Continuous-time Quantum Monte Carlo - Hybridization-expansion Algorithm for Fermions (I)

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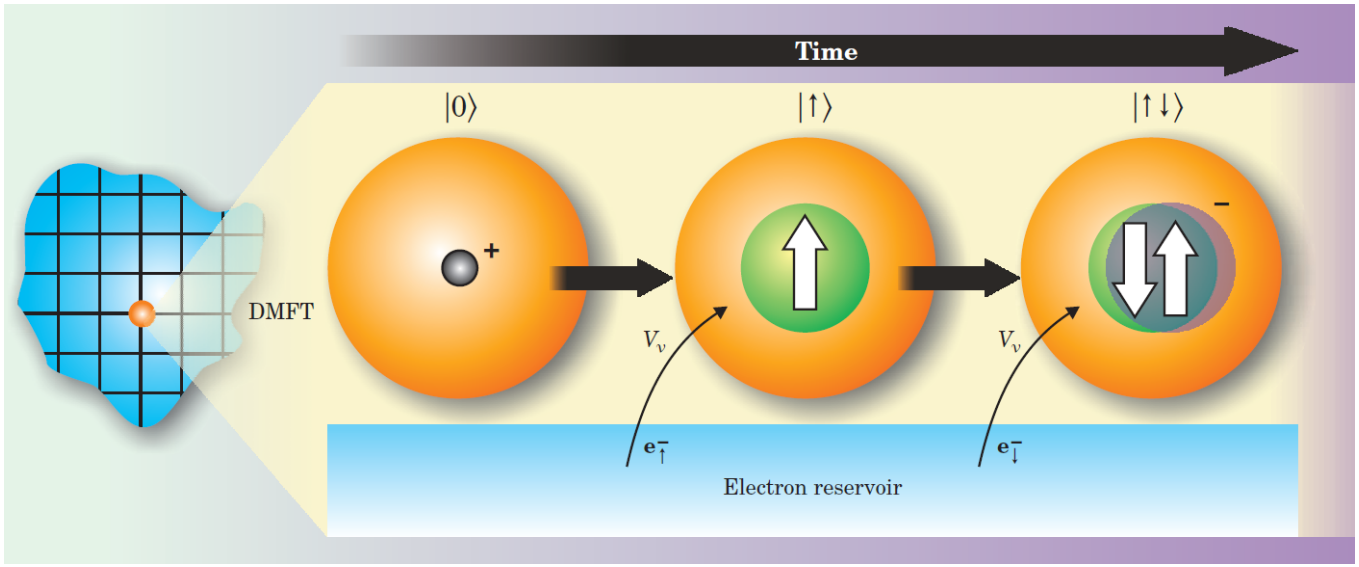
Quantum Impurity Problems



G. Kotliar and D. Vollhardt, Phys. Today March, 53 (2004)

- Quantum Impurity Problems(QIPs) were initially constructed to describe the quantum mechanical properties of an impurity or imperfection such as a magnetic atom, dislocation, or a substitutional ion in a lattice.
- Many-body lattice problems, such as heavy fermion systems, Mott metal-insulator transition, nonconventional superconductivity could be mapped to QIPs with dynamical mean field theory (DMFT).

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Quantum Impurity Model

A quantum impurity model may be represented as a Hamiltonian H_{QI}

$H_{\mathbf{QI}} = H_{\mathbf{loc}} + H_{\mathbf{bath}} + H_{\mathbf{hyb}}$

$$H_{\mathrm{loc}} = H^0_{\mathrm{loc}} + H^I_{\mathrm{loc}} = \sum_{ab} E^{ab} d^\dagger_a d_b + \sum_{pqrs} I^{pqrs} d^\dagger_p d^\dagger_q d_r d_s \quad (1)$$

$$H_{\mathrm{bath}} = \sum_{k\alpha} \varepsilon_{k\alpha} c^\dagger_{k\alpha} c_{k\alpha} \quad (2)$$

$$H_{\mathrm{hyb}} = \sum_{k\alpha b} (V^{\alpha b}_k c^\dagger_{k\alpha} d_b + \mathrm{h.c.}) \quad (3)$$

H_{loc} describes the "impurity" (a system with a finite (typically small) number of degrees of freedom), H_{bath} describes the noninteracting system, and H_{hyb} gives the coupling between the impurity and bath.

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Anderson Impurity Model

The Anderson impurity model describes a localized electronic level, subject to a local Coulomb interaction, which is coupled to a band of non-interacting conduction electrons. In the single-impurity single-orbital case, its Hamiltonian reads

$$\begin{aligned} H_{\mathrm{AIM}} &= \underbrace{\sum_{k\sigma} \varepsilon_k c_{k\sigma}^{\dagger} c_{k\sigma}}_{H_{\mathrm{bath}}} + \underbrace{\sum_{\sigma} \varepsilon_0 d_{\sigma}^{\dagger} d_{\sigma} + U n_{\uparrow} n_{\downarrow}}_{H_{\mathrm{loc}}} \\ &+ \underbrace{\sum_{k\sigma} \left(V_k c_{k\sigma}^{\dagger} d_{\sigma} + h.c. \right)}_{H_{\mathrm{hyb}}} \end{aligned} \tag{4}$$

ε_0 is the level energy and $U n_{\uparrow} n_{\downarrow}$ is the interaction term.

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Basic Idea of CT-QMC

In CT-QMC, the Hamiltonian $H = H_a + H_b$ is split into two parts. The partition function $Z = \mathrm{Tr}[e^{-\beta H}]$ is written in the interaction representation with respect to H_a and expands in powers of H_b,

$$\begin{aligned} Z =& \mathrm{Tr}\ T_\tau e^{-\beta H_a} \exp\left[-\int_0^\beta d\tau H_b(\tau)\right] \\ =& \sum_k (-1)^k \int_0^\beta d\tau_1 \ldots \int_{\tau_{k-1}}^\beta d\tau_k \\ & \times \mathrm{Tr}\left[e^{-\beta H_a} H_b(\tau_k) H_b(\tau_{k-1}) \ldots H_b(\tau_1)\right] \end{aligned} \tag{5}$$

The impurity Green's function $(0 < \tau < \beta)$ or the "solution" of the impurity model is then given by

$$G(\tau) = \frac{1}{Z}\mathrm{Tr}[e^{-(\beta-\tau)H} d e^{-\tau H} d^\dagger] \tag{6}$$

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CT-QMC Expansion Algorithms

There are several expansion algorithms with different choices of H_b. The most widely used ones are:

- CT-INT (Interaction expansion, $H_b = H^I_{\text{loc}}$): works well for clusters, single orbital models, has sign problem with repulsive interactions, is not good for general electric structure Hamiltonians.
- CT-HYB (Hybridization expansion, $H_b = H_{\text{hyb}}$): works well for multi-orbital systems, handles low temperature and strong interactions more efficiently, is not good for clusters.

Some other expansion algorithms that either consider an additional auxiliary field decomposition (for clusters) or exchange coupling (for Kondo problems) have been developed as well.

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Hybridization Expansion (I)

In CT-HYB, we separate bath and impurity operators and obtain

$$H_b = H_{\text{hyb}} = \underbrace{\sum_{pj} (V_p^j c_p^\dagger d_j}_{\tilde{H}_{\text{hyb}}} + \underbrace{\sum_{pj} V_p^{j*} d_j^\dagger c_p)}_{\tilde{H}_{\text{hyb}}^\dagger} \tag{7}$$

$$\begin{aligned} Z = & \sum_{k=0}^{\infty} \int_0^\beta d\tau_1 \dots \int_{\tau_{k-1}}^\beta d\tau_k \int_0^\beta d\tau_1' \dots \int_{\tau_{k-1}'}^\beta d\tau_k' \\ & \sum_{\substack{j_1,\cdots j_k \\ j_1',\cdots j_k'}} \sum_{\substack{p_1,\cdots p_k \\ p_1',\cdots p_k'}} V_{p_1}^{j_1} V_{p_1'}^{j_1'*} \cdots V_{p_k}^{j_k} V_{p_k'}^{j_k'*} \\ & \times \text{Tr}_d \left[T_\tau e^{-\beta H_{\text{loc}}} d_{j_k}(\tau_k) d_{j_k'}^\dagger(\tau_k') \cdots d_{j_1}(\tau_1) d_{j_1'}^\dagger(\tau_1') \right] \\ & \times \text{Tr}_c \left[T_\tau e^{-\beta H_{\text{bath}}} c_{p_k}^\dagger(\tau_k) c_{p_{k'}}(\tau_k') \cdots c_{p_1}^\dagger(\tau_1) c_{p_1'}(\tau_1') \right] \end{aligned} \tag{8}$$

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Hybridization Expansion (II)

The bath partition function could be integrated out

$$Z_{\text{bath}} = \text{Tr} e^{-\beta H_{\text{bath}}} = \prod_{\sigma} \prod_{p} (1 + e^{-\beta \varepsilon_p}), \tag{9}$$

With the anti-periodic hybridization function $\mathbf{\Delta}$,

$$\Delta_{lm}(\tau) = \sum_{p} \frac{V_p^{l*} V_p^{m}}{e^{\varepsilon_p \beta} + 1} \times \begin{cases} -e^{-\varepsilon_p(\tau-\beta)}, & 0 < \tau < \beta \\ e^{-\varepsilon_p \tau}, & -\beta < \tau < 0 \end{cases}, \tag{10}$$

and by separating the contributions from each spin, we obtain

$$\begin{aligned} Z &= Z_{\text{bath}} \prod_{j} \sum_{k_j=0}^{\infty} \int_0^{\beta} d\tau_1^j \ldots \int_{\tau'^j_{k_j-1}}^{\beta} d\tau'^j_{k_j} \\ &\times \text{Tr}_d \left[T_\tau e^{-\beta H_{\text{loc}}} d_j(\tau_{k_j}^j) d_j^\dagger(\tau_{k_j}'^j) \ldots d_j(\tau_1^j) d_j^\dagger(\tau_1'^j) \right] \det \mathbf{\Delta}_j. \end{aligned} \tag{11}$$

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Monte Carlo Method

Monte Carlo methods are the only practical choices to do very high dimension integrations such as equation 11.
For $x \in \mathcal{C}$ with weight $p(x)$, we have the partition function

$$Z = \int_C dx\ p(x) \tag{12}$$

The expectation value of a quantity A is given by

$$\langle A \rangle_p = \frac{1}{Z} \int_C dx\ A(x)p(x) \tag{13}$$

With M configurations x_i in a Monte Carlo procedure,

$$\langle A \rangle_p \approx \langle A \rangle_{MC} \equiv \frac{1}{M} \sum_{i=1}^{M} A(x_i). \tag{14}$$

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Markov Process

A Markov process defines a transition matrix W_{xy} which specifies the probability to go from state x to state y in one step of the Markov process.
The Markov process will converge exponentially from any initial state to a stationary distribution $p(x)$ if two conditions are satisfied.

- Ergodicity: for all x and y there exists an integer $N < \infty$ such that for all $n \geq N$ the probability $(W^n)_{xy} \neq 0$.
- Balance: the distribution $p(x)$ satisfies the detailed balance condition

$$\frac{W_{xy}}{W_{yx}} = \frac{p(y)}{p(x)}$$

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Metropolis-Hastings Algorithm

An update from a configuration x to a new configuration y is proposed with a probability W_{xy}^{prop} but accepted only with probability W_{xy}^{acc}. If the proposal is rejected the old configuration x is used again.

$$W_{xy}^{\text{acc}} = \min\left[1, \frac{p(y)W_{yx}^{\text{prop}}}{p(x)W_{xy}^{\text{prop}}}\right]. \tag{15}$$

$$W_{xy} = W_{xy}^{\text{prop}} W_{xy}^{\text{acc}} \tag{16}$$

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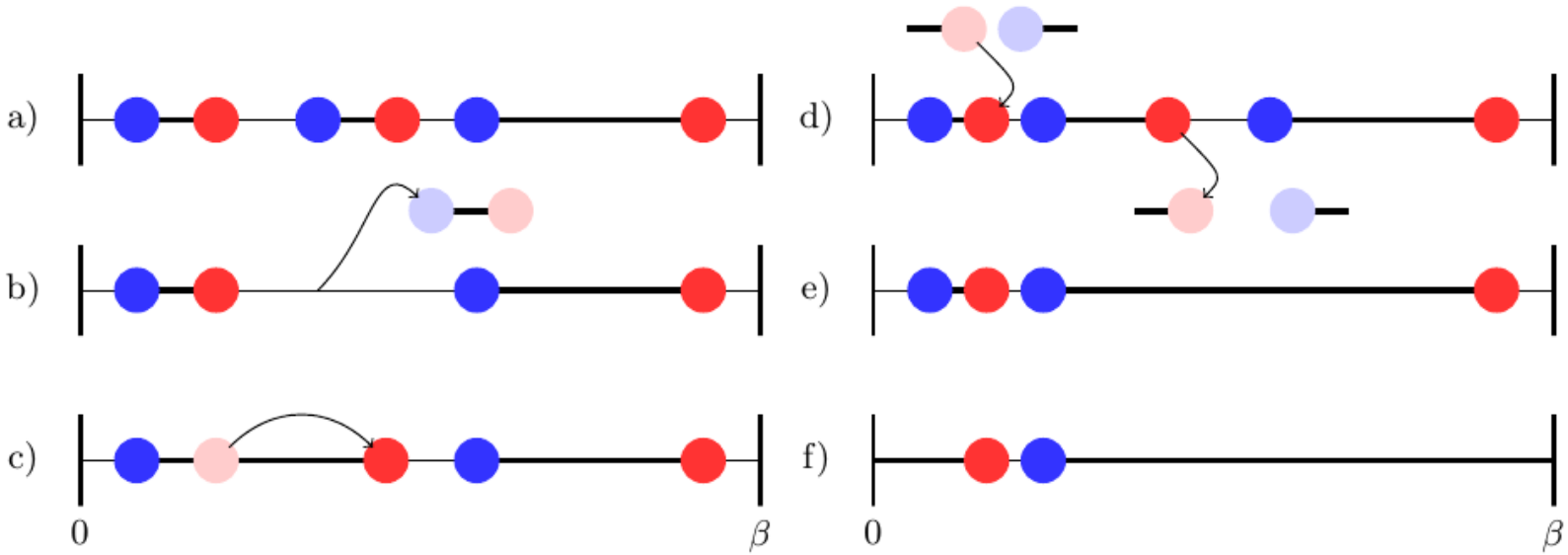
Hybridization Update Diagrams

(a) original configuration; (b) removal of a segment; (c) shift of an end point of a segment; (d) insertion of an antisegment; (e) removal of an antisegment; (f) removal of another antisegment such that the remaining segment "wraps" around β.



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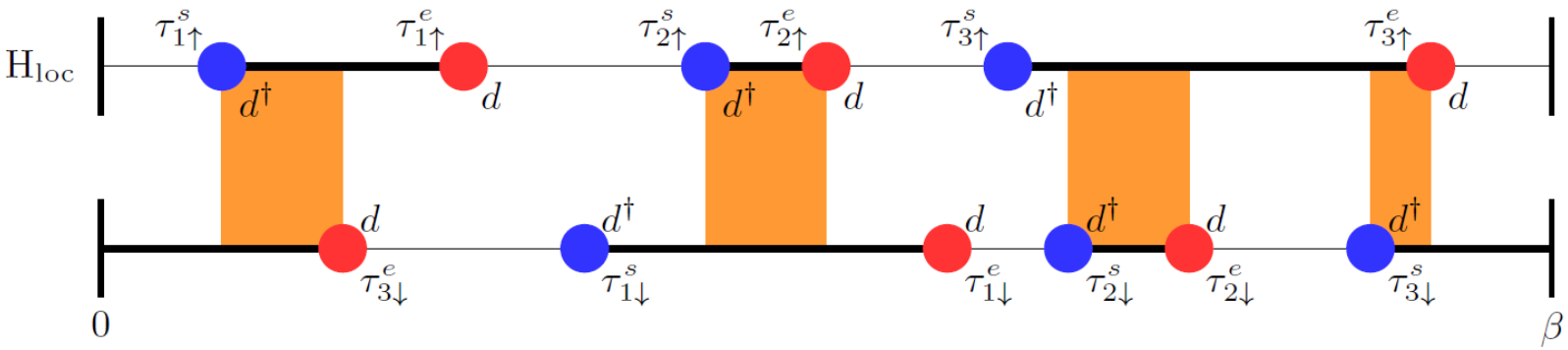
Segment Representation

Segment representation make it possible to treat interaction by looking at overlap of lines. Extension to density - density interactions for multiple orbitals is made straightforward as well.



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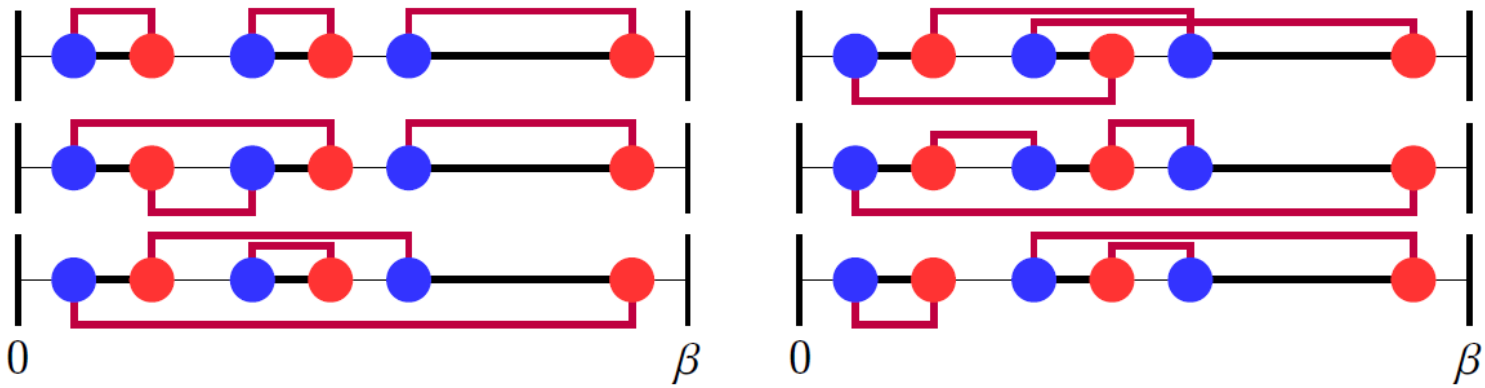
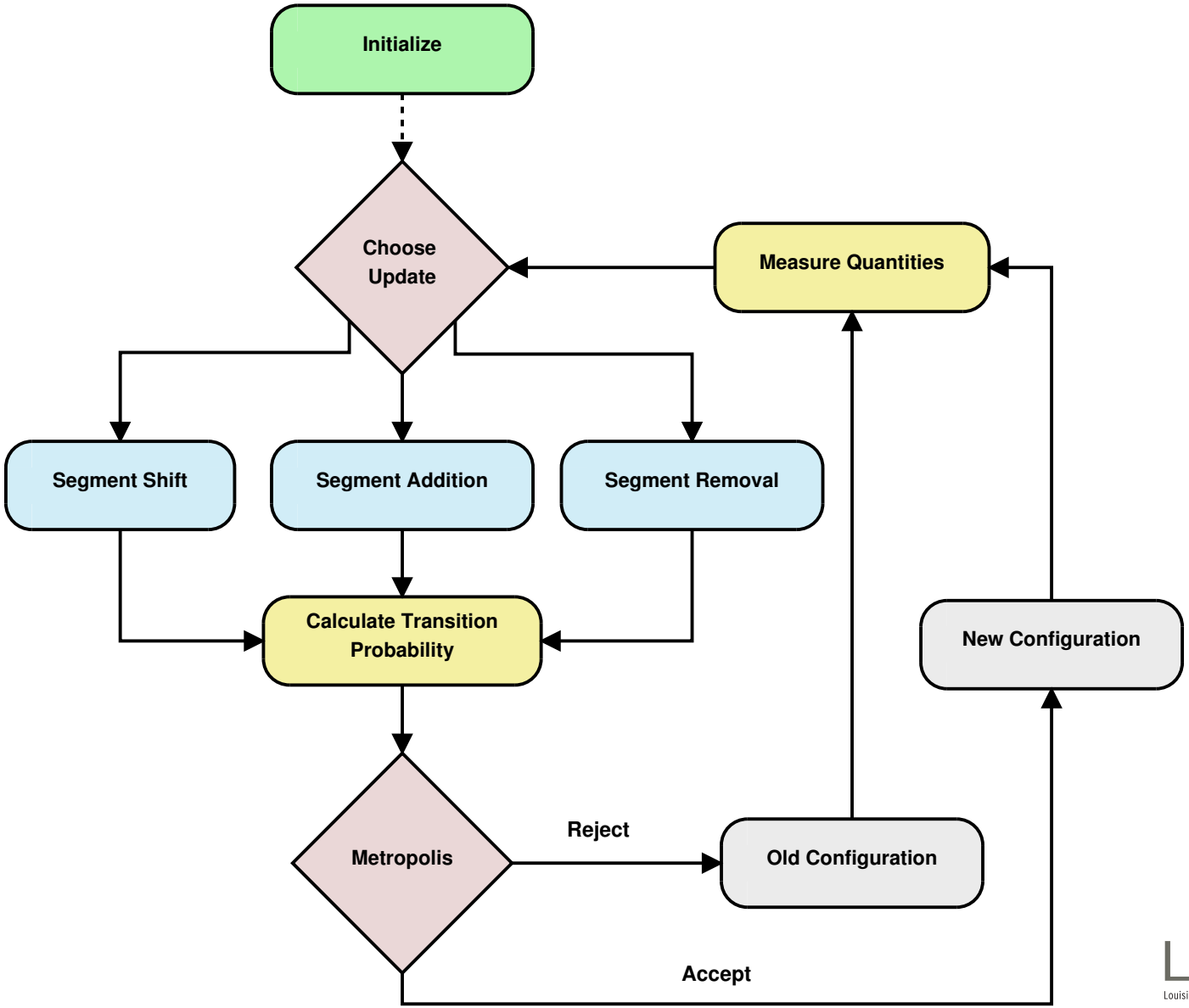
Segment Representation

Possible hybridization lines of a particular segment configuration.



CTQMC Workflow



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