]} = \underbrace{\sum_{n} \int_0^{\beta} d\tau_1 \sum_{s_1} \cdots \int_0^{\tau_{n-1}} d\tau_n \sum_{s_n}}_{\textit{Sum} \text{ with Monte Carlo}} \underbrace{\left(-\frac{U}{2}\right)^n \det\left[M_n\left(\tau_1, s_1 \cdots, \tau_n, s_n\right)\right]}_{\text{Weight}}$$

Importance sampling (See notes Appendix A)

→ Importance of high precision tests. L=2, βt=10, U/t=2

Double occupancy: 0.378765 +/- 0.000050, Exact: 0.378732

Double occupancy: 0.378564 +/- 0.000027

(Bad random number generator!)

$$\langle O \rangle = \frac{\sum_C W(C) O(C)}{\sum_C W(C)} = \frac{1}{N}\sum_{n=1}^{N} O(C_n) \pm \sqrt{\frac{\left\langle \left(O - \langle O \rangle\right)^2 \right\rangle}{N}}$$

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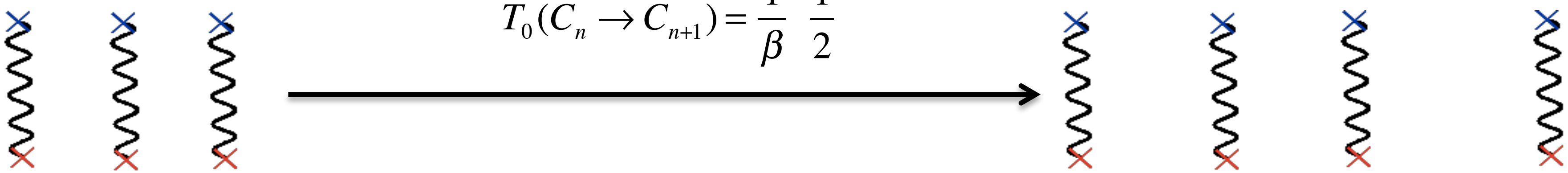
Importance sampling (See notes Appendix A)

$$P_{C\to C'} = \min\left(\frac{T^0_{C'\to C} W(C')}{T^0_{C\to C'} W(C)}, 1\right)$$

Adding

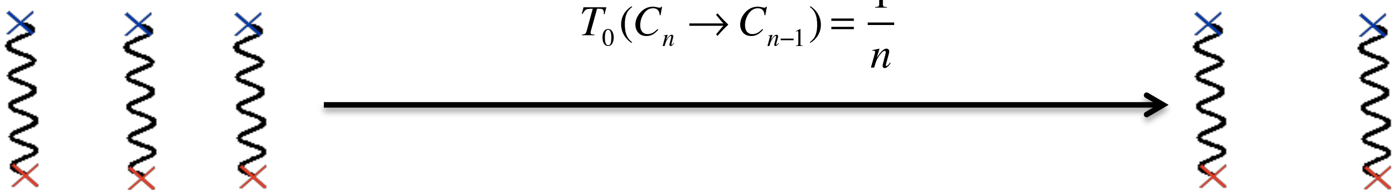
$$T_0(C_n \to C_{n+1}) = \frac{1}{\beta}\,\frac{1}{2}$$



$[\tau_1, s_1][\tau_2, s_2][\tau_3, s_3]$ $\longrightarrow$ $[\tau_1, s_1][\tau_2, s_2][\tau_3, s_3],\quad [\tau_4, s_4]$

Removing

$$T_0(C_n \to C_{n-1}) = \frac{1}{n}$$



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$$\frac{\mathrm{Tr}\left[e^{-\beta H}\right]}{\mathrm{Tr}\left[e^{-\beta H_0}\right]} = \underbrace{\sum_n \int_0^\beta d\tau_1 \sum_{s_1} \cdots \int_0^{\tau_{n-1}} d\tau_n \sum_{s_n}}_{\textit{Sum}\text{ with Monte Carlo}} \underbrace{\left(-\frac{U}{2}\right)^n \det\left[M_n\left(\tau_1, s_1 \cdots, \tau_n, s_n\right)\right]}_{\text{Weight}}$$

Importance sampling (See notes Appendix A)

$$P_{C\to C'} = \min\left(\frac{T^0_{C'\to C} W(C')}{T^0_{C\to C'} W(C)}, 1\right)$$

$$P_{C_n\to C_{n+1}} = \min\left(-\frac{U\beta}{(n+1)} \frac{\prod_\sigma \det \mathbf{M}_\sigma(C_{n+1})}{\prod_\sigma \det \mathbf{M}_\sigma(C_n)}, 1\right)$$

$$P_{C_{n+1}\to C_n} = \min\left(-\frac{(n+1)}{U\beta} \frac{\prod_\sigma \det \mathbf{M}_\sigma(C_n)}{\prod_\sigma \det \mathbf{M}_\sigma(C_{n+1})}, 1\right)$$

Thus, to accept or remove a move we have to compute the ratio of two determinants.

Useful identities:

(1) $$(\mathbf{A}+\mathbf{u}\otimes\mathbf{v})^{-1}=\mathbf{A}^{-1}-\frac{\mathbf{A}^{-1}\mathbf{u}\otimes\mathbf{v}\mathbf{A}^{-1}}{1+\mathbf{v}\cdot\mathbf{A}^{-1}\mathbf{u}}$$

$A\in\mathbb{C}^{n\times n},\ u\in\mathbb{C}^{n},\ v\in\mathbb{C}^{n}$

$u\otimes v\in\mathbb{C}^{n\times n},\ (u\otimes v)_{i,j}=u_i v_j$

$u\bullet v=\sum_i u_i v_i$

(2) $$\det(\mathbf{A}+\mathbf{u}\otimes\mathbf{v})=\det(\mathbf{A})\left(1+\mathbf{v}\cdot\mathbf{A}^{-1}\mathbf{u}\right)$$

From (1) and (2) follows

$$\det\left(\mathbf{A}+\mathbf{u}_1\otimes\mathbf{v}_1+\mathbf{u}_2\otimes\mathbf{v}_2\right)=$$
$$\det(\mathbf{A})\left[\left(1+\mathbf{v}_1\cdot\mathbf{A}^{-1}\mathbf{u}_1\right)\left(1+\mathbf{v}_2\cdot\mathbf{A}^{-1}\mathbf{u}_2\right)-\left(\mathbf{v}_2\cdot\mathbf{A}^{-1}\mathbf{u}_1\right)\left(\mathbf{v}_1\cdot\mathbf{A}^{-1}\mathbf{u}_2\right)\right]$$

Adding a Vertex

$$\frac{\det \mathbf{M}_\sigma(C_{n+1})}{\det \mathbf{M}_\sigma(C_n)} = \frac{\det \begin{pmatrix} \mathbf{M}_\sigma(C_n) & & & \begin{matrix} g_0(\tau_1,\tau') \\ \vdots \\ g_0(\tau_n,\tau') \end{matrix} \\ g_0(\tau',\tau_1) & \ldots & g_0(\tau',\tau_n) & g_0(\tau',\tau') - \alpha_\sigma(s') \end{pmatrix}}{\det \mathbf{M}_\sigma(C_n)}$$

$$= \frac{\det \left(\begin{pmatrix} \mathbf{M}_\sigma(C_n) & & \begin{matrix} 0 \\ \vdots \\ 0 \end{matrix} \\ 0 & \ldots 0 & 1 \end{pmatrix} + \mathbf{u}_1 \otimes \mathbf{v}_1 + \mathbf{u}_2 \otimes \mathbf{v}_2 \right)}{\det \mathbf{M}_\sigma(C_n)}$$

with

$$\mathbf{u}_1 = (g_0(\tau_1,\tau'), \ldots, g_0(\tau_n,\tau'), g_0(\tau',\tau') - \alpha_\sigma(s') - 1)\,, \quad (\mathbf{v}_1)_i = \delta_{i,n+1}$$

and

$$(\mathbf{u}_2)_i = \delta_{i,n+1}, \quad \mathbf{v}_2 = (g_0(\tau',\tau_1), \ldots, g_0(\tau',\tau_n), 0).$$

$$\frac{\det \mathbf{M}_\sigma(C_{n+1})}{\det \mathbf{M}_\sigma(C_n)} = g_0(\tau',\tau') - \alpha_\sigma(s') - \sum_{i,j=1}^{n} g_0(\tau',\tau_i) \left[M_\sigma^{-1}(C_n) \right]_{i,j} g_0(\tau_j,\tau')\,.$$

If $M^{-1}(C_n)$ is known then computing the ratio involves n^2 operations.

Removing a Vertex

$$\frac{\det \mathbf{M}_\sigma(C_{n-1})}{\det \mathbf{M}_\sigma(C_n)} = \frac{\det \begin{pmatrix} g_0(\tau_1,\tau_1)-\alpha_\sigma(s_1) & \dots & g_0(\tau_1,\tau_{n-1}) & 0 \\ \vdots & & \vdots & \vdots \\ g_0(\tau_{n-1},\tau_1) & \dots & g_0(\tau_{n-1},\tau_{n-1})-\alpha_\sigma(s_{n-1}) & 0 \\ 0 & \dots & 0 & 1 \end{pmatrix}}{\det \mathbf{M}_\sigma(C_n)}$$

$$= \frac{\det\left[\mathbf{M}_\sigma(C_n) + \mathbf{u}_1 \otimes \mathbf{v}_1 + \mathbf{u}_2 \otimes \mathbf{v}_2\right]}{\det \mathbf{M}_\sigma(C_n)}$$

with

$$\mathbf{u}_1 = -\Big(\left[M_\sigma(C_n)\right]_{1,n}, \dots, \left[M_\sigma(C_n)\right]_{n,n} - 1\Big), \quad (\mathbf{v}_1)_i = \delta_{i,n}$$

and

$$(\mathbf{u}_2)_i = \delta_{i,n}, \quad \mathbf{v}_2 = -\Big(\left[M_\sigma(C_n)\right]_{n,1}, \dots, \left[M_\sigma(C_n)\right]_{n,n-1}, 0\Big).$$

$$\frac{\det \mathbf{M}_\sigma(C_{n-1})}{\det \mathbf{M}_\sigma(C_n)} = \left[M_\sigma^{-1}(C_n)\right]_{n,n}$$

If $M^{-1}(C_n)$ is known then computing the ratio is negligible.

Upgrading $M_\sigma^{-1}(C_{n\pm1})$

If the move is accepted then you have to upgrade $M_\sigma^{-1}(C_{n\pm1})$

But $$M_\sigma(C_{n\pm1}) = M_\sigma(C_n) + u_1^\pm \otimes v_1^\pm + u_2^\pm \otimes v_2^\pm$$

and $M_\sigma^{-1}(C_n)$ is present in memory.

→ Use $\left(\mathbf{A} + \mathbf{u} \otimes \mathbf{v}\right)^{-1} = \mathbf{A}^{-1} - \dfrac{\mathbf{A}^{-1}\mathbf{u} \otimes \mathbf{v}\mathbf{A}^{-1}}{1 + \mathbf{v} \cdot \mathbf{A}^{-1}\mathbf{u}}$ recursively to carry out the update.

→ Required number of operations n^2

What is the average expansion parameter?

Consider H = H_0 + H_1

$$\langle n \rangle = \frac{1}{Z}\sum_n \frac{(-1)^n n}{n!}\int_0^\beta \mathrm{d}\tau_1 \quad \cdots \quad \int_0^\beta \mathrm{d}\tau_n \, \langle T \hat{H}_1(\tau_1) \quad \cdots \quad \hat{H}_1(\tau_n)\rangle_0$$

(m=n-1)

$$= -\frac{1}{Z}\sum_m \frac{(-1)^m}{m!}\int_0^\beta \mathrm{d}\tau_1 \cdots \int_0^\beta \mathrm{d}\tau_m \int_0^\beta \mathrm{d}\tau \, \langle T \hat{H}_1(\tau_1)\cdots \hat{H}_1(\tau_m)\hat{H}_1(\tau)\rangle_0$$

$$= -\int_0^\beta \mathrm{d}\tau \langle \hat{H}_1(\tau)\rangle \; .$$

What is the average expansion parameter?

Consider $H = H_0 + H_1$

$$\langle n\rangle = \frac{1}{Z}\sum_n \frac{(-1)^n n}{n!}\int_0^\beta d\tau_1 \cdots \int_0^\beta d\tau_n \langle T\hat{H}_1(\tau_1) \cdots \hat{H}_1(\tau_n)\rangle_0$$

(m=n-1)

$$= -\frac{1}{Z}\sum_m \frac{(-1)^m}{m!}\int_0^\beta d\tau_1 \cdots \int_0^\beta d\tau_m \int_0^\beta d\tau \langle T\hat{H}_1(\tau_1)\cdots\hat{H}_1(\tau_m)\hat{H}_1(\tau)\rangle_0$$

$$= -\int_0^\beta d\tau \langle \hat{H}_1(\tau)\rangle .$$

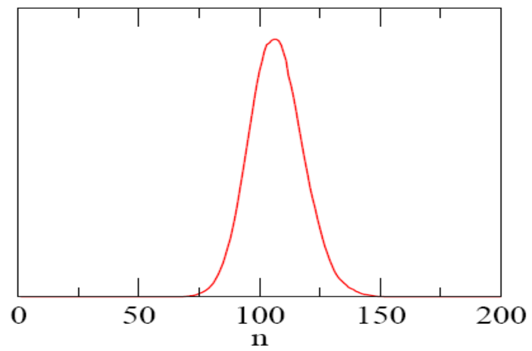
For

$$H_1 = H_U = \frac{U}{2}\sum_{s=\pm 1}\left(n_\uparrow^d - [1/2 - s\delta]\right)\left(n_\downarrow^d - [1/2 + s\delta]\right)$$

$$\langle n\rangle = -\beta U\left[\langle(\hat{n}_\uparrow - 1/2)(\hat{n}_\downarrow - 1/2)\rangle - \delta^2\right]$$

→ Time to update each vertex (a sweep) ~ n^3 ~ $(\beta U)^3$

What is the average expansion parameter?



Histogram of expansion parameter.

For

$$H_1 = H_U = \frac{U}{2} \sum_{s=\pm 1} \left(n_{\uparrow}{}^{d} - \left[1/2 - s\delta \right] \right) \left(n_{\downarrow}{}^{d} - \left[1/2 + s\delta \right] \right)$$

$$\langle n \rangle = -\beta U \left[\langle (\hat{n}_{\uparrow} - 1/2)(\hat{n}_{\downarrow} - 1/2) \rangle - \delta^2 \right]$$

→ Time to update each vertex (a sweep) ~ n^3 ~ $(\beta U)^3$

$$\frac{\mathrm{Tr}\left[e^{-\beta H}\right]}{\mathrm{Tr}\left[e^{-\beta H_0}\right]} = \underbrace{\sum_n \int_0^\beta d\tau_1 \sum_{s_1} \cdots \int_0^{\tau_{n-1}} d\tau_n \sum_{s_n}}_{\equiv \sum_C} \underbrace{(-1)^n \left\langle T\; H_U\left[\tau_1, s_1\right] \cdots H_U\left[\tau_n, s_n\right] \right\rangle_0}_{\equiv W(C)}$$

$$H_U\left[\tau_1, s_1\right] = \frac{U}{2}\left[n_\uparrow(\tau_1) - \alpha_\uparrow(s_1)\right]\left[n_\downarrow(\tau_1) - \alpha_\downarrow(s_1)\right]$$

Measurements.

$$G^\sigma(\tau,\tau') \equiv \left\langle T\, \hat{d}^+_\sigma(\tau) \hat{d}_\sigma(\tau') \right\rangle = \frac{\sum_C (-1)^n \left\langle T\; H_U\left[\tau_1, s_1\right] \cdots H_U\left[\tau_n, s_n\right]\; \hat{d}^+_\sigma(\tau) \hat{d}_\sigma(\tau') \right\rangle_0}{\sum_C W(C)} = \frac{\sum_C W(C)\, G^\sigma_C(\tau,\tau')}{\sum_C W(C)}$$

$$G^\sigma{}_C(\tau,\tau') \equiv \frac{\left\langle T\; H_U\left[\tau_1, s_1\right] \cdots H_U\left[\tau_n, s_n\right]\; \hat{d}^+_\sigma(\tau) \hat{d}_\sigma(\tau') \right\rangle_0}{\left\langle T\; H_U\left[\tau_1, s_1\right] \cdots H_U\left[\tau_n, s_n\right] \right\rangle_0} = G^\sigma{}_0(\tau,\tau') - \sum_{\alpha,\beta=1}^{n} G^\sigma{}_0(\tau,\tau_\alpha) \left(M^\sigma{}_n{}^{-1}\right)_{\alpha\beta} G^\sigma{}_0(\tau_\beta,\tau')$$

$$G^{\sigma}{}_{C}(\tau,\tau') \equiv \frac{\left\langle T\ H_U\left[\tau_1,s_1\right]\cdots H_U\left[\tau_n,s_n\right]\ \hat{d}^{+}_{\sigma}(\tau)\hat{d}_{\sigma}(\tau')\right\rangle_0}{\left\langle T\ H_U\left[\tau_1,s_1\right]\cdots H_U\left[\tau_n,s_n\right]\right\rangle_0} = G^{\sigma}{}_{0}(\tau,\tau') - \sum_{\alpha,\beta=1}^{n} G^{\sigma}{}_{0}(\tau,\tau_\alpha)\left(M^{\sigma}{}_{n}{}^{-1}\right)_{\alpha\beta} G^{\sigma}{}_{0}(\tau_\beta,\tau')$$

Follows from:

$$\frac{\left\langle T\ H_U\left[\tau_1,s_1\right]\cdots H_U\left[\tau_n,s_n\right]\ \hat{d}^{+}_{\sigma}(\tau)\hat{d}_{\sigma}(\tau')\right\rangle_0}{\left\langle T\ H_U\left[\tau_1,s_1\right]\cdots H_U\left[\tau_n,s_n\right]\right\rangle_0} = \frac{\det\begin{pmatrix} M^{\sigma}(C_n) & \cdots & & G_0^{\sigma}(\tau_1,\tau') \\ & \ddots & & \vdots \\ & & & G_0^{\sigma}(\tau_n,\tau') \\ G_0^{\sigma}(\tau,\tau_1) & \cdots & G_0^{\sigma}(\tau,\tau_n) & G_0^{\sigma}(\tau\ ,\tau') \end{pmatrix}}{\det\left(M^{\sigma}(C_n)\right)}$$

$$= \frac{\det\left[\begin{pmatrix} M^{\sigma}(C_n) & \cdots & & 0 \\ & \ddots & & \vdots \\ & & & 0 \\ 0 & \cdots & 0 & 1 \end{pmatrix} + u_1 \otimes v_1 + u_2 \otimes v_2\right]}{\det\left(M^{\sigma}(C_n)\right)}$$

Use:

$$\det\left(\mathbf{A} + \mathbf{u}_1 \otimes \mathbf{v}_1 + \mathbf{u}_2 \otimes \mathbf{v}_2\right) =$$

$$\det(\mathbf{A})\left[\left(1 + \mathbf{v}_1 \cdot \mathbf{A}^{-1}\mathbf{u}_1\right)\left(1 + \mathbf{v}_2 \cdot \mathbf{A}^{-1}\mathbf{u}_2\right) - \left(\mathbf{v}_2 \cdot \mathbf{A}^{-1}\mathbf{u}_1\right)\left(\mathbf{v}_1 \cdot \mathbf{A}^{-1}\mathbf{u}_2\right)\right]$$

$$\frac{\mathrm{Tr}\left[e^{-\beta H}\right]}{\mathrm{Tr}\left[e^{-\beta H_0}\right]} = \underbrace{\sum_n \int_0^\beta d\tau_1 \sum_{s_1} \cdots \int_0^{\tau_{n-1}} d\tau_n \sum_{s_n}}_{\textit{Sum} \text{ with Monte Carlo}} \underbrace{\left(-\frac{U}{2}\right)^n \det\left[M_n\left(\tau_1, s_1 \cdots, \tau_n, s_n\right)\right]}_{\text{Weight}}$$

Measurements.

$$G^\sigma{}_C(\tau,\tau') \equiv \frac{\left\langle T\ H_U\left[\tau_1,s_1\right]\cdots H_U\left[\tau_n,s_n\right]\ \hat{d}^+_\sigma(\tau)\hat{d}_\sigma(\tau')\right\rangle_0}{\left\langle T\ H_U\left[\tau_1,s_1\right]\cdots H_U\left[\tau_n,s_n\right]\right\rangle_0} = G^\sigma{}_0(\tau,\tau') - \sum_{\alpha,\beta=1}^{n} G^\sigma{}_0(\tau,\tau_\alpha)\left(M^\sigma{}_n{}^{-1}\right)_{\alpha\beta} G^\sigma{}_0(\tau_\beta,\tau')$$

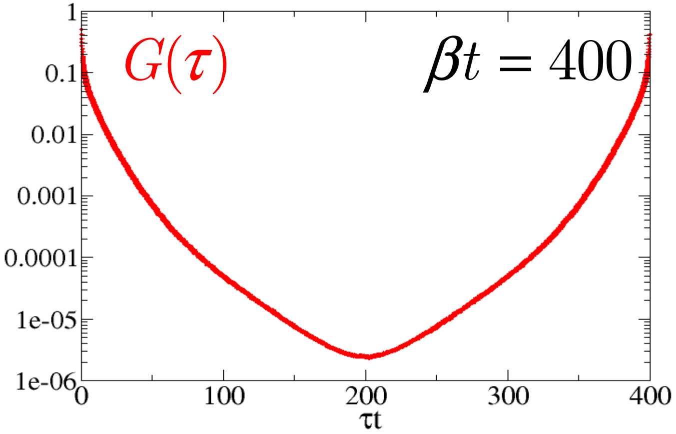
Wick theorem applies for each configuration C of vertices (See notes)

Direct calculation of Matsubara Green functions is possible

$$G^\sigma{}_C(i\omega_m) = G^\sigma{}_0(i\omega_m) - G^\sigma{}_0(i\omega_m)\sum_{\alpha,\beta=1}^{n} e^{-i\omega_m\tau_\alpha}\left(M^\sigma{}_n{}^{-1}\right)_{\alpha\beta} G^\sigma{}_0(\tau_\beta,0)$$

Examples.

a) Particle-hole symmetric Anderson Model, U/t=4.

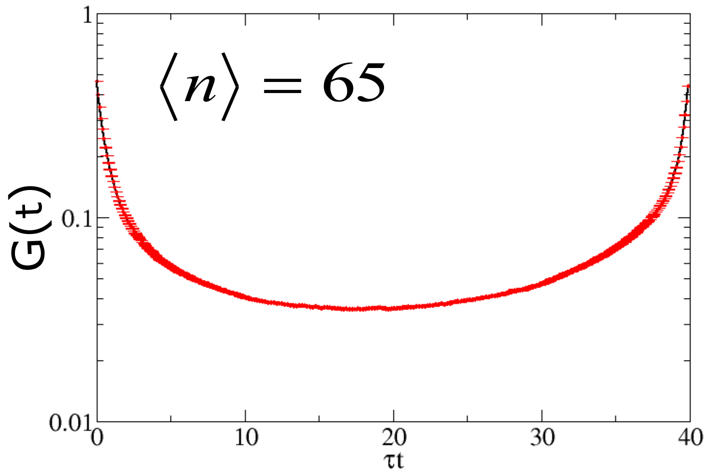


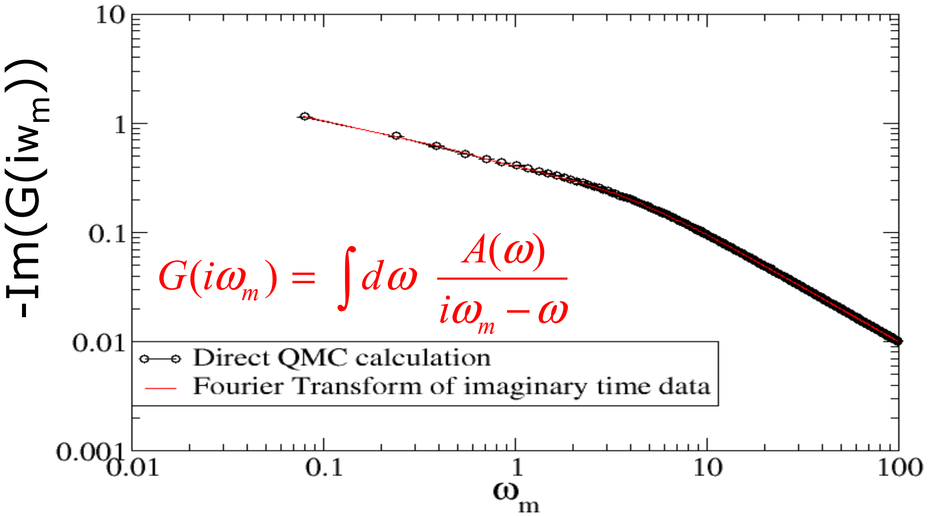
$$\langle n \rangle = 270$$

Hirsch-Fye: $L_{\text{Trot}} = 400/0.2 \quad (\Delta\tau t = 0.2)$

Speedup: $(2000/270)^3 \approx 400$

b) Off particle-hole Symmetry, U/t=4 βt=40.





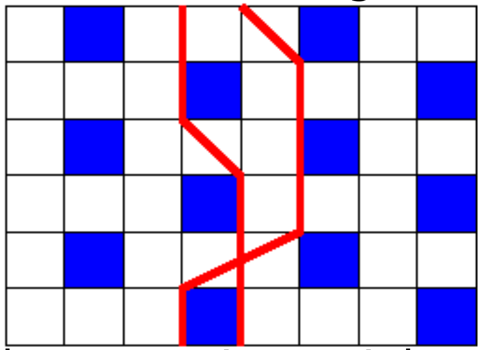
Speedup $(200/65)^3 \approx 30$

Direct calculation of $G(iw_m)$ is possible.

Sign problem – a simple example.

Consider: $H = -t_1 \sum_i c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i - t_2 \sum_i c_i^\dagger c_{i+2} + c_{i+2}^\dagger c_i, \quad t_1, t_2 > 0, \quad \{c_i^\dagger, c_j\} = \delta_{i,j}$

World line configuration:



has negative weight.

$$\langle O \rangle = \frac{\sum_c W(c) O(c)}{Z} \equiv \frac{\frac{1}{Z'} \sum_c |W(c)| \operatorname{sign}(c) O(c)}{Z/Z'}$$

$$Z = \sum_c W(c) \qquad Z' = \sum_c |W(c)| \ \text{ and } \ \operatorname{sign}(c) = W(c) / |W(c)|$$

But: Z´ is the partition function of H with fermions replaced by hard core bosons. Thus:

$$Z / Z' \approx e^{-\beta V \delta} \ \text{ with } \ \delta = \left(E_0^F - E_0^B\right) / V > 0$$

For practical purposes we will need:

$$\frac{\Delta(Z/Z')}{Z/Z'} << 1 \quad \text{but} \quad \Delta(Z/Z') \approx 1/\sqrt{\text{CPU}} \ \text{ so that CPU} >> \ e^{2\beta V \delta}$$

Note:

- Had we formulated everything in Fourier space........
- Hamiltonian H with $t_1>0$ and $t_2<0$ and hard core bosons yields a sign problem. This corresponds essentially to a frustrated spin chain. Thus the sign problem is not limited to fermionic systems.
- δ is formulation dependent.

Continuous-time QMC Solvers for Electronic Systems in Fermionic and Bosonic Baths

F.F. Assaad (DMFT@25, Juelich, September 2014)

Goal: Detailed overview of CT-INT.

Outline

- Weak coupling CT-QMC – Basics.
  – Add ons: Retarded interactions:
  phonon degrees of freedom.
- Selected applications. Topological insulators, electron-phonon interaction.
- Conclusions.

Julius-Maximilians-
UNIVERSITÄT
WÜRZBURG

Phonons (bosonic baths) Integrate out phonons in favor of a retarded interaction.

Hubbard-Holstein:

$$\hat{H} = \sum_{i,j,\sigma} t_{i,j}\ \hat{c}^{+}_{i,\sigma}\hat{c}_{j,\sigma} \quad + U\sum_{i}\hat{n}_{i,\uparrow}\hat{n}_{i,\downarrow} \ + g\sum_{i}\hat{Q}_{i}(\hat{n}_{i}-1) + \sum_{i}\frac{\hat{P}_{i}^{2}}{2M} + \frac{k}{2}\hat{Q}_{i}^{2}$$

Integrate out the phonons

$$Z = \int\left[dc^{+}dc\right]\ \exp\left[-S_{0} - U\int_{0}^{\beta} d\tau\ \ n_{i\uparrow}(\tau)n_{i\downarrow}(\tau)\ + \int_{0}^{\beta} d\tau \int_{0}^{\beta} d\tau' \sum_{i,j}[n_{i}(\tau)-1]D^{0}(i-j,\tau-\tau')[n_{j}(\tau')-1]\right]$$

$$D^{0}(i-j,\tau-\tau') = \delta_{i,j}\frac{g^{2}}{2k}P(\tau-\tau')$$

$$P(\tau) = \frac{\omega_{0}}{2(1-e^{-\beta\omega_{0}})}\left[e^{-|\tau|\omega_{0}} + e^{-(\beta-|\tau|)\omega_{0}}\right],\quad \omega_{0} = \sqrt{k/M}$$

Attractive, retarded interaction (time scale $1/w_0$).

Antiadiabatic limit: $\lim_{\omega_0\to\infty} P(\tau) = \delta(\tau)$ → Attractive Hubbard.

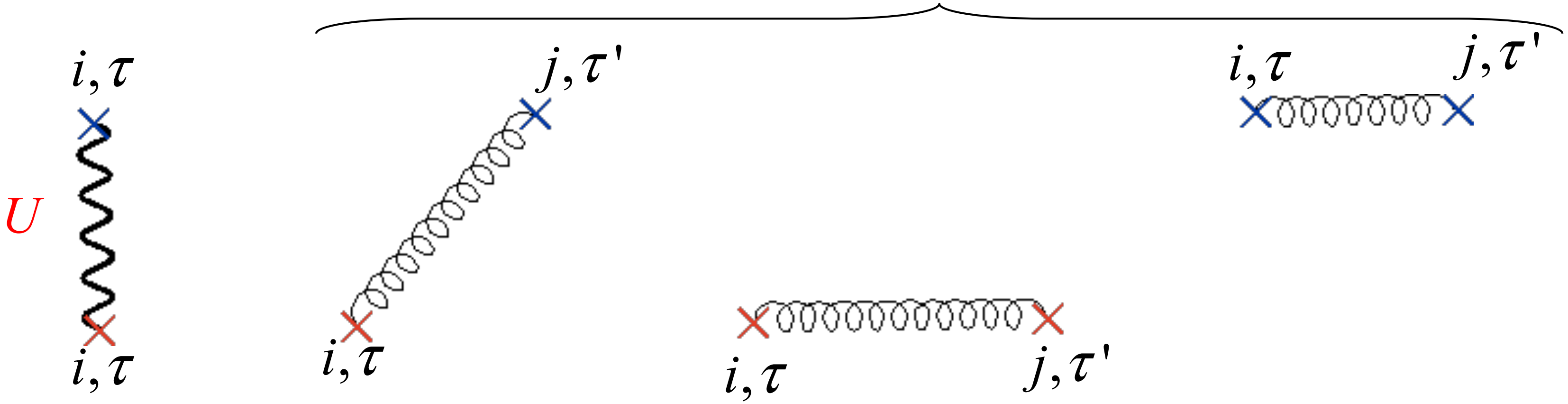
Phonons (bosonic baths) Integrate out phonons in favor of a retarded interaction.

$$Z = \int \left[dc^{+} dc \right] \exp\left[-S_0 - U \int_0^{\beta} d\tau \; n_{i\uparrow}(\tau) n_{i\downarrow}(\tau) \; + \; \int_0^{\beta} d\tau \int_0^{\beta} d\tau' \sum_{i,j} [n_i(\tau) - 1] D^0(i-j, \tau - \tau') [n_j(\tau') - 1] \right]$$

QMC: Expand both in Hubbard and retarded phonon interaction.

Vertices:

Hubbard. Phonon. $D^0(i-j, \tau-\tau')$



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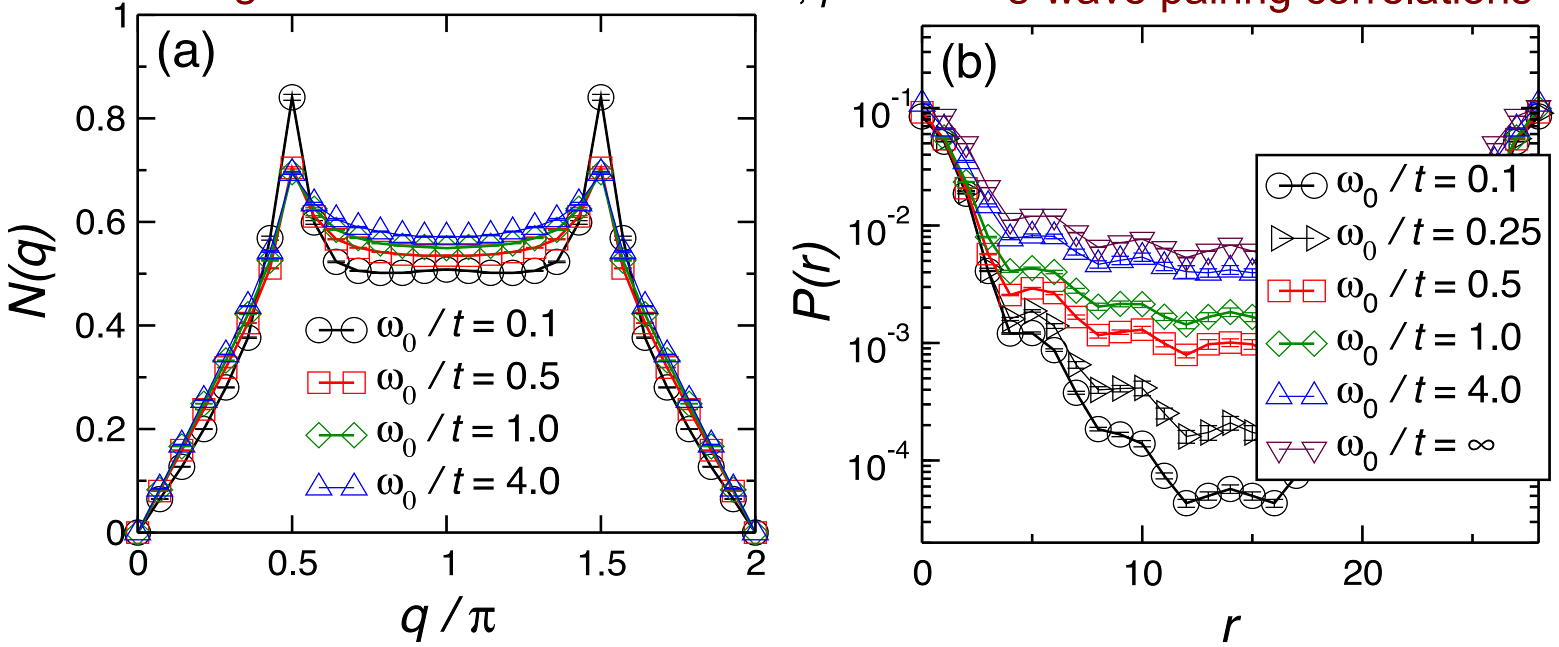
Bosonic Baths → Electron-phonon problems

M. Hohenadler, FFA. J. Phys.: Condens. Matter 25, 014005 (2013)

Peierls to superfluid crossover in the one-dimensional quarter filled Holstein model @ $g^2/Wk=0.35$

$$\hat{H} = \sum_{i,j,\sigma} t_{i,j}\, \hat{c}^{+}_{i,\sigma}\hat{c}_{j,\sigma} + g\sum_i \hat{Q}_i(\hat{n}_i - 1) + \sum_i \frac{\hat{P}_i^2}{2M} + \frac{k}{2}\hat{Q}_i^2, \qquad \omega_0 = \sqrt{\frac{k}{M}}$$

Charge correlation   L=28, βt=40   s-wave pairing correlations



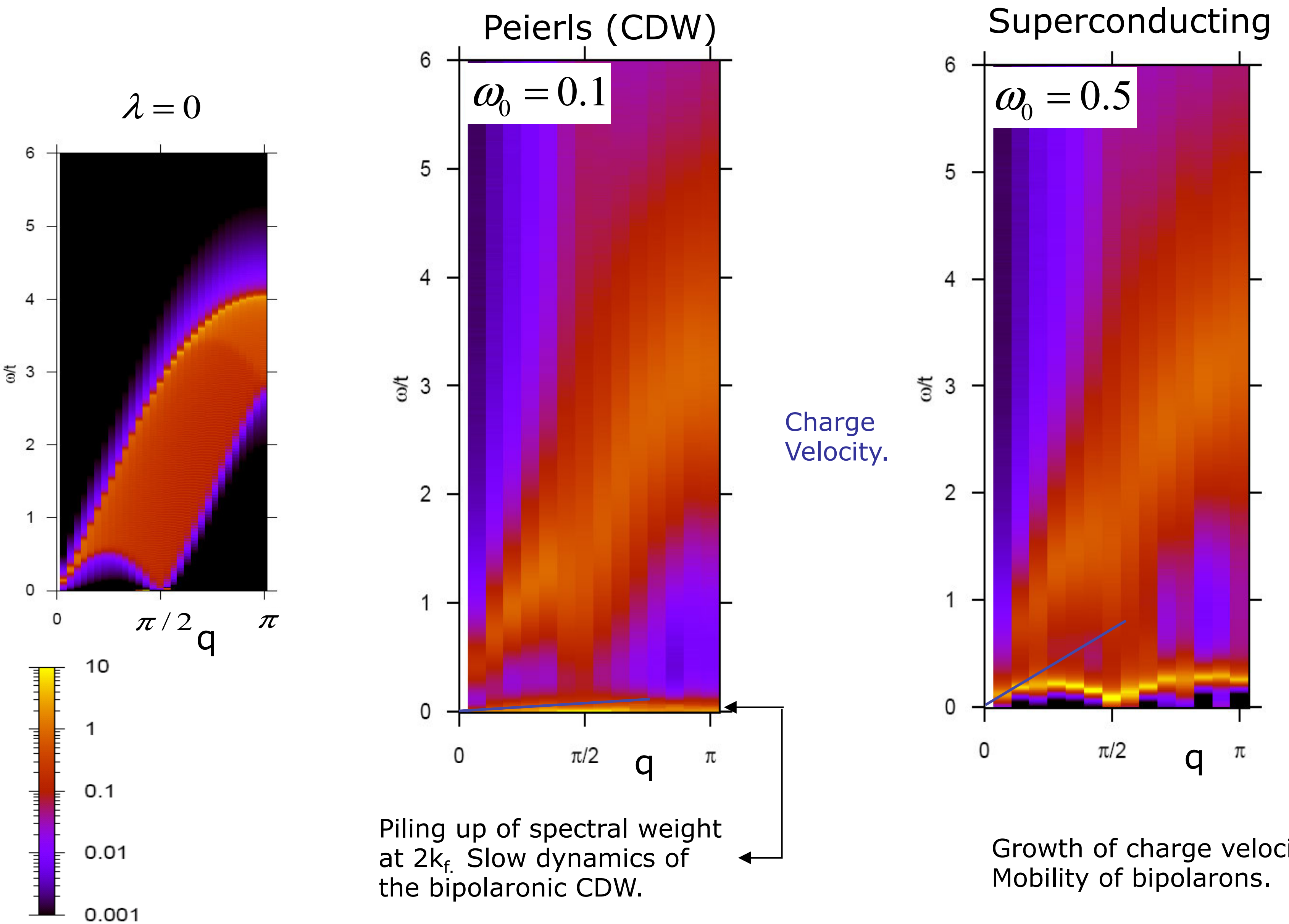
$\omega_0 << t$ Pairs of electrons form a commensurate CDW (diagonal LRO) → Peierls instability

$\omega_0 >> t$ Pairs condense to form an s-wave superconductor (off diagonal LRO).

Charge dynamical structure factor @ $\lambda/t = 0.35$

$$N(q,\omega) = \frac{1}{Z}\sum_{n,m} e^{-\beta E_m} \left|\langle n|\hat{n}\ (q)|m\rangle\right|^2 \delta(E_n - E_m - \omega)$$

$$\beta t = 40,\ \ \rho = 0.5$$



Piling up of spectral weight at $2k_{f.}$ Slow dynamics of the bipolaronic CDW.

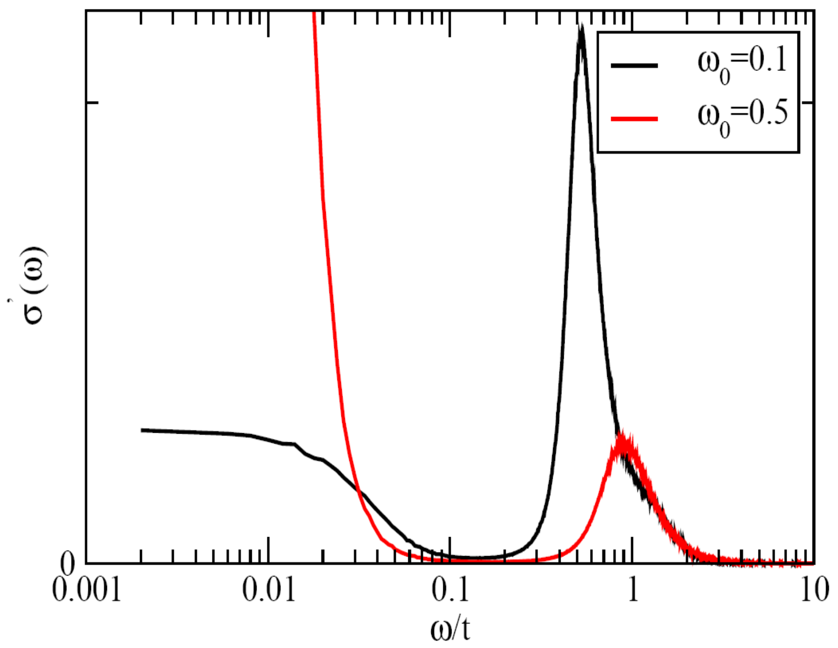
Growth of charge velocity. Mobility of bipolarons.

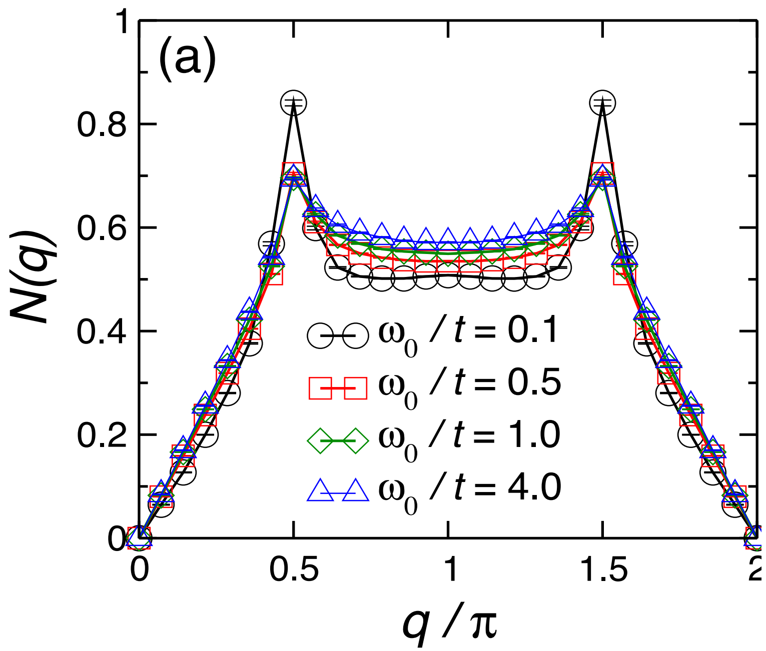
Optical Conductivity.

Continuity equation: $$\sigma'(\mathbf{q},\omega) = \frac{\omega}{\mathbf{q}^2}\left(1-e^{-\beta\omega}\right)N(\mathbf{q},\omega)$$

Long wavelength limit: $N(\mathbf{q},\omega) \approx N(\mathbf{q})\delta\left(v_c\mathbf{q}-\omega\right)$ with $N(\mathbf{q}) \approx \alpha\mathbf{q}$

$$\rightarrow \ \sigma'(\omega) = \lim_{\mathbf{q}\to 0}\sigma'(\mathbf{q},\omega) \approx \alpha v_c \delta(\omega)$$ at T=0.

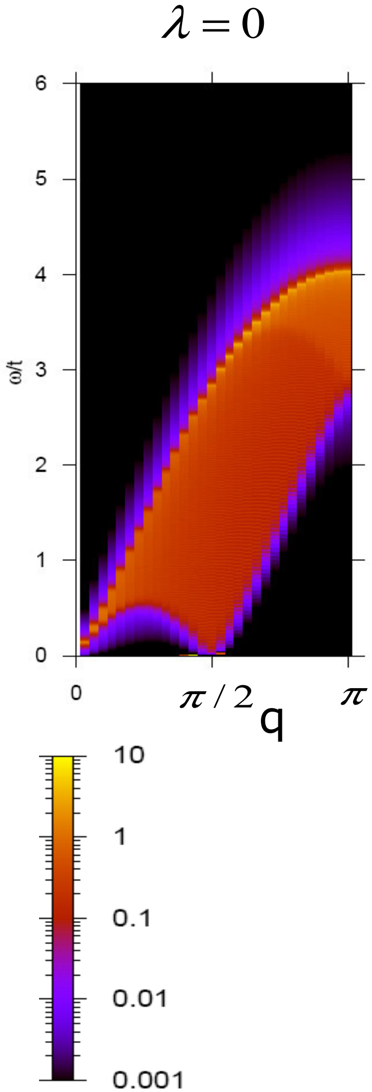


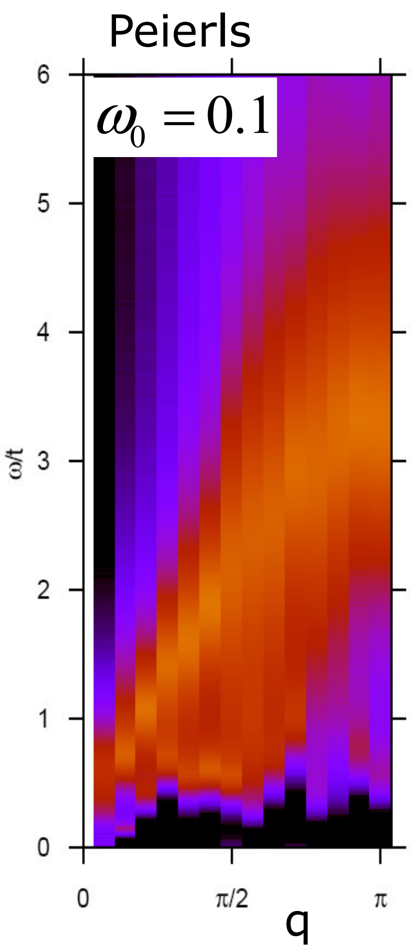


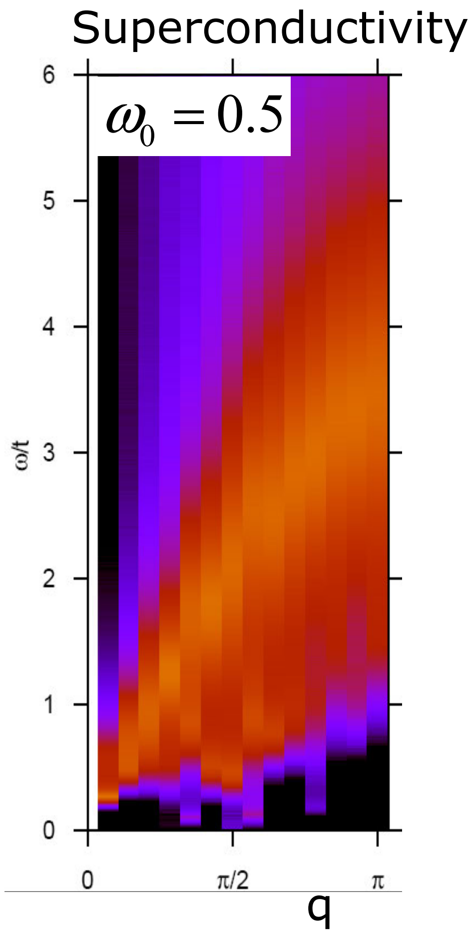
Spin dynamical structure factor @ λ/t =0.35

$$S(q,\omega)=\frac{1}{Z}\sum_{n,m} e^{-\beta E_m}\left|\langle n|\hat{S}_z(q)|m\rangle\right|^2 \delta(E_n-E_m-\omega)$$

$\beta t = 40, \ \rho = 0.5$







Suppression of low energy spectral weight.

Interpretation: $\Delta_{sp}>0$, $\Delta_c=0$

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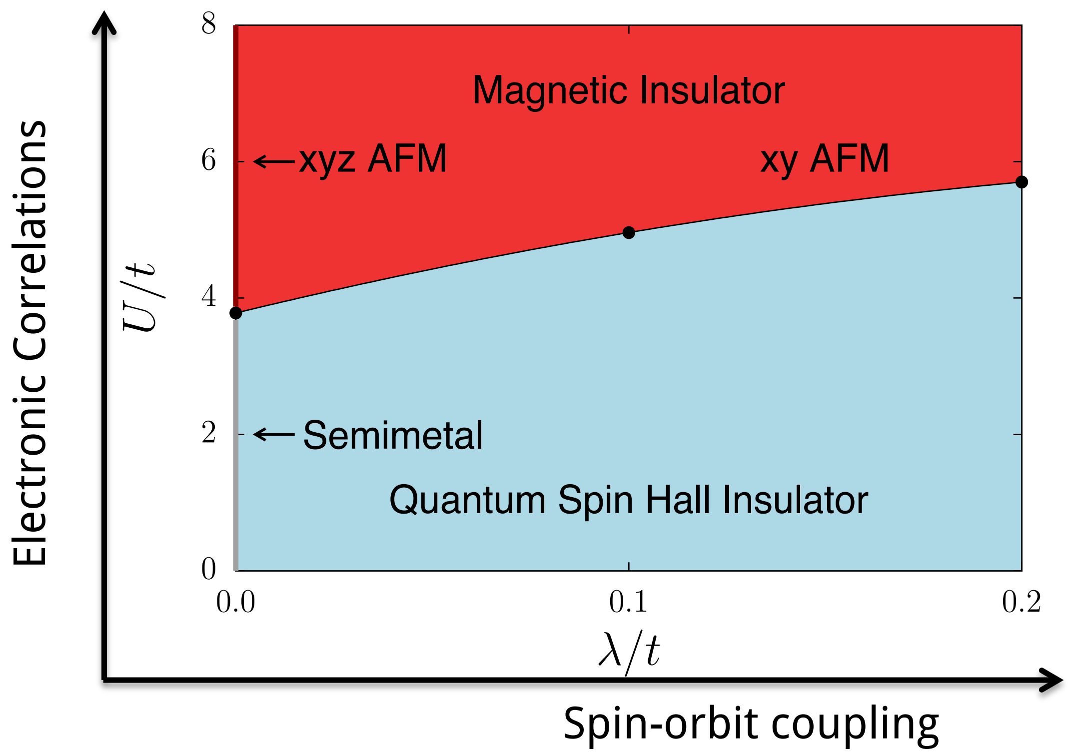
Fermionic Baths → Correlation effects on edge state of quantum Spin Hall states

Phases of the Kane Mele Hubbard model

S. Rachel & K. Le Hur, PRB 82, 075106, (2010)

M. Hohenadler et al. PRB 85 (2012)



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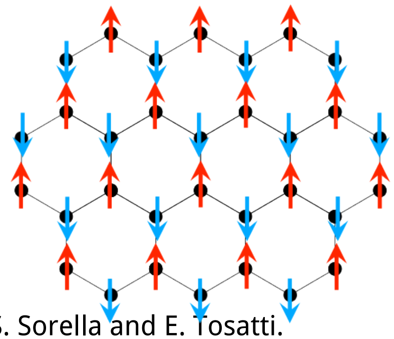


S. Sorella and E. Tosatti. EPL, 19, 699, (1992)

T. Paiva et al. Phys. Rev. B, 72, 085123 (2005)

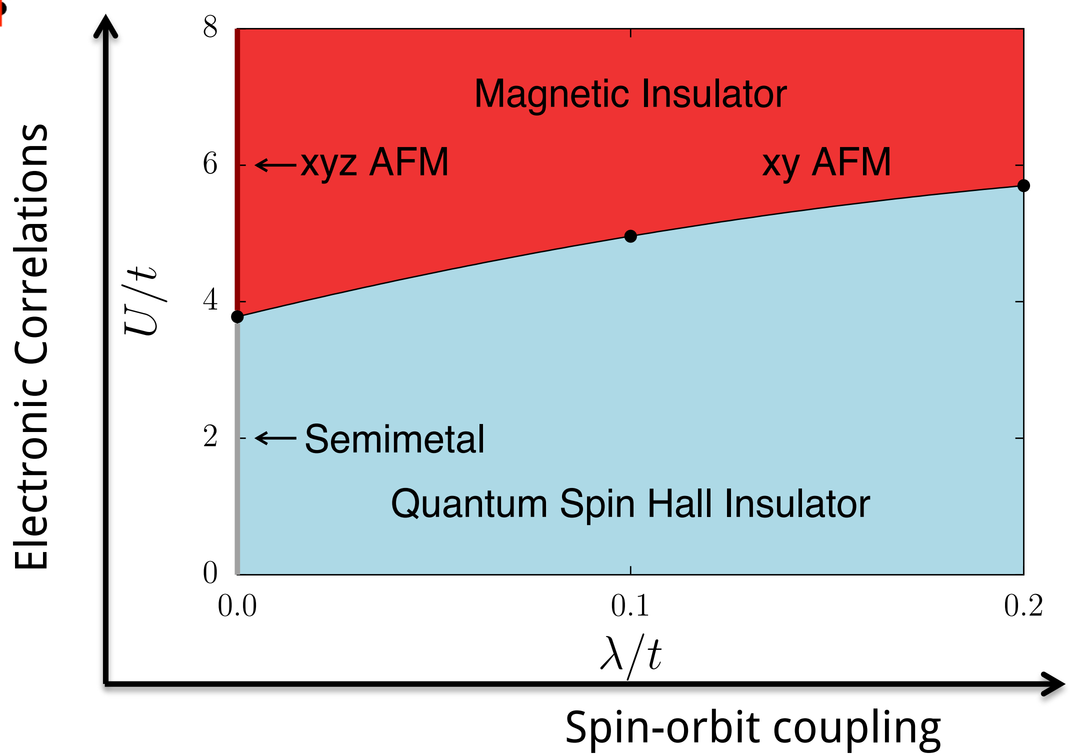
Z. Y. Meng et al. Nature 464, 847 (2010)

S. Sorella et al. Scientific Reports 2, 992 (2012)

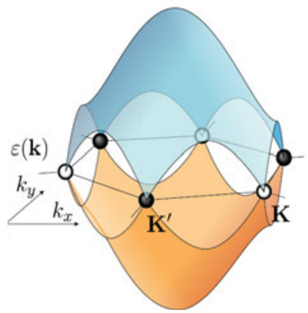
F. Assaad & I. Herbut PRX 3, 031010 (2013)

B. Clark arXiv:1305.0278

Antiferromagnetic
Mott insulator



Dirac fermions



Tight binding model on
Honeycomb lattice at
half-filling

Symmetries
SU(2) spin ✓
Sublattice ✓
Time reversal ✓

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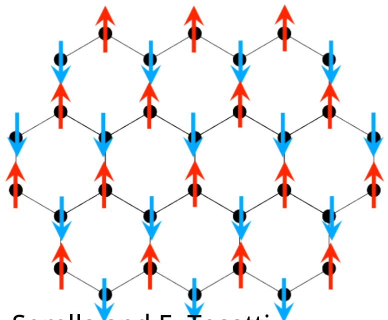

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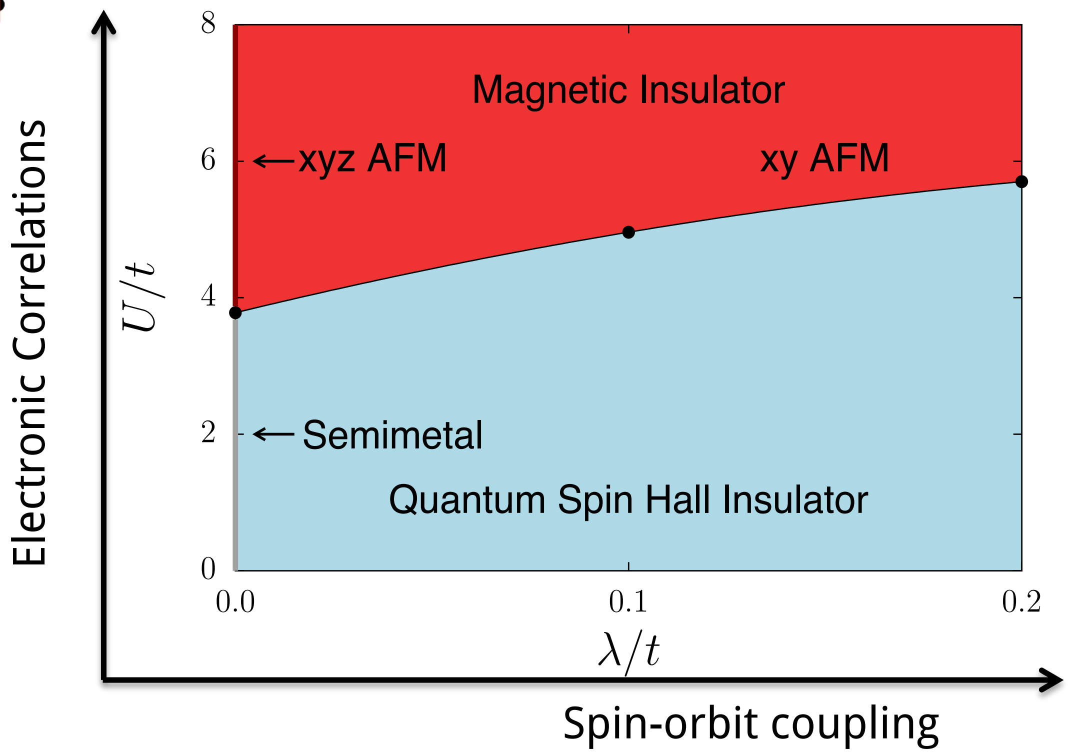
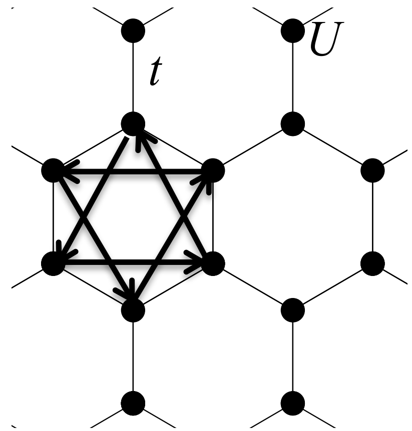
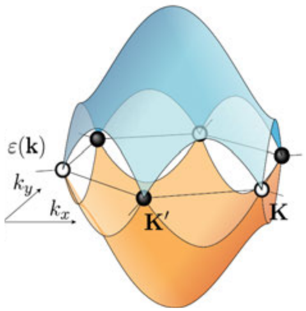


$$\overset{\mathbf{i}\qquad\quad\mathbf{j}}{\longrightarrow} = i\lambda\left(\hat{c}_{\mathbf{i}}^{\dagger}\sigma_z\hat{c}_{\mathbf{j}} - \hat{c}_{\mathbf{j}}^{\dagger}\sigma_z\hat{c}_{\mathbf{i}}\right)$$



Haldane model in each spin sector

Dirac fermions

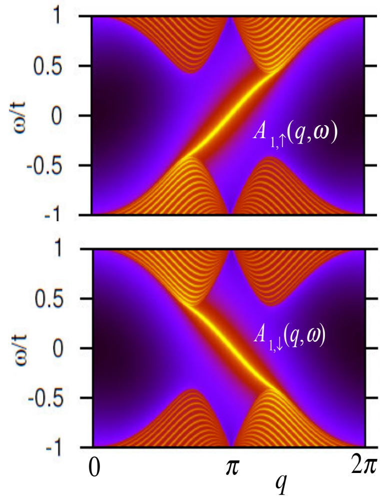


Tight binding model on Honeycomb lattice at half-filling

Symmetries
SU(2) spin ✓
Sublattice ✓
Time reversal ✓

SU(2) spin → U(1) spin
Sublattice ✗
Time reversal ✓

Opens gap → Quantum spin Hall with robust helical edge states.



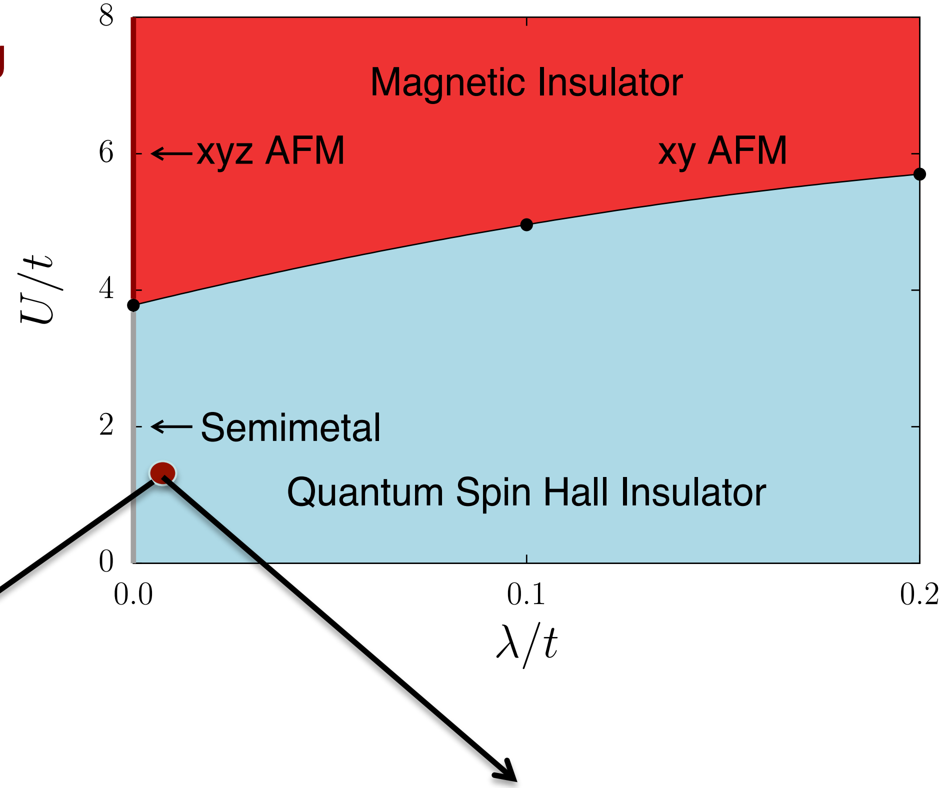
Fermionic Baths → Correlation effects on edge state of quantum Spin Hall states

Phases of the Kane Mele Hubbard model

S. Rachel & K. Le Hur, PRB 82, 075106, (2010)

M. Hohenadler et al. PRB 85 (2012)

Question: Elastic backward scattering is forbidden due to time reversal symmetry. What about inelastic scattering?

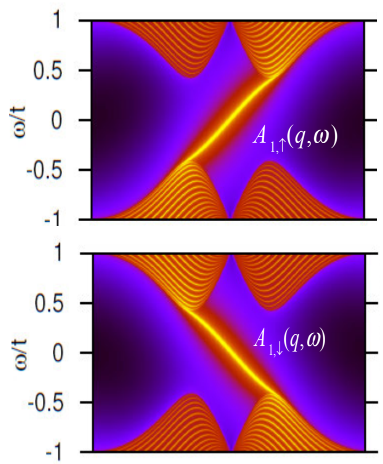


Bulk: U/W << 1

Ground state of bulk is well described by mean field

Edge: U/v_F >> 1 ($v_F \sim \lambda$)

Edge states are exponentially localized
Strongly correlated problem

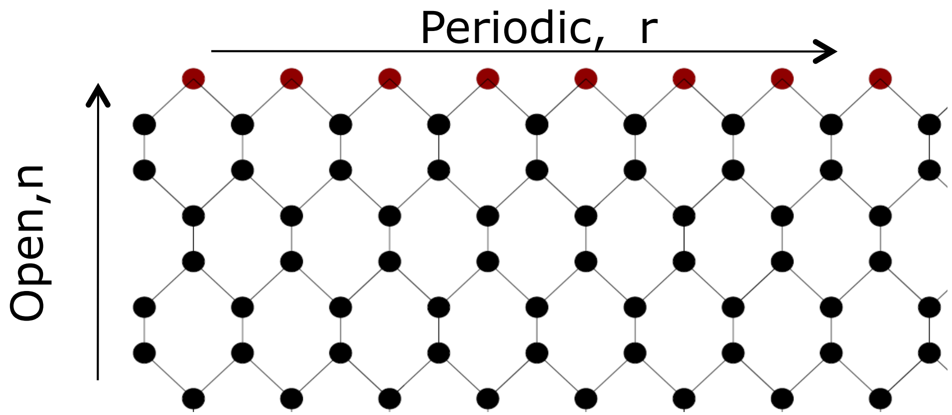


Fermionic Baths → Correlation effects on edge state of quantum Spin Hall states

M. Hohenadler, T. C. Lang and F. F. Assaad
Phys. Rev. Lett. 106, 100403 (2011)

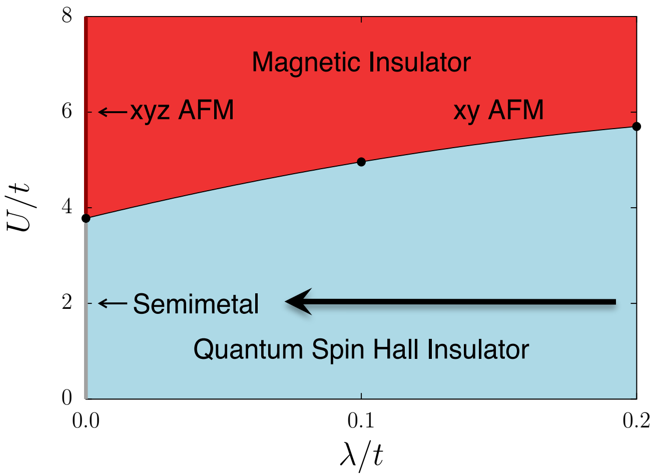
M. Hohenadler and F. F. Assaad
Phys. Rev. B 85, 081106(R) (2012)

→ Paramagnetic mean field for bulk. Retain all the fluctuations on the edge.



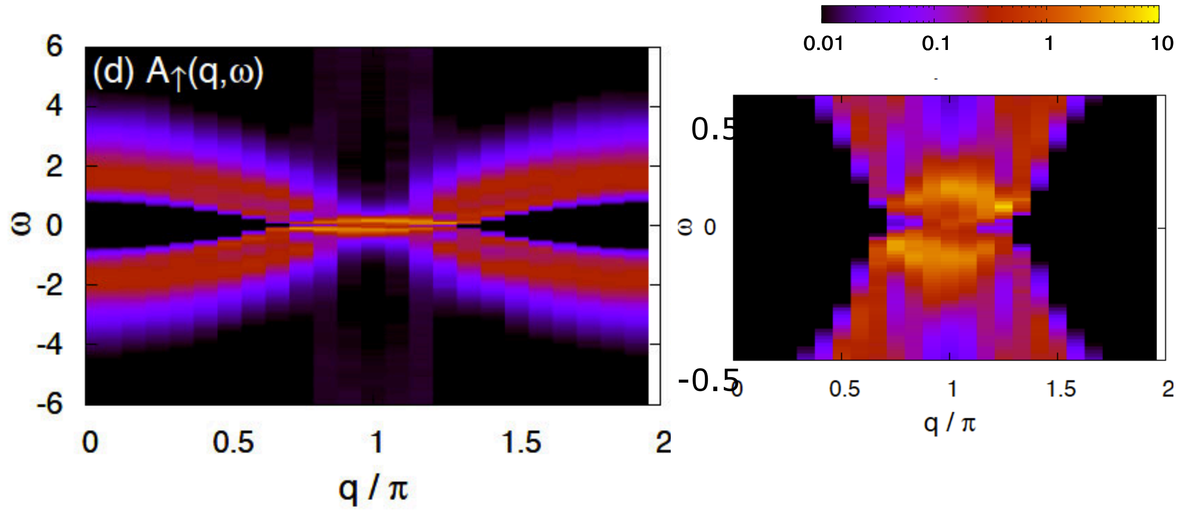
$$S = \int_0^\beta d\tau \int_0^\beta d\tau' \sum_{r,r',\sigma} c^\dagger_{r,\sigma}(\tau) \underbrace{G^{-1}_{0,\sigma}(r-r',\tau-\tau')}_{\text{Green function of the model on the ribbon (e.g. paramagnetic mean-field)}} c_{r',\sigma}(\tau') + U\int_0^\beta d\tau \sum_r \left(n_{r,\uparrow}(\tau)-\frac{1}{2}\right)\left(n_{r,\downarrow}(\tau)-\frac{1}{2}\right)$$

Fermionic Baths → Correlation effects on edge state of quantum Spin Hall states



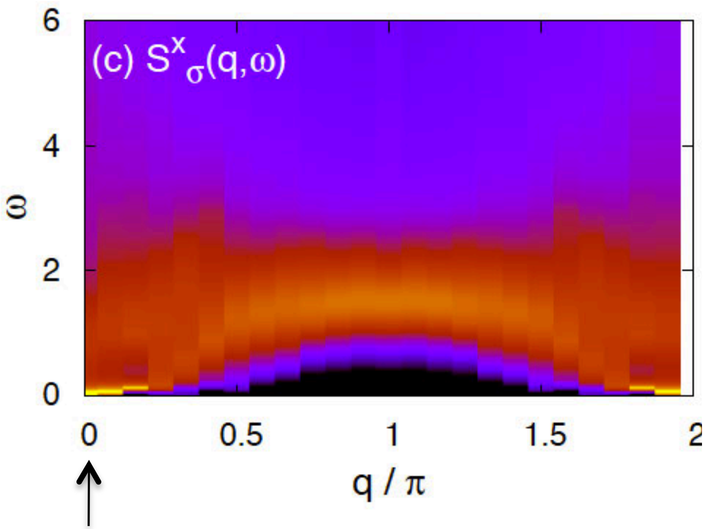
Single particle spectral function

Strong coupling: $\lambda / t = 0.05, U / t = 2$



Dynamic spin-structure factor

at $\lambda / t = 0.1, U / t = 2$



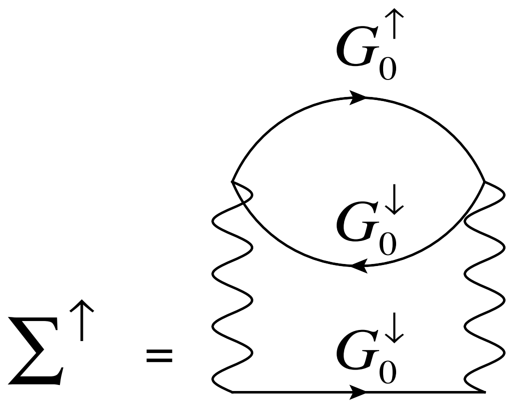
$2k_f$

$$S^x_\sigma(q,\omega) = \frac{1}{Z}\sum_{n,m} e^{-\beta E_n} \left|\langle m | S^x(q) | n \rangle\right|^2 \delta(E_m - E_n - \omega)$$

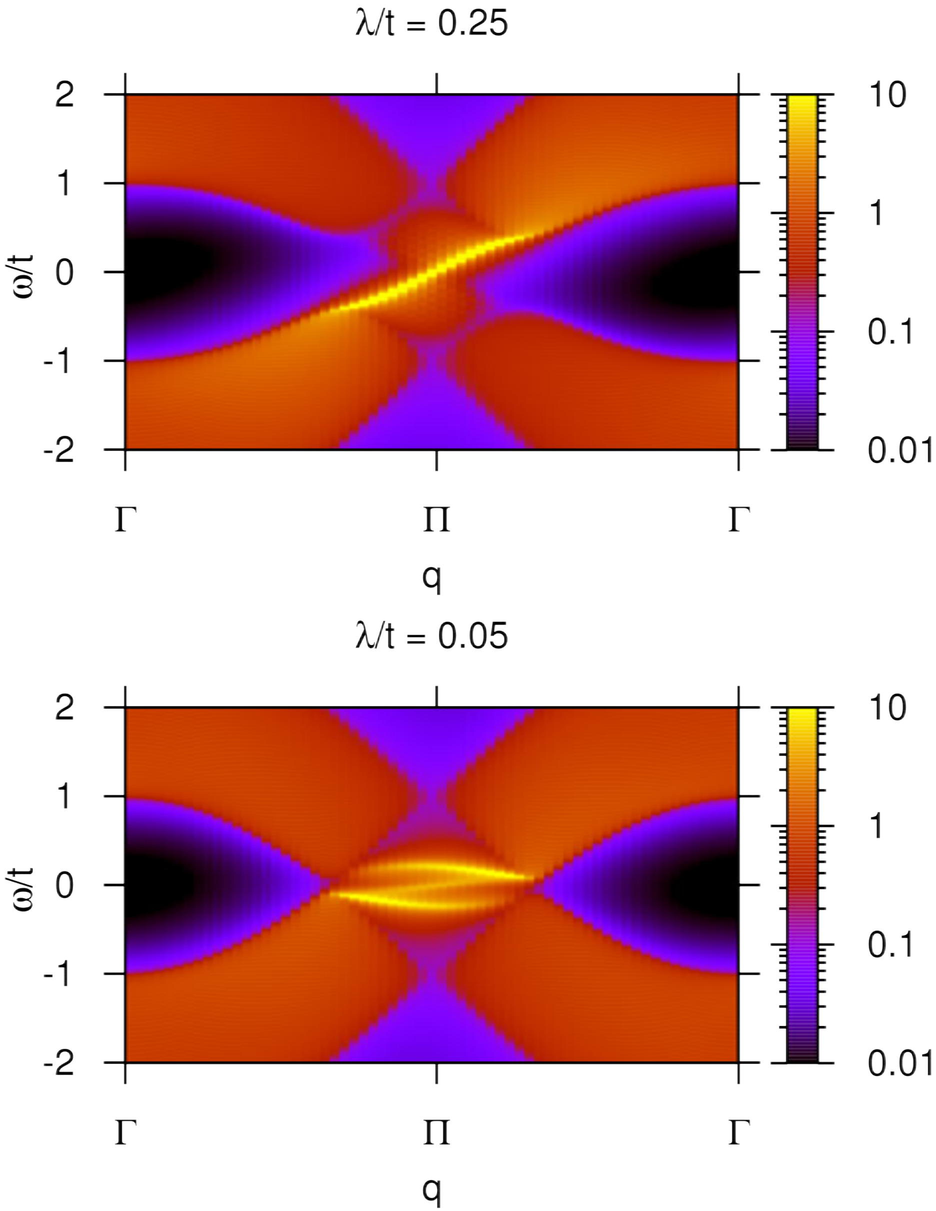
→ Inelastic scattering between left (spin do) and right (spin up) movers reduces substantially the spectral weight of the helical edge state.

$$H_U = -\frac{U}{2}\sum_q S_q^+ S_q^- + S_q^- S_q^+$$

Second order perturbation theory.



Single particle spectral function U/t=2



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- Weak coupling CT-QMC – Basics.
  – Add ons: Retarded interactions:
  phonon degrees of freedom.
- Selected applications. Topological insulators, electron-phonon interaction.
- Conclusions.

CT-INT is a very flexible action based QMC method which allows to tackle correlated electron problems embedded in fermionic and bosonic baths. In the absence of negative sign problem, it scales polynomially in the number of interacting degrees of freedom.