Ultracold fermion theory @ UQ

P. D. Drummond, J. F. Corney, K. Kheruntsyan, X.-J. Liu, H. Hu*

Australian Centre for Quantum Atom Optics
*Scuola Normale Superiore, Pisa.

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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
- apply simple theoretical models to high accuracy
- 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

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Quantum field theory: K&D 2000

\[ H_0 = \sum_{i=m,1,2} \int dx \left[ \frac{\hbar^2}{2m_i} |\nabla \Psi_i|^2 + E_M \Psi_M^+ \Psi_M \right] \]

\[ H_s = \sum_{ij} \frac{\hbar U_{ij}}{2} \int dx \Psi_i^+ \Psi_j \Psi_j \Psi_i \]

\[ H_{M\Rightarrow A_1+A_2} = \frac{\hbar \chi}{2} \int dx \left[ \Psi_M^+ \Psi_1 \Psi_2 + H.c. \right] \]

- \( \Psi_{1,2,M}(t, x) \) – field operators \([a_{1,2}(k), b(k)]\)

- \( E_M \) – ’bare’ energy detuning; \( U_{ij} \) – s-wave scattering

- \( \chi \) – atom-molecule coupling \((A_1 + A_2 \Leftrightarrow M)\)

- One year BEFORE Timmermans or Holland et al :-)}
Coherent quantum superposition

- **EXACT** quantum ground-state solution, for \( N = 2 \):

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

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

- Renormalised binding energy vs B-field

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

\( s = 2 \) for fermions [K&D 2004]
Molecular binding energy in $^{40}\text{K}_2$

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

\begin{align*}
\text{our theory} \\
\text{JILA’03 $^{40}\text{K}_2$ exp.} \\
(B_0 = 224 \text{ G})
\end{align*}
Bosonic case: $^{85}\text{Rb}_2$ 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 $^6\text{Li}_2$? [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 \( \alpha \) to obtain correct density
Variational solution

Including renormalization, we obtain two basic gap equations:

\[ 1 = \tilde{U}_0 \int_0^K \frac{q^2 dq}{4\pi^2} \left[ \frac{1}{\varepsilon_q} - \frac{1}{E_q} \right] \]

\[ n = 2 \left[ \frac{\chi_0 \Delta}{\varepsilon_0 \tilde{U}_0} \right]^2 + \int_0^K \frac{q^2 dq}{2\pi^2} \left[ 1 - \frac{U_q}{E_q} \right] \]

✔ 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

\[ \hat{H} = -t \sum_{\langle i,j \rangle, \sigma} \hat{a}^+_i \sigma \hat{a}_j \sigma + U \sum_j \hat{n}_{j, \uparrow} \hat{n}_{j, \downarrow} \]

- Simplest model of an interacting Fermi gas
- Describes ultracold gas in an optical lattice
- Weak-coupling limit \( \rightarrow \) BCS transitions
- Relevance to high-\( T_c \) superconductors?
- Test theories of strongly interacting fermions
Fermionic vs Bosonic Hubbard physics!

Fermions

Bosons

|1⟩
|2⟩

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TRAPPED 1D FERMI GAS

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

- Includes 1D trap potential
- Use local density approximation
- Based on exact solution for 1D Hubbard model
Energy Bands in Mott-Insulator regime

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

Interactions $\implies$ Mott insulator at half-filling (not yet seen).
Characteristic parameters

- Effective mass: \( m^* = \frac{\hbar^2}{(2td^2)} \)
- Dimensionless trapping frequency: \( \omega = \frac{\hbar \omega_0 (m/m^*)^{1/2}}{t} \)
- Coupling constant \( \kappa = \frac{U^2}{(8t^2N\omega)} \)
- Effective filling factor \( \nu = \frac{\sqrt{2N\omega}}{\pi} \)
Phase-diagram vs filling $\nu$ and coupling $\kappa$
Cross-over: Filling vs $v$, at $\kappa = 1$
Luttinger approximation

Luttinger long-wavelength Hamiltonian:

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

- Density and phase velocity \( u_\rho, u_\sigma \)
- Luttinger exponents \( K \)

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

(a)

(b)

(c)

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Collective mode frequency vs filling factor

(b)

(d)
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
Quantum Monte Carlo is a standard technique. However, 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 $\hat{\rho}$ in operator basis $\hat{\Lambda}$:

$$\hat{\rho} = \int P(\vec{\lambda})\hat{\Lambda}(\vec{\lambda})d\vec{\lambda}$$

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

✔ Choose basis to match PHYSICAL state

✔ Choose gauge to stabilize equations

✔ Choose algorithm to reduce sampling variance
1. **Evolution:** \( \partial \hat{\rho} / \partial t = \hat{L}[\rho] \)

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

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

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

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

6. **Noise:** \( D = B^TB, \partial \vec{\lambda} / \partial t = A + B \vec{\zeta} \)
APPLICATIONS: STATIC CALCULATIONS

◊ Grand canonical distribution: \( \hat{\rho} = \exp(- (\hat{H} - \mu \hat{N}) \tau) \)

\[ \text{⇒} \quad \hat{\rho} \text{ is the unnormalised density operator} \]
\[ \text{⇒} \quad \tau = 1/k_B T \text{ is the inverse temperature,} \]
\[ \text{⇒} \quad \mu \text{ the chemical potential} \]

◊ Rewrite as equation for temperature evolution:

\[ d\hat{\rho}/d\tau = - \left[ (\hat{H} - \mu \hat{N}), \hat{\rho} \right]_+ / 2 \]
1 site: bosons cf fermions

- $g_2(0)$ (Fermi)
- $g_2(0)$ (Bose)
- log<N> (Bose)
- analytic
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