Ultracold fermion theory @ UQ

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Fermion theory @UQ

- Revisit our effective field theory for coupled atom-molecule systems
- **Analytic result for molecular binding energy**
- Simple variational theory for BEC/BCS crossover
- New results for fermion collective modes in lattices,
- New Gaussian technique for fermion problems
- **Solution to Fermi/Hubbard sign problem**

Simplicity of Ultracold Atoms

✔ underlying interactions well understood, few parameters

✔ interactions can be tuned

✔ helps understanding of many-body physics

$\longrightarrow$ apply simple theoretical models to high accuracy

$\longrightarrow$ novel experimental tests of methods, QFT

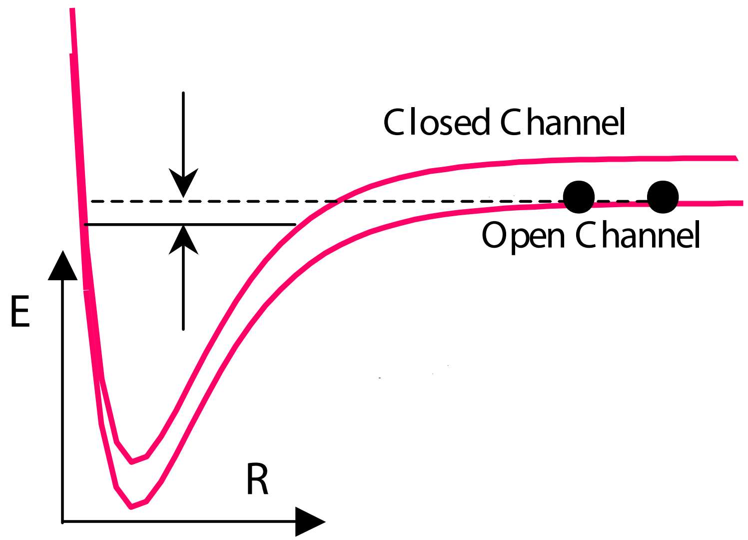
✔ new tests of massive particle quantum measurements?

Recent experiments

- Fermi BCS-BEC experiments: JILA, Duke, Rice, Innsbruck, MIT, Paris (ENS)
- Bosonic lattice experiments: NIST, Max Planck, Texas
- Fermi lattice experiments: Florence (LENS), Zurich
- **EXPERIMENTS PLANNED AT ACQAO:**
  - Swinburne: Lithium-6
  - (?) ANU: Helium-3*

I: Feshbach Resonance and BEC-BCS

- Tunable interactions in ultra-cold quantum gases
- Coherent conversion of an atomic gas to a BEC of molecules
- Studies of the BCS-BEC crossover regime



Quantum field theory: K&D 2000

$$H_0 = \sum_{i=m,1,2} \int d\mathbf{x} \left[\frac{\hbar^2}{2m_i} |\nabla \hat{\Psi}_i|^2 + E_M \hat{\Psi}_M^\dagger \hat{\Psi}_M \right]$$

$$H_s = \sum_{ij} \frac{\hbar U_{ij}}{2} \int d\mathbf{x} \hat{\Psi}_i^\dagger \hat{\Psi}_j^\dagger \hat{\Psi}_j \hat{\Psi}_i$$

$$H_{M \rightleftarrows A_1 + A_2} = \frac{\hbar \chi}{2} \int d\mathbf{x} \left[\hat{\Psi}_M^\dagger \hat{\Psi}_1 \hat{\Psi}_2 + H.c. \right]$$

- $\hat{\Psi}_{1,2,M}(t,\mathbf{x})$ – field operators [$a\hat{_{1,2}}(\mathbf{k})$, $\hat{b}(\mathbf{k})$]
- E_M – 'bare' energy detuning; U_{ij} – s-wave scattering
- χ – atom-molecule coupling ($A_1 + A_2 \rightleftarrows M$)
- **One year BEFORE Timmermans or Holland et al :-)**

Coherent quantum superposition

- **EXACT** quantum ground-state solution, for $N = 2$:

$$\left|\Psi^{(N)}\right\rangle = \left[\hat{a}_0^\dagger + \sum_k G_k \hat{b}_k^\dagger \hat{c}_{-k}^\dagger\right]^{N/2} |0\rangle$$

coherent superposition of a molecule with a pair of correlated atoms: “dressed” molecule (K&D 2000)

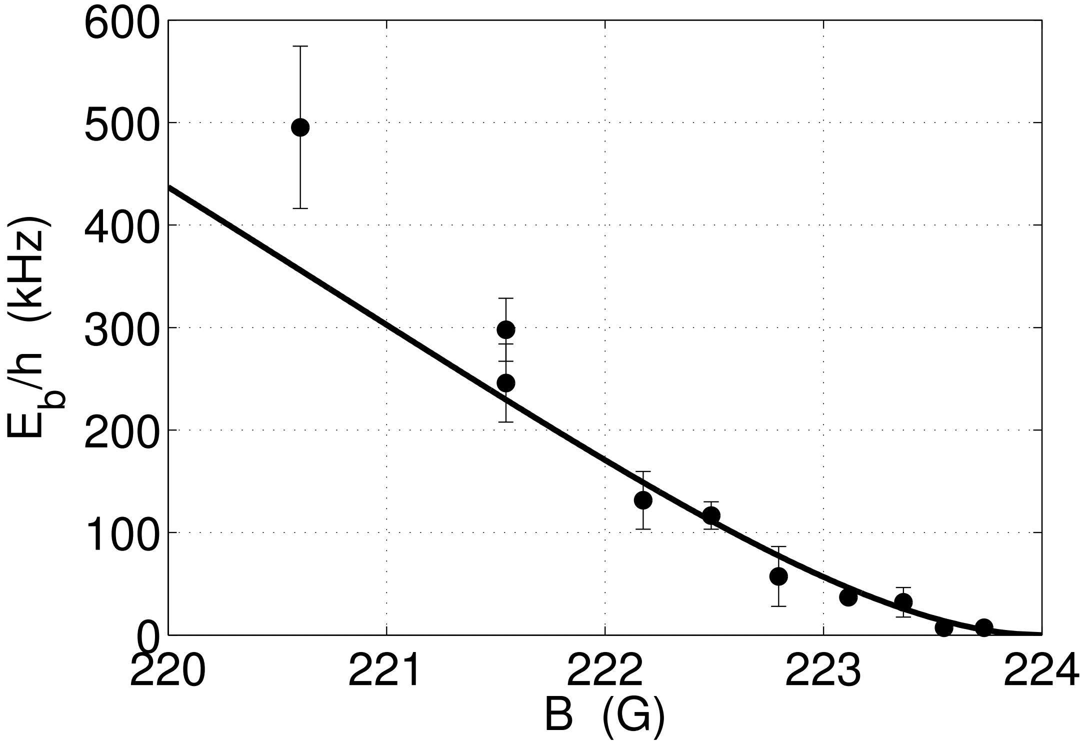
- Renormalised binding energy vs B-field

$$B = B_0 - \frac{1}{\Delta\mu}\left(E_b + \frac{sC\hbar\chi_0^2\sqrt{E_b}}{1 - 2CU_0\sqrt{E_b}}\right), \qquad (E_b \equiv -E)$$

$s = 2$ for fermions[K&D 2004]

Molecular binding energy in ^{40}K$_2$

Here, $s = 2; C = m^{3/2}/(8\pi\hbar^2)$

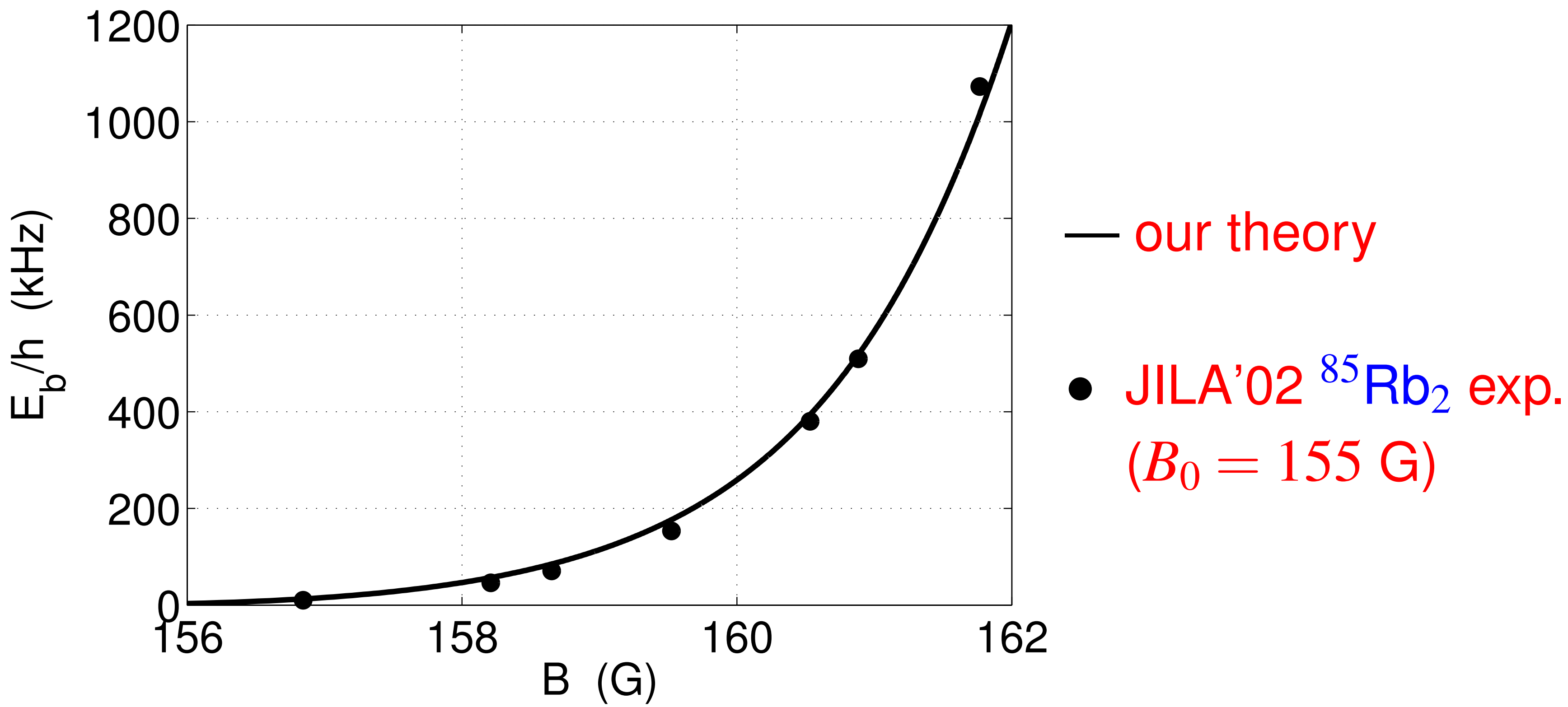


— our theory

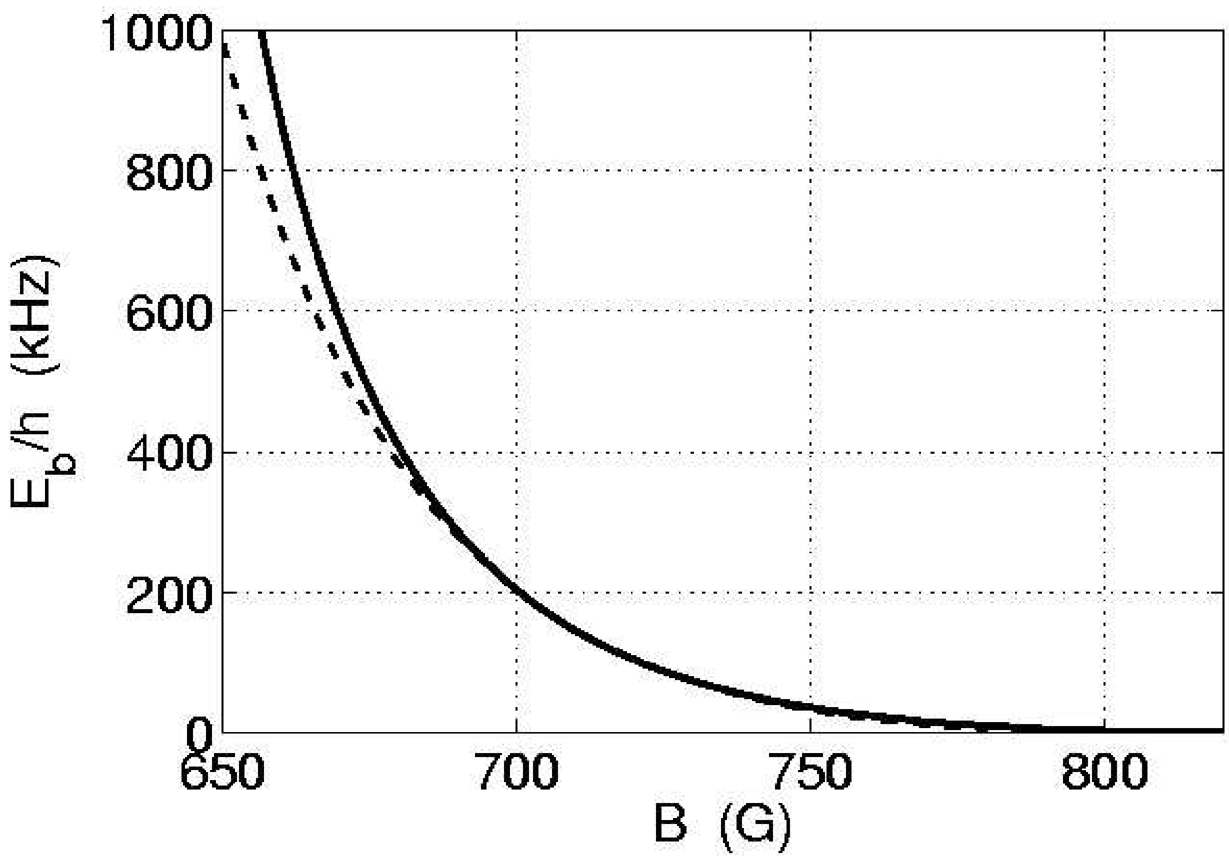
● JILA'03 ^{40}K$_2$ exp. ($B_0 = 224$ G)

Bosonic case: $^{85}Rb_2$ dimers [JILA 2002]

The same result, with $s = 1$, applies to the bosonic version of the theory [P.D.Drummond et al., PRL **81**, 3055 (1998)]



How about $^6Li_2$? [Our theory vs Kokkelmans]



Variational ansatz: many-body ground-state

- **Same expression**, but with an exponential form for simplicity:

$$|\Psi\rangle = \exp\left\{\alpha\left[\hat{a}_0^\dagger + \sum_k G_k \hat{b}_k^\dagger \hat{c}_{-k}^\dagger\right]\right\}|0\rangle$$

- **A BEC of modified dressed molecules**
- Example of a Fermi-Bose Gaussian state(!)
- Vary the correlation function G_k to minimize the energy
- Vary α to obtain correct density

Variational solution

Including renormalization, we obtain two basic gap equations:

$$
\begin{aligned}
1 &= \widetilde{U}_0 \int_0^K \frac{q^2 dq}{4\pi^2} \left[\frac{1}{\varepsilon_q} - \frac{1}{E_q} \right] \\
n &= 2 \left[\frac{\chi_0 \Delta}{\varepsilon_0^a \widetilde{U}_0} \right]^2 + \int_0^K \frac{q^2 dq}{2\pi^2} \left[1 - \frac{U_q}{E_q} \right]
\end{aligned}
$$

✔ Can solve numerically to obtain ground-state energy

Conclusions

- Reduces to standard Leggett single-channel BCS crossover model for broad resonance

- Similar to Green's function calculations (Holland, Griffin, Ho etc)

- New features for narrow resonance, ($\Delta E \leq E_f$) high density

- Finite temperature and non mft effects under investigation

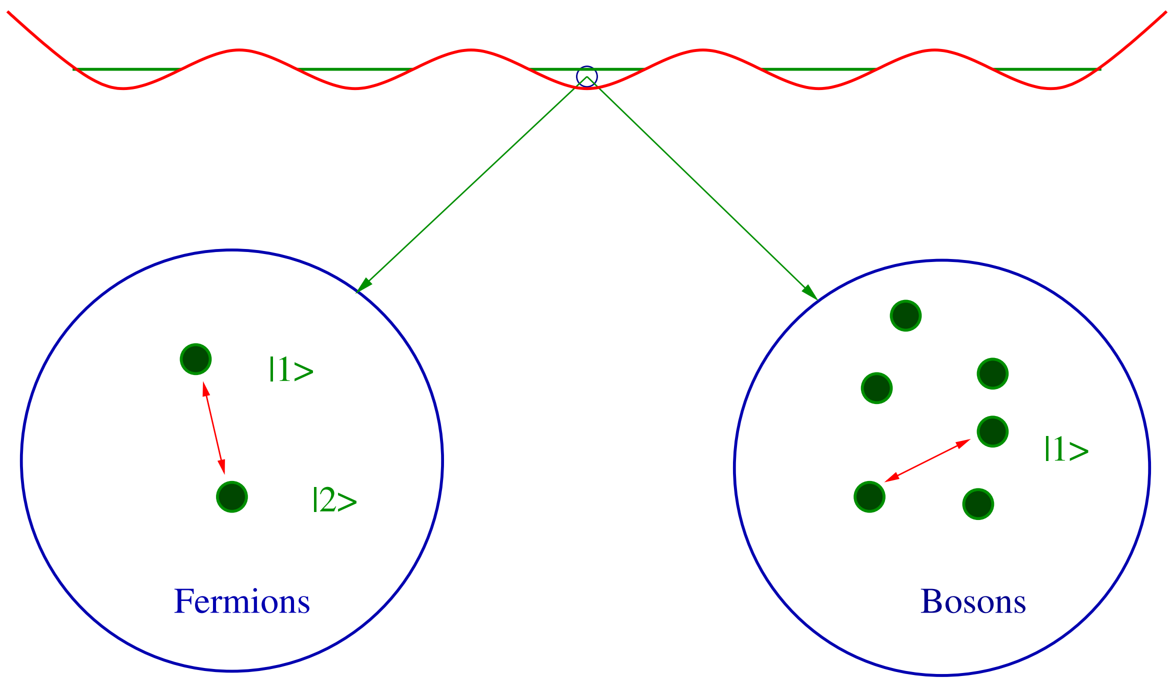
- **Role of universality, strong coupling physics?**

II: Hubbard Model Mott transition

$$\widehat{H} = -t \sum_{\langle i,j \rangle,\sigma} \widehat{a}^{\dagger}_{i,\sigma} \widehat{a}_{j,\sigma} + U \sum_{j} \widehat{n}_{j,\uparrow} \widehat{n}_{j,\downarrow}$$

- Simplest model of an interacting Fermi gas
- Describes ultracold gas in an optical lattice
- Weak-coupling limit $\Longrightarrow$ BCS transitions
- Relevance to high-T_c superconductors?
- Test theories of strongly interacting fermions

Fermionic vs Bosonic Hubbard physics!



TRAPPED 1D FERMI GAS

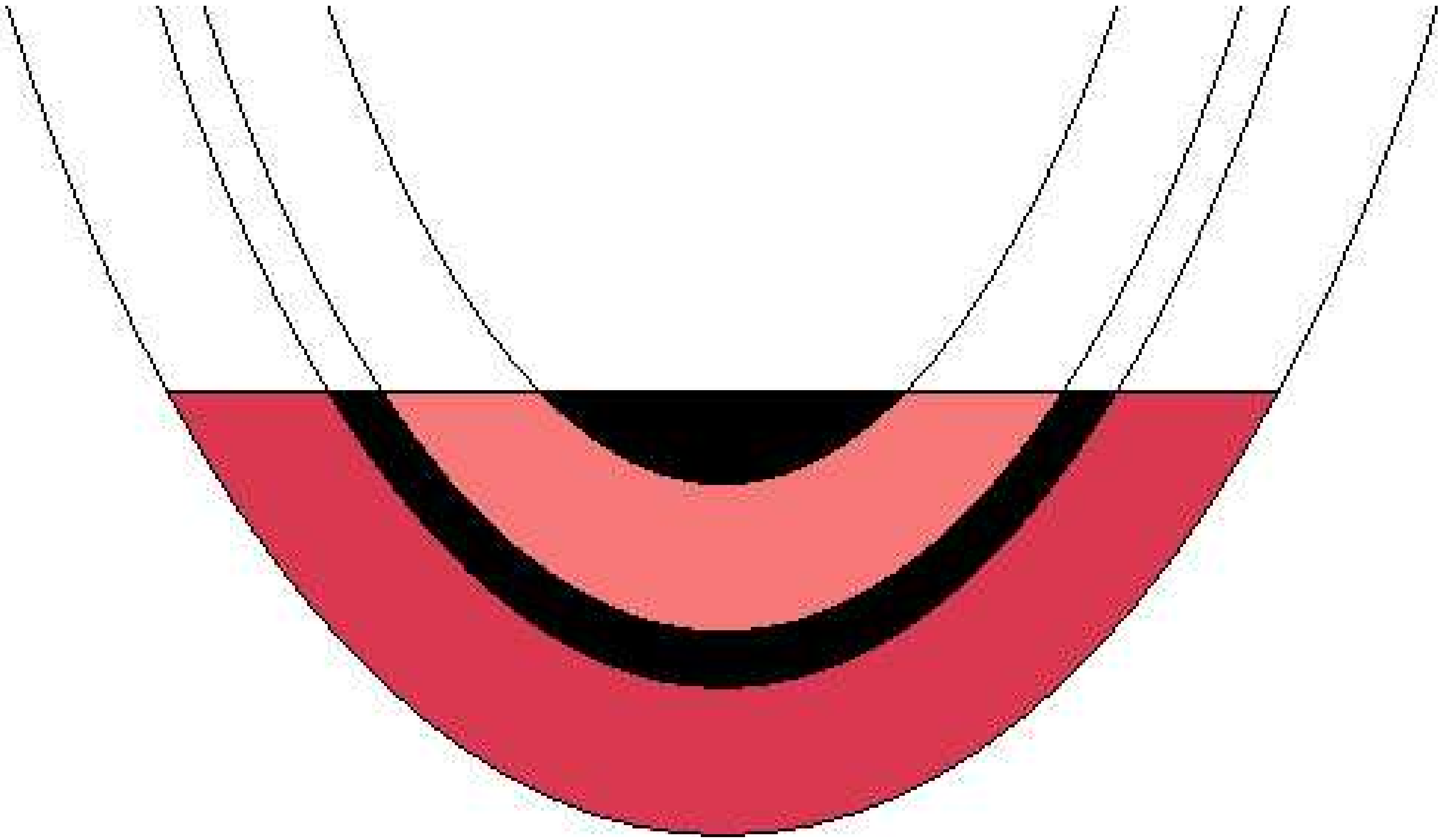
$$\mathcal{H} = -t\sum_{j\sigma}\left(\widehat{a}^{\dagger}_{j,\sigma}\widehat{a}_{j+1,\sigma} + h.c.\right) + U\sum_{j}\widehat{n}_{j,\uparrow}\widehat{n}_{j,\downarrow} + \sum_{j\sigma}\frac{m\omega_0^2 d^2}{2} j^2 \widehat{n}_{j,\sigma},$$

- Includes 1D trap potential
- Use local density approximation
- Based on exact solution for 1D Hubbard model

Energy Bands in Mott-Insulator regime

No interactions $\Longrightarrow$ band insulator when band fills (observed).

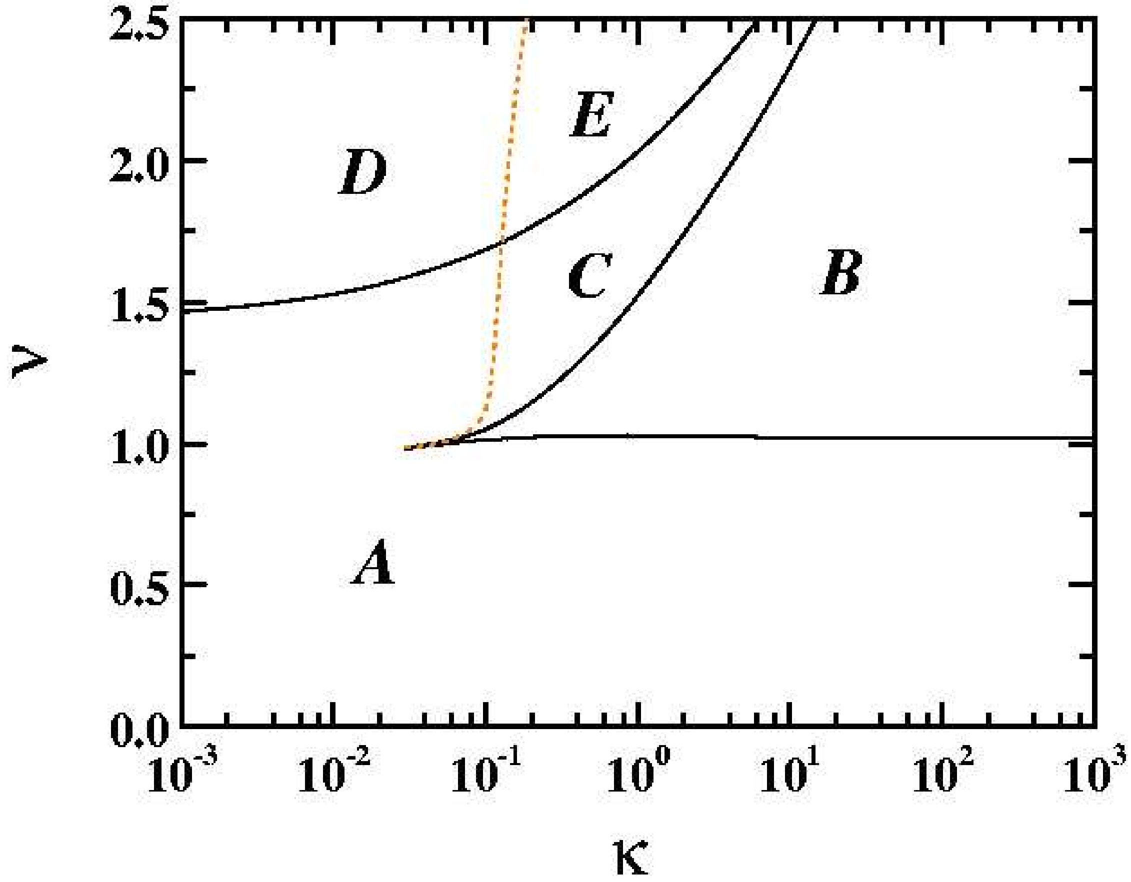
Interactions $\Longrightarrow$ Mott insulator at half-filling (not yet seen).



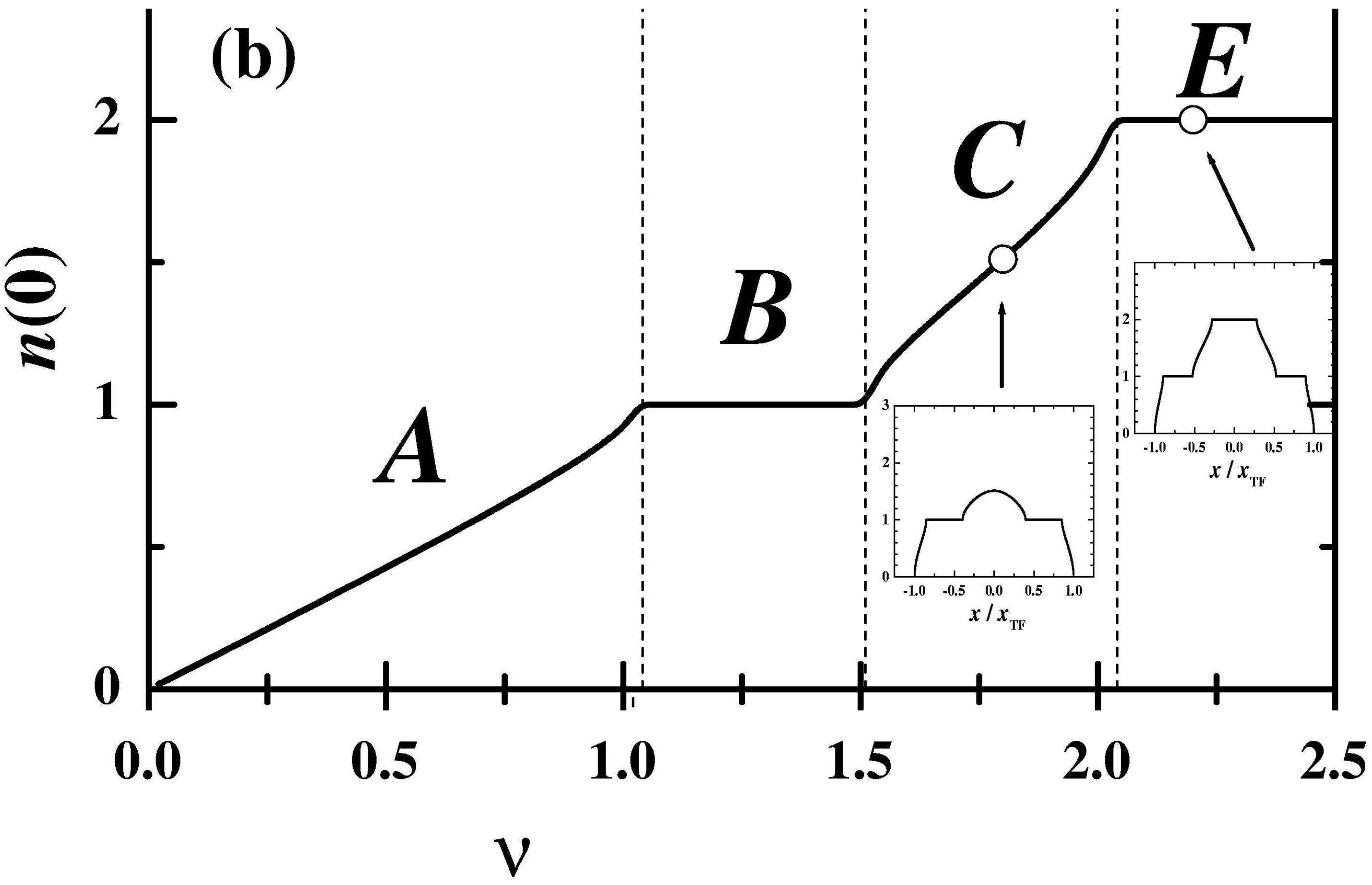
Characteristic parameters

- Effective mass: $m^* = \hbar^2/\left(2td^2\right)$
- Dimensionless trapping frequency: $\omega = \hbar\omega_0\,(m/m^*)^{1/2}/t$.
- Coupling constant $\kappa = U^2/\left(8t^2N\omega\right)$
- Effective filling factor $\nu = \sqrt{2N\omega}/\pi$

Phase-diagram vs filling ν and coupling κ



Cross-over: Filling vs ν , at $\kappa = 1$



Luttinger approximation

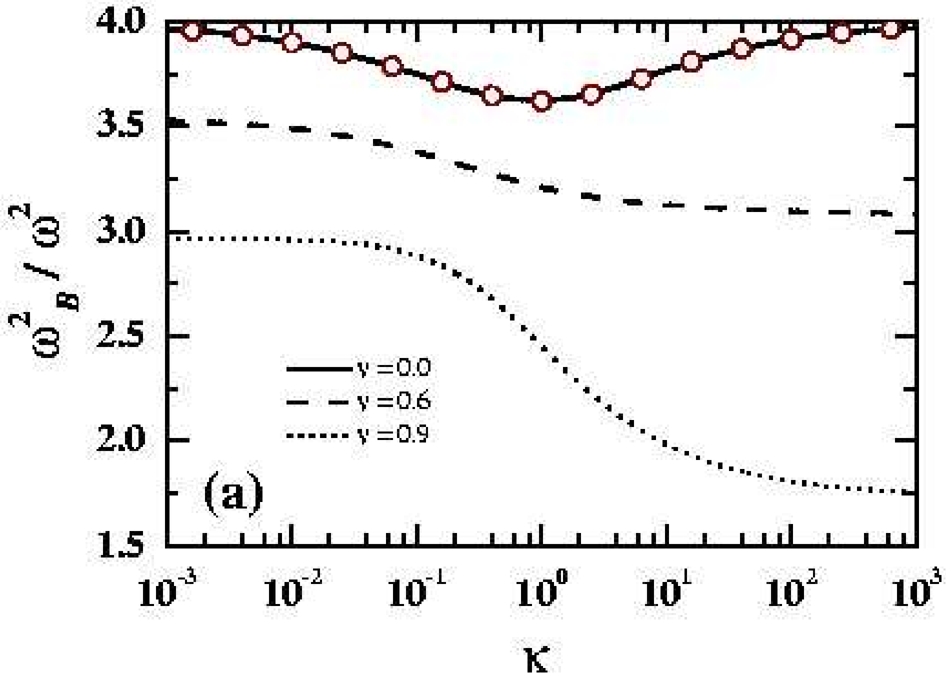
Luttinger long-wavelength Hamiltonian:

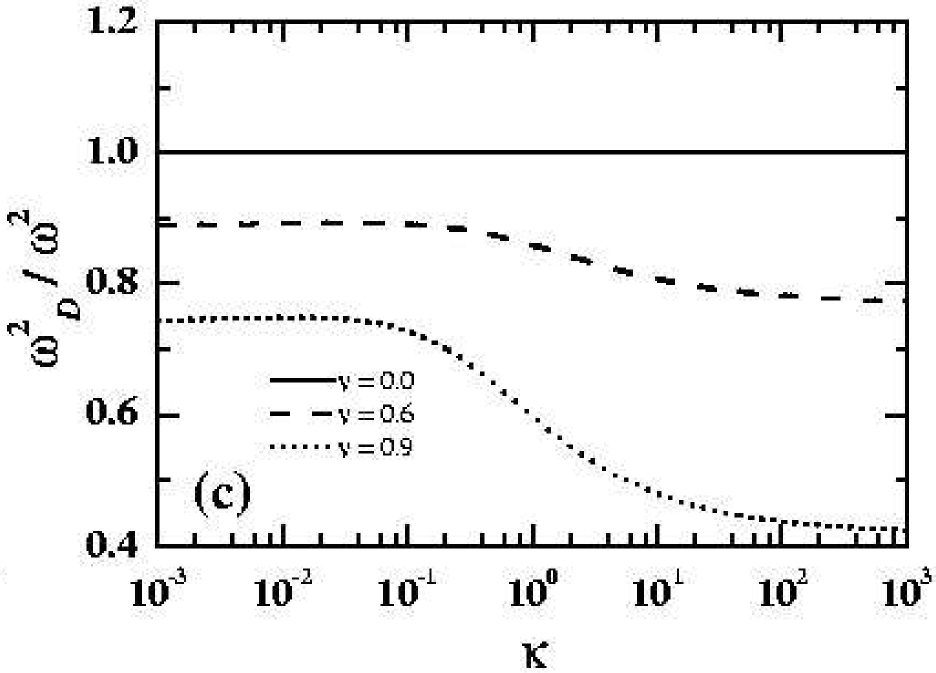
$$\mathcal{H}_{\mathrm{LL}} = \sum_{\nu=\rho,\sigma} \int dx \frac{u_\nu(x)}{2} \left[K_\nu(x) \Pi_\nu^2 + \frac{1}{K_\nu(x)} \left(\frac{\partial \phi_\nu}{\partial x} \right)^2 \right].$$

- Density and phase velocity u_ρ, u_σ
- Luttinger exponents K

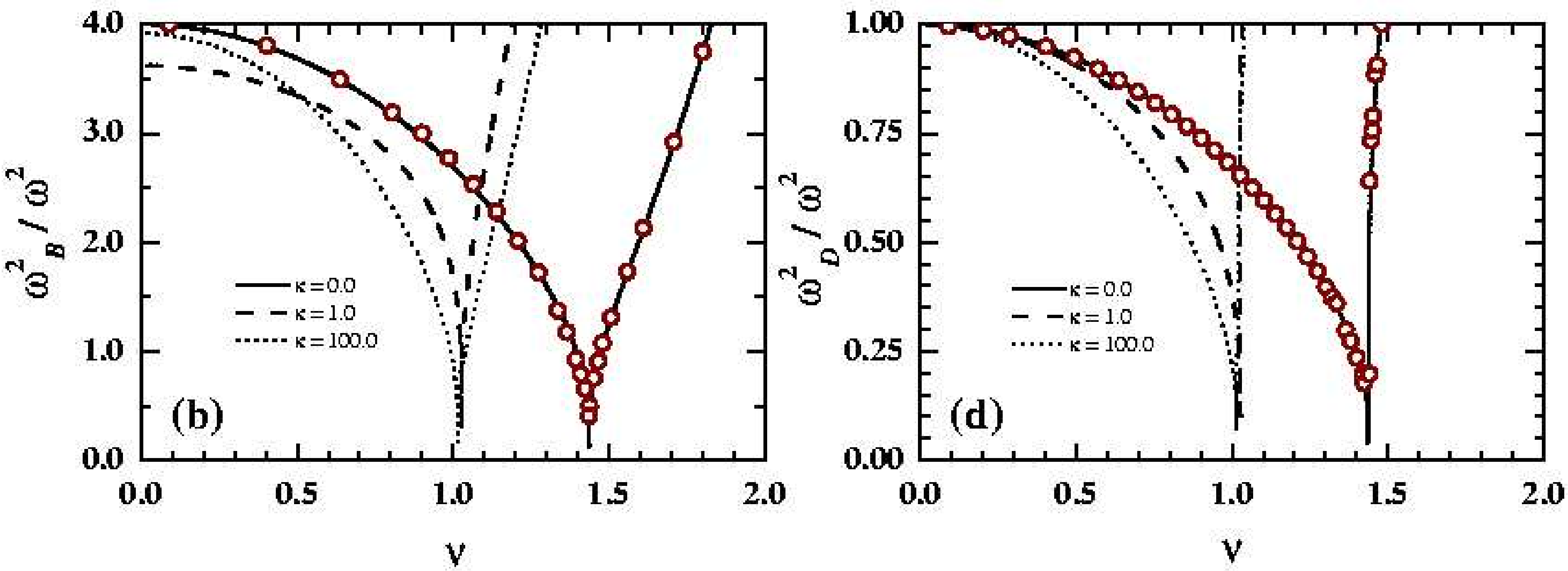
Use local-density approximation, solve for collective mode frequency.

Collective mode frequency vs coupling





Collective mode frequency vs filling factor



Conclusions

- Solved for collective fermionic modes in a trap+lattice
- Frequency dip signature of metal-insulator transition, BUT
  - Linearized method (small displacements)
  - Zero temperature only
  - No damping calculated!
- **Unsolved problem for large trap displacements**

III: Quantum simulation with Gaussian operators

- Quantum field theory calculation WITHOUT approximation?
- Using Gaussian operator basis
- Treat **covariances** as phase-space variables.
- Simulates both ***fermions*** and ***bosons***
- Can treat thermal ensembles and dynamics
- **NO: anticommutators, determinants, Fermi sign problem**

QMC sign problem

- Quantum Monte Carlo is a standard technique
- Except for special cases, fermionic QMC suffers from sign problems:

$$\langle A \rangle \sim \frac{\langle sA \rangle}{\langle s \rangle}$$

- published results almost always have approximations!
- sign problem increases with dimension, lattice size, interaction strength
- **QMC doesn't work at all for quantum dynamics!**

General expansion

Expand state density operator $\widehat{\rho}$ in operator basis $\widehat{\Lambda}$:

$$\widehat{\rho} = \int P(\overrightarrow{\lambda})\widehat{\Lambda}(\overrightarrow{\lambda})d\overrightarrow{\lambda}$$

- $P(\overrightarrow{\lambda})$ is a probability distribution, sampled stochastically
- $\overrightarrow{\lambda}$ constitutes a phase-space

Strategy

- ✔ Choose basis to match PHYSICAL state
- ✔ Choose gauge to stabilize equations
- ✔ Choose algorithm to reduce sampling variance

OUTLINE

1. **Evolution:** $\partial\widehat{\rho}/\partial t = \widehat{L}[\widehat{\rho}]$

2. **Phase space**: $\overrightarrow{\lambda} = (\Omega, \alpha)$

3. **Basis:** $\widehat{\Lambda}(\overrightarrow{\lambda})$: $\widehat{\rho} = \int P(\overrightarrow{\lambda})\widehat{\Lambda}(\overrightarrow{\lambda})d^{2p)}\overrightarrow{\lambda}$

4. **Identities**: $\partial\widehat{\rho}/\partial t = \int P(\overrightarrow{\lambda})[\mathcal{L}\widehat{\Lambda}(\overrightarrow{\lambda})]d^{2p}\overrightarrow{\lambda}$

5. **Partial integration:** $\partial P/\partial t = \mathcal{L}'P = [-\overrightarrow{\partial}\mathbf{A} + \frac{1}{2}\overrightarrow{\partial}\mathbf{D}\overrightarrow{\partial}]P(\overrightarrow{\lambda})$

6. **Noise**: $\mathbf{D} = \mathbf{B}^T\mathbf{B}$, $\partial\overrightarrow{\lambda}/\partial t = \mathbf{A} + \mathbf{B}\overrightarrow{\zeta}$

APPLICATIONS: STATIC CALCULATIONS

- ♢ Grand canonical distribution: $\widehat{\rho} = \exp(-(\widehat{H} - \mu\widehat{N})\tau)$

  $\Longrightarrow$ $\widehat{\rho}$ is the unnormalised density operator

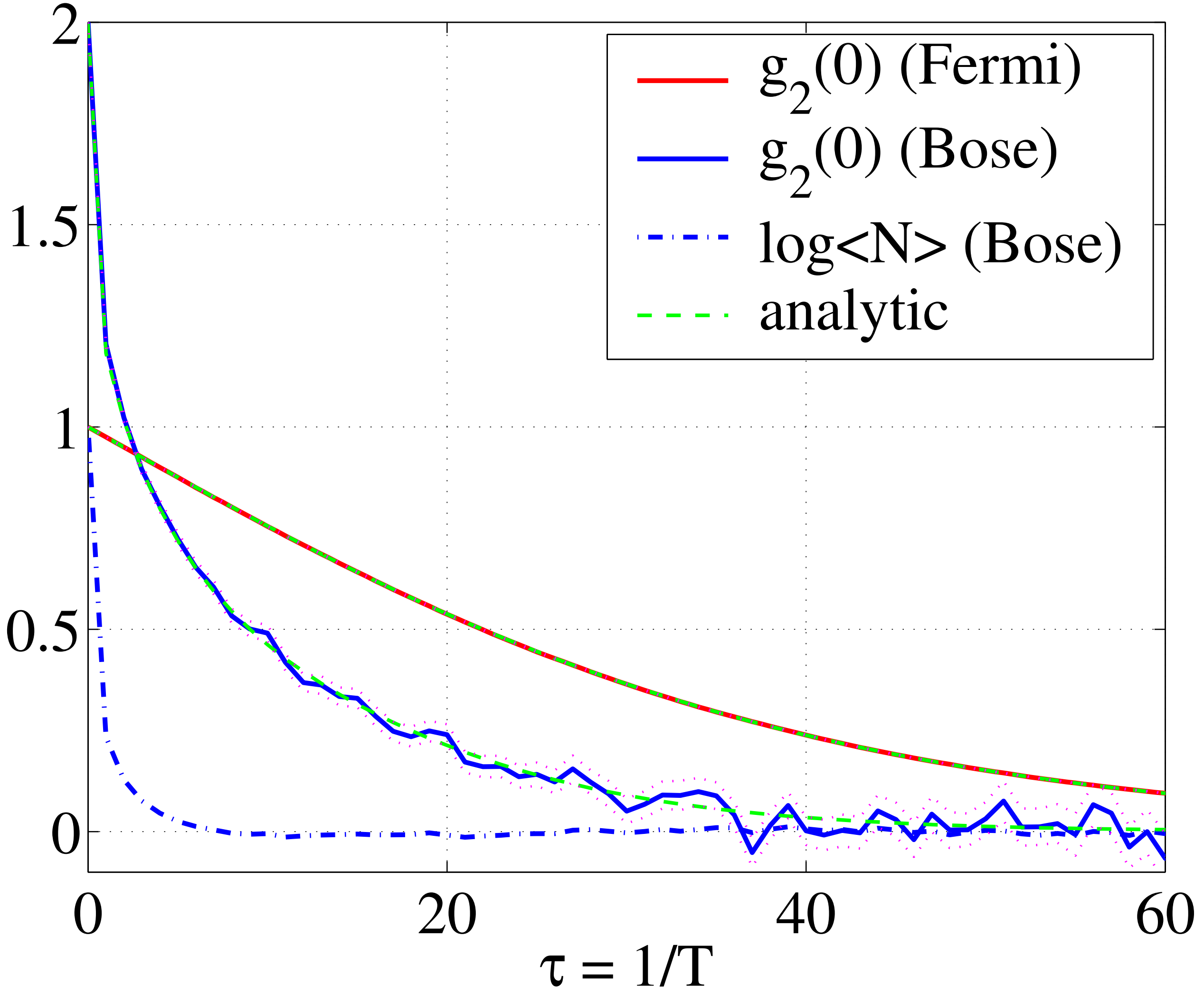
  $\Longrightarrow$ $\tau = 1/k_B T$ is the inverse temperature,

  $\Longrightarrow$ μ the chemical potential

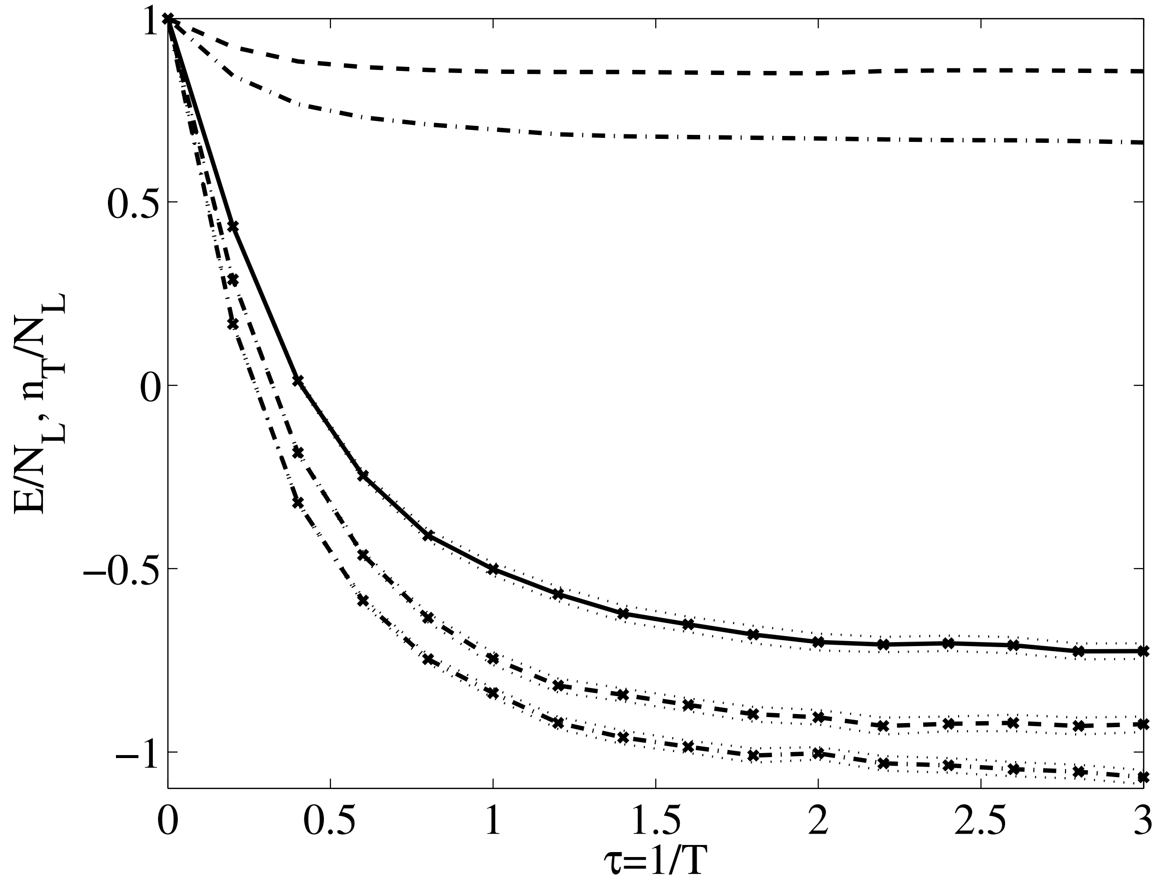
- ♢ Rewrite as equation for temperature evolution:

$$d\widehat{\rho}/d\tau = -\left[(\widehat{H} - \mu\widehat{N}), \widehat{\rho}\right]_{+}/2$$

1 site: bosons cf fermions



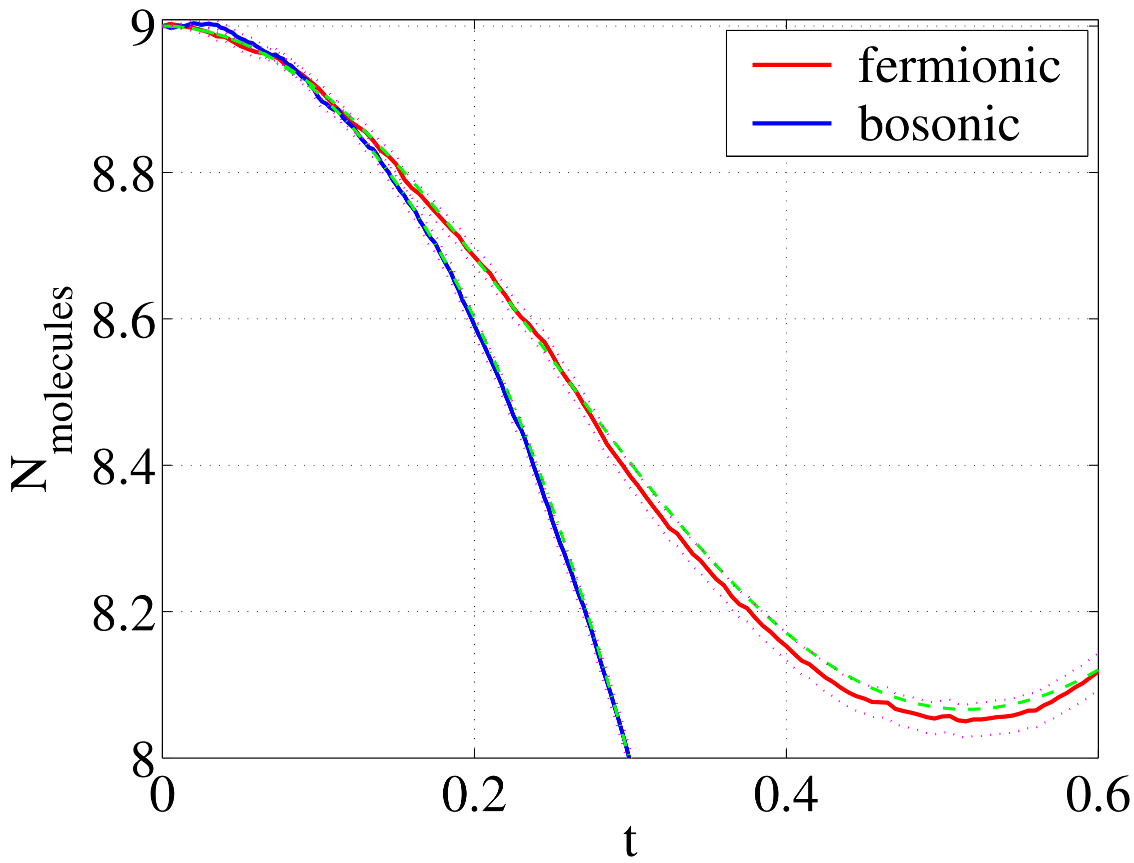
2D Lattice-256 sites: no Fermi sign problem



Quantum dynamics: bosons into fermions

- Ultracold molecules converted to fermionic atoms?
- Experiments at JILA, Innsbruck, MIT, Duke Uni, Paris (ENS)
- Single-well bosonic photoassociation observed in Texas, Max-Planck
- What about molecular dissociation in an optical lattice?
- Pauli blockade limits down-conversion to fermionic atoms.
- Simple test of Fermi-Bose quantum simulation

Pauli blockade: CAN NIST DO THIS?



- You can't run, you can't hide....

Summary: fermions@UQ

- Our Feshbach field-theory model is well-confirmed
- Simple, physical approach to BEC/BCS crossover
- Theory of Mott 1D, zero temperature case
- **FREQUENCY DIP AT MOTT INSULATOR TRANSITION**
- new exact technique for dynamic & static Fermi calculations
- can calculate correlations at any temperature - 1D, 2D or 3D
- **SOLVES THE USUAL FERMI SIGN PROBLEM**