Implementing a Self-Corrected Chemical Potential Scheme in Determinant Quantum Monte Carlo Simulations

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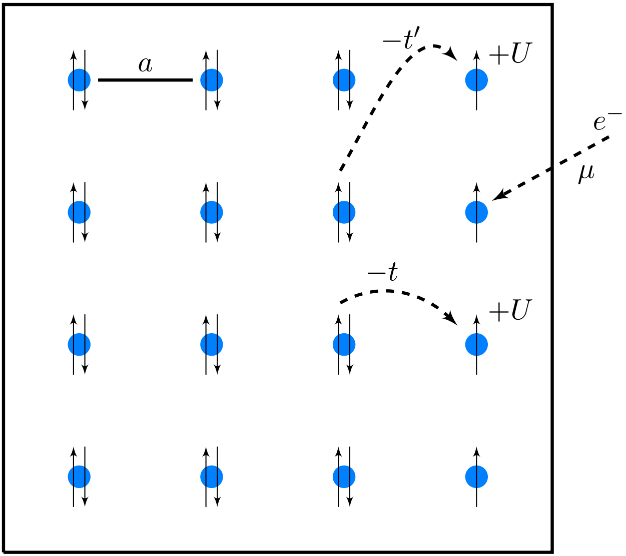
Many-Body Problem in Solid-State Physics

- Quantum Mechanics - spatial/spin/energy states based on system Hamiltonian

$$\hat{H} = -\sum_i \frac{\hbar^2}{2m_e}\nabla_i^2 - \sum_I \frac{\hbar^2}{2m_I}\nabla_I^2 + \frac{1}{2}\sum_I \sum_{J\neq I} \frac{ke^2 Z_I Z_J}{|\mathbf{R}_I - \mathbf{R}_J|} - \sum_i \sum_I \frac{ke^2 Z_I}{|\mathbf{r}_i - \mathbf{R}_I|} + \frac{1}{2}\sum_i \sum_{j\neq i} \frac{ke^2}{|\mathbf{r}_i - \mathbf{r}_j|}$$

- Determinant Quantum Monte Carlo (DQMC) simulations - approximate the partition function $Z(\hat{H})$ using auxiliary field sampling (system configurations)
- Favors more significant contributions to Z through acceptance/rejection scheme
(S. Johnston et al., *Phys. Rev. B* **87**, 235133 (2013))
- Compute expectation values for macroscopic properties - energy, magnetization, electron filling, etc.

2D Repulsive Hubbard Model

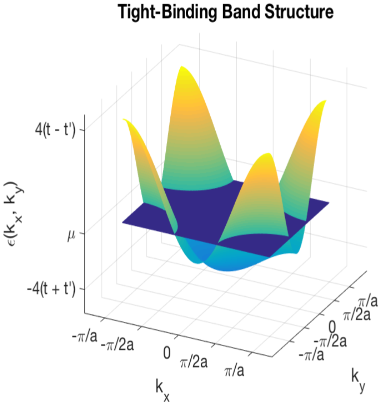


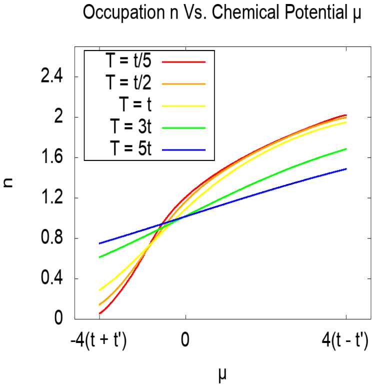
Model Hamiltonian and Interactions

$$\hat{H} = \hat{H}_t + \hat{H}_U + \hat{H}_\mu$$
$$= -t \sum_{<i,j>,\sigma} (\hat{c}^\dagger_{i,\sigma}\hat{c}_{j,\sigma} + \hat{c}^\dagger_{j,\sigma}\hat{c}_{i,\sigma}) + U \sum_{i=1}^{N} \hat{n}_{i\uparrow}\hat{n}_{i\downarrow} - \mu \sum_{i,\sigma} \hat{n}_{i,\sigma}$$

- Electrons can diffuse to and from surroundings to reach equilibrium
- Competition of allowed electron behaviors captured here
- Green's functions as field propagators
(M. Jarrell, *Z. F. Physik B - Condensed Matter* **90**, 2 (1993))

Non-Interacting Case: Band and Occupation Results

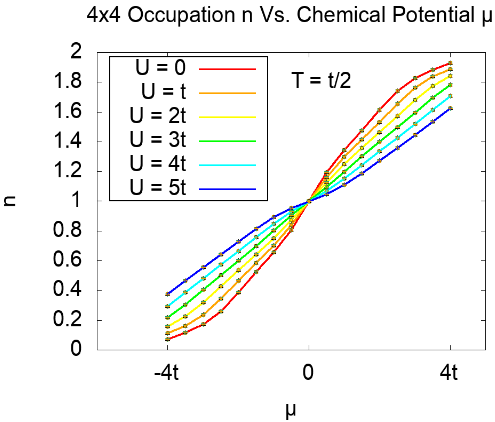




$$\epsilon = -2t[\cos(k_x a) + \cos(k_y a)] - 4t' \cos(k_x a)\cos(k_y a)$$

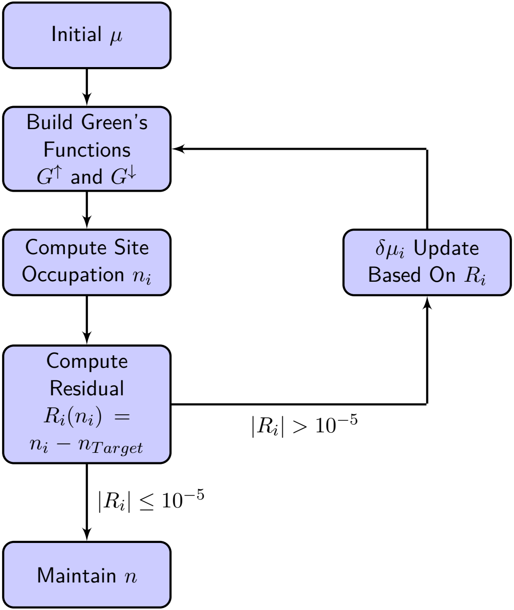
$$n = \frac{2}{N} \sum_{k_x} \sum_{k_y} \frac{1}{e^{\beta(\epsilon(k_x,k_y)-\mu)} + 1}$$

$U \geq 0$: DQMC Average Occupations ($t' = 0$)



- Small error bars - 20,000 warmup/measurement sweeps
- Flattening near half-filling - Mott Gap formation
  (F. Ohkawa, arXiv:cond-mat/0606644 (2007))
- Maintain desired filling - accurate initial input for μ (overhead runs)

Occupation-Based Feedback Loop During Warmups



Chemical Potential Response

$$n = \frac{1}{N}\sum_{i}^{N}[(1 - G_{ii}^{\uparrow}) + (1 - G_{ii}^{\downarrow})]$$

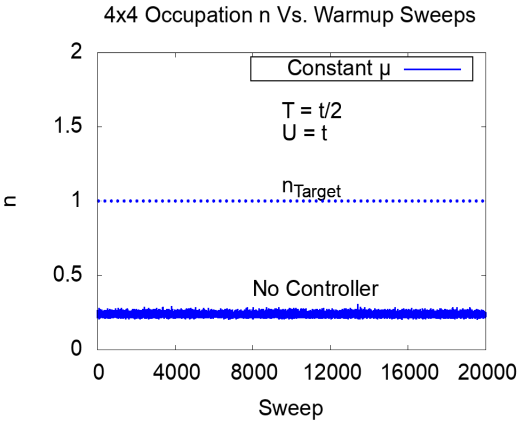
(i refers to site spatial index)

- Occupation n starts with a nonzero residual from the target: $R_i = n_i - n_{Target}$ (i refers to simulation sweep index)
- Correction feedback to the chemical potential μ as a response (Z. Zhao et al., *IEEE Transactions on Systems, Man, and Cybernetics* **23**, 5 (1993))
- Implement and test a proportional-integral-derivative (PID) controller for μ

$$\begin{aligned}\delta\mu_i &= \delta\mu_{P,i} + \delta\mu_{I,i} + \delta\mu_{D,i} \\ &= -K_P R_i - K_I \left(\int_0^t R(t')dt'\right)_i - K_D \left(\frac{dR}{dt}\right)_i\end{aligned}$$

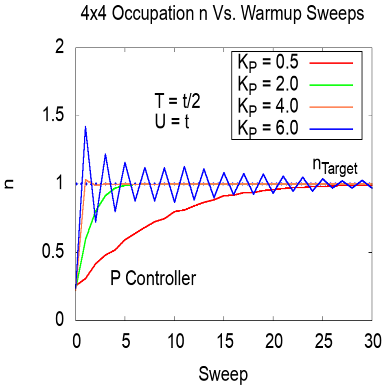
- Tune the influence of each term - gain coefficients K_P, K_I, and K_D

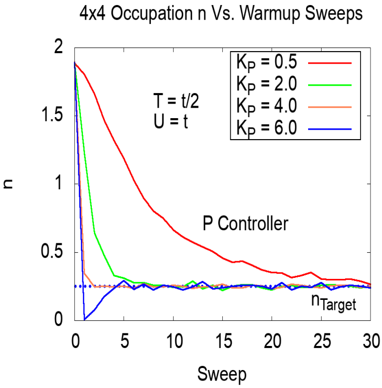
Occupation During Warmups



$$\mu_0 = -3t$$

P-Controller Convergence

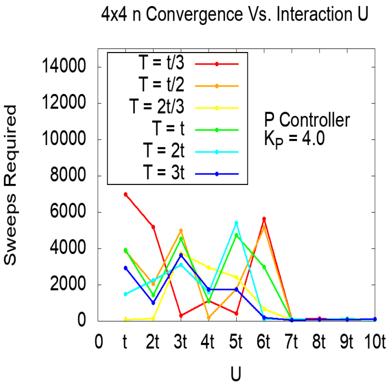


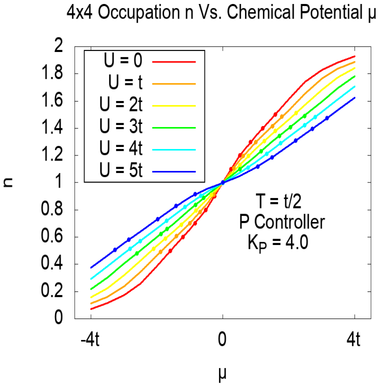


$$\mu_0 = -3t$$
$$n_{Target} = 1$$

$$\mu_0 = 4t$$
$$n_{Target} = 0.25$$

P-Controller Robustness and Accuracy

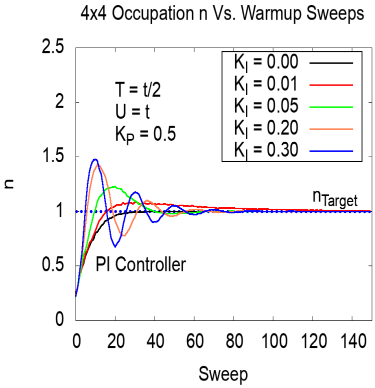




Warmup sweeps until
$R < 10^{-5}$

(μ, n) after measurements
$\mu_0 = -3t$

PI-Controller Convergence



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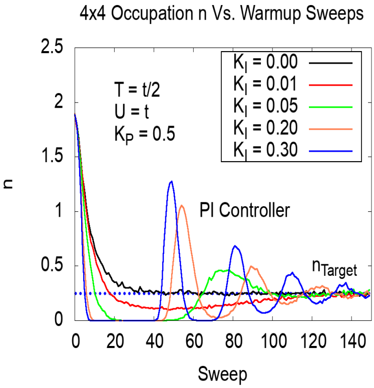

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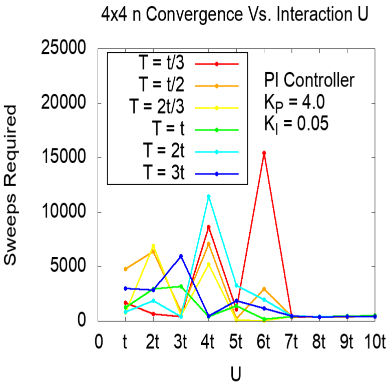
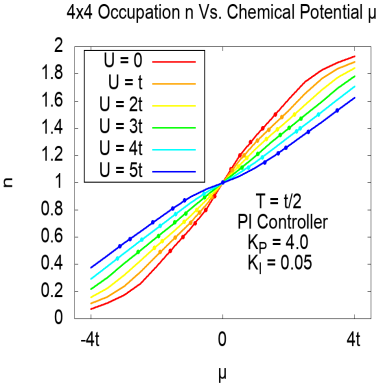
PI-Controller Robustness and Accuracy

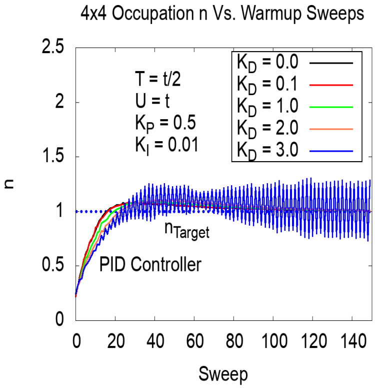


Warmup sweeps until
$R < 10^{-5}$

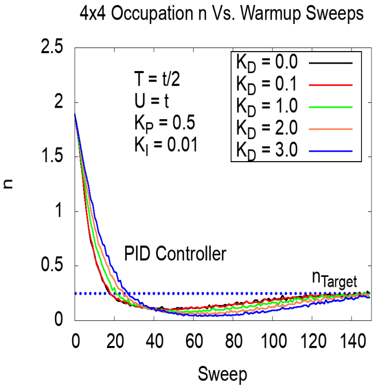


(μ, n) after measurements
$\mu_0 = -3t$

PID-Controller Convergence



$$\mu_0 = -3t$$
$$n_{Target} = 1$$



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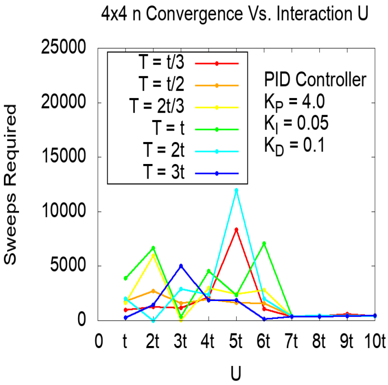
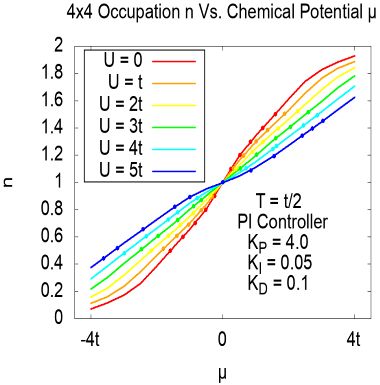
PID-Controller Robustness and Accuracy





Warmup sweeps until $R < 10^{-5}$

(μ, n) after measurements $\mu_0 = -3t$

- P controller seems the most reliable, but optimize K_P and R_{Tol} for $U \geq 3t$

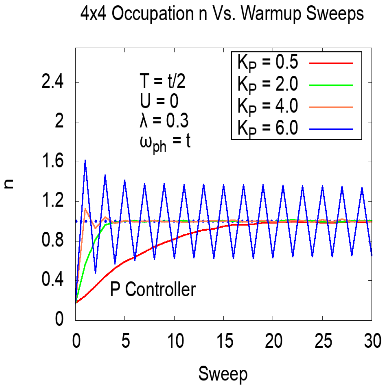
2D Holstein Lattice Model

- More realistic models - atoms spatially displace from equilibrium as optical phonons

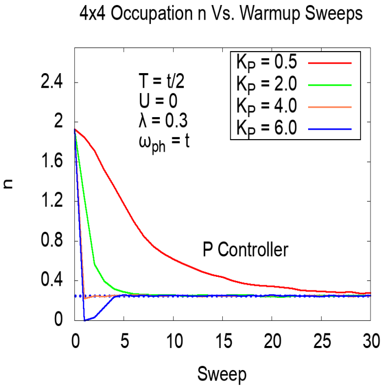
$$\hat{H} = \hat{H}_t + \hat{H}_U + \hat{H}_\mu + \hat{H}_{Ion} + \hat{H}_{e-ph}$$
$$= -t \sum_{<i,j>,\sigma} (\hat{c}^\dagger_{i,\sigma}\hat{c}_{j,\sigma} + \hat{c}^\dagger_{j,\sigma}\hat{c}_{i,\sigma}) + U \sum_{i=1}^{N} \hat{n}_{i\uparrow}\hat{n}_{i\downarrow} - \mu \sum_{i,\sigma} \hat{n}_{i,\sigma} +$$
$$\sum_I \left(\frac{m_I \omega_{ph}^2}{2} \hat{X}_i^2 - \frac{\hbar^2}{2m_I} \nabla_I^2 \right) - g \sum_{i,\sigma} \hat{n}_{i,\sigma} \hat{X}_i$$

- Electron occupations, ion displacements, and ion velocities as additional degrees of freedom
- Dimensionless electron-phonon coupling strength $\lambda = g^2/W\omega_{ph}^2$
(S. Johnston et al., *Phys. Rev. B* **87**, 235133 (2013))

P-Controller Convergence for Holstein

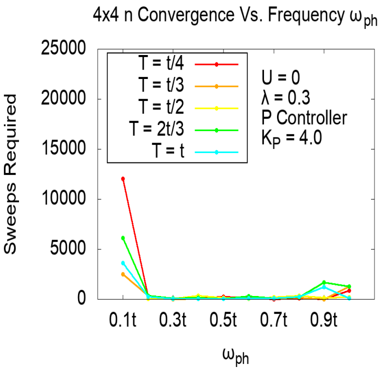


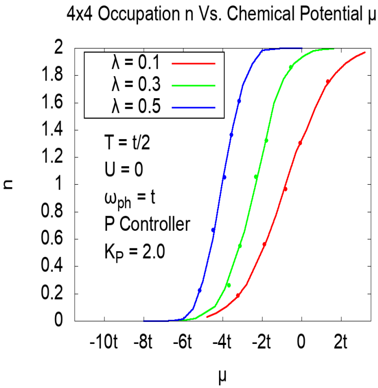
$$\mu_0 = -3t$$
$$n_{Target} = 1$$



$$\mu_0 = 4t$$
$$n_{Target} = 0.25$$

P-Controller Robustness and Accuracy for Holstein

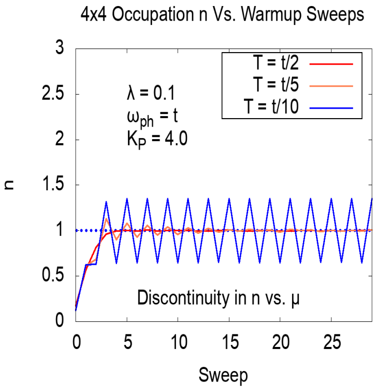




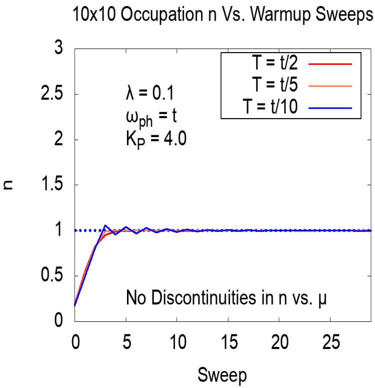
Warmup sweeps until
$R < 10^{-5}$

(μ, n) after measurements
$\mu_0 = -3t$ (imaginary time $\delta\tau = 0.2$)

Low Temperature Complications for Holstein



Overshoots at low T

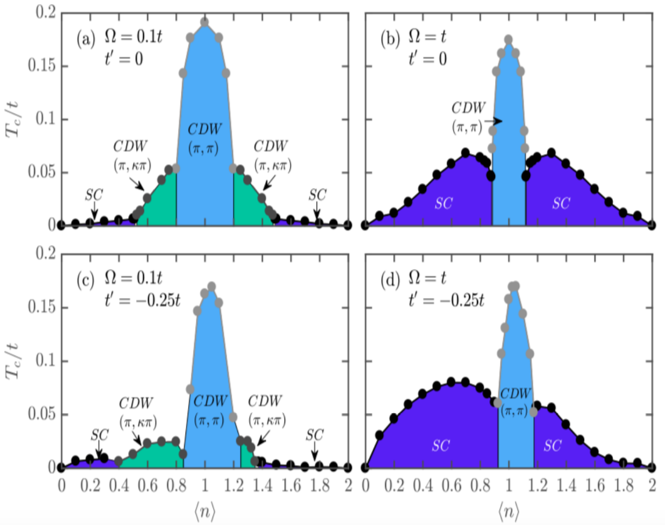


Converges at low T

Conclusions and Future Directions

- DQMC warmups/measurements: system partition function Z
- Fixing μ also fixes electron filling n
- Hubbard/Holstein P-controller each sweep for convergence/reliability
- $\delta\mu = -K_P(n - n_{Target})$
- Optimize K_P for each phase-space regime especially:
  - Large Hubbard U
  - Large Holstein λ
  - Low T (also increase lattice size)
- Future steps: prevent occupation drifting with a stricter deactivation condition for $\delta\mu$
- Competing interactions and ordered phases for Hubbard-Holstein

Maintaining n For $T < t/10$: Phase Diagrams



(P. Dee et al., arXiv:1811.03676 (2018))

References

[1] F. Ohkawa, arXiv:cond-mat/0606644 (2007).

[2] M. Jarrell, *Z. F. Physik B - Condensed Matter* **90**, 2 (1993).

[3] P. Dee, K. Nakatsukasa, Y. Wang, and S. Johnston, arXiv:1811.03676 (2018).

[4] S. Johnston, E. Nowadnick, F. Kung, B. Moritz, R. Scalettar, and T. Devereaux, *Phys. Rev. B* **87**, 235133 (2013).

[5] Z. Zhao, M. Tomizuka, and S. Isaka, *IEEE Transactions on Systems, Man, and Cybernetics* **23**, 5 (1993).