Lecture 2: Ultracold fermions

Fermions in optical lattices. Fermi Hubbard model. Current state of experiments

Lattice modulation experiments

Doublon lifetimes

Stoner instability
Ultracold fermions in optical lattices
Fermionic atoms in optical lattices

\[ \mathcal{H} = -t \sum_{\langle ij \rangle \sigma} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} - \mu \sum_i n_i \]

Experiments with fermions in optical lattice, Kohl et al., PRL 2005
Quantum simulations with ultracold atoms

$YBa_2Cu_3O_7$

Antiferromagnetic and superconducting $T_c$ of the order of 100 K

Atoms in optical lattice

Antiferromagnetism and pairing at sub-micro Kelvin temperatures

Same microscopic model

$$\mathcal{H} = -t \sum_{\langle ij \rangle \sigma} c_{i\sigma} \dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} - \mu \sum_i n_i$$
Positive U Hubbard model


Antiferromagnetic insulator

D-wave superconductor
Repulsive Hubbard model at half-filling

\[ T \sim U \]

\[ T_N \sim t e^{-\sqrt{2\pi} \left( \frac{t}{U} \right)^{1/2}} \]

\[ T_N \sim \frac{t^2}{U} \]

current experiments

Mott state without AF order
Signatures of incompressible Mott state of fermions in optical lattice

Suppression of double occupancies

Compressibility measurements
Lattice modulation experiments with fermions in optical lattice.

Probing the Mott state of fermions

Sensarma, Pekker, Lukin, Demler, PRL (2009)

Related theory work: Kollath et al., PRL (2006)
Huber, Ruegg, PRB (2009)
Orso, Iucci, et al., PRA (2009)
Lattice modulation experiments
Probing dynamics of the Hubbard model

Modulate lattice potential $V_0$

Measure number of doubly occupied sites

$t \sim \exp(-\sqrt{V_0/E_R})$

$U \sim \left(\frac{V_0}{E_R}\right)^{3/4}$

Main effect of shaking: modulation of tunneling

$\mathcal{H}_{\text{pert}}(\tau) = \lambda t \cos \omega \tau \sum_{\langle ij \rangle \sigma} c_i^\dagger c_j^\sigma$

Doubly occupied sites created when frequency $\omega$ matches Hubbard $U$
Lattice modulation experiments
Probing dynamics of the Hubbard model

Mott state

Regime of strong interactions $U \gg t$.

Mott gap for the charge forms at $T \sim U$

Antiferromagnetic ordering at $T_N \sim J = \frac{4t^2}{U}$

“High” temperature regime $T_N << T << U$

All spin configurations are equally likely. Can neglect spin dynamics.

“Low” temperature regime $T \leq T_N$

Spins are antiferromagnetically ordered or have strong correlations
Schwinger bosons and Slave Fermions

Bosons

\[ c_{i\sigma}^\dagger = a_{i\sigma}^\dagger h_i + \sigma a_{i-\sigma} d_i^\dagger \]

Fermions

Constraint:

\[ a_{i\sigma}^\dagger a_{i\sigma} + d_i^\dagger d_i + h_i^\dagger h_i = 1 \]

Singlet Creation

\[ A_{ij}^\dagger = a_{i\uparrow}^\dagger a_{j\downarrow}^\dagger - a_{i\downarrow}^\dagger a_{j\uparrow}^\dagger \]

Boson Hopping

\[ F_{ij}^\dagger = a_{i\uparrow}^\dagger a_{j\uparrow}^\dagger + a_{i\downarrow}^\dagger a_{j\downarrow}^\dagger \]
Schwinger bosons and slave fermions

Fermion hopping

\[ c_{i\uparrow}^\dagger c_{j\uparrow} + c_{i\downarrow}^\dagger c_{j\downarrow} + \text{h.c.} = (d_{i\uparrow}^\dagger d_{j\downarrow} - h_{i\uparrow}^\dagger h_{j\downarrow}) F_{ij} + d_{i\uparrow}^\dagger h_{j\downarrow}^\dagger A_{ij} + \text{h.c.} \]

Propagation of holes and doublons is coupled to spin excitations. Neglect spontaneous doublon production and relaxation.

Doublon production due to lattice modulation perturbation

\[ \mathcal{H}(\tau) = \lambda t \sin \omega \tau \sum_{\langle ij \rangle} (d_{i\uparrow}^\dagger h_{j\downarrow}^\dagger A_{ij} + \text{h.c.}) \]

Second order perturbation theory. Number of doublons

\[ N_d(\tau) = t^2 \lambda^2 \int_0^\tau dt' \int_0^\tau dt'' \sin[\omega t'] \sin[\omega t''] \sum_{\langle ij \rangle\langle lm \rangle} \langle A_{ij}^\dagger(t') d_i(t') h_j(t') h_m^\dagger(t'') d_l^\dagger(t'') A_{lm}(t'') \rangle \]
“Low” Temperature \( T \ll T_N \)

Schwinger bosons Bose condensed

Propagation of holes and doublons strongly affected by interaction with spin waves

Assume independent propagation of hole and doublon (neglect vertex corrections)

Self-consistent Born approximation

\[
\begin{array}{c}
\text{Spectral function for hole or doublon} \\
\text{Sharp coherent part:} \\
\text{dispersion set by } t^2/U, \text{ weight by } t/U \\
\text{Incoherent part:} \\
\text{dispersion } 4t \times \text{dimension} \\
\end{array}
\]

Oscillations reflect shake-off processes of spin waves
“Low” Temperature $T << T_N$

Rate of doublon production

- Sharp absorption edge due to coherent quasiparticles
- Broad continuum due to incoherent part
- Spin wave shake-off peaks
“High” Temperature

Calculate self-energy of doublons and holes interacting with incoherent spin excitations (Schwinger bosons) in the non-crossing approximation

\[ T_N << T << U \]

Sensarma et al., PRL (2009)
Tokuno et al. arXiv:1106.1333

Equivalent to Retraceable Path Approximation

Brinkmann & Rice, 1970

In calculating spectral function consider paths with no closed loops
“High” Temperature

\[ T_N << T << U \]

Spectral Fn. of single hole

Doublon production rate

Experiment:
R. Joerdens et al.,

Theory:
Sensarma et al., PRL (2009)
Tokuno et al. arXiv:1106.1333
Temperature dependence

Reduced probability to find a singlet on neighboring sites

D. Pekker et al., unpublished
Fermions in optical lattice.  
Decay of repulsively bound pairs

Experiments: ETH group  
Theory: Sensarma, Pekker, et. al.

Ref: N. Strohmaier et al., PRL 2010
Fermions in optical lattice.
Decay of repulsively bound pairs

Doublons – repulsively bound pairs
What is their lifetime?

Direct decay is not allowed by energy conservation

Excess energy $U$ should be converted to kinetic energy of single atoms

Decay of doublon into a pair of quasiparticles requires creation of many particle-hole pairs
Fermions in optical lattice.
Decay of repulsively bound pairs

Experiments: N. Strohmaier et. al.
Relaxation of doublon- hole pairs in the Mott state

Energy $U$ needs to be absorbed by spin excitations

- Energy carried by spin excitations
  $\sim J = 4t^2/U$

- Relaxation requires creation of $\sim U^2/t^2$ spin excitations

Relaxation rate

$$W \sim t(t/U)^{U^2/t^2}$$

Sensarma et al., PRL 2011

Very slow, not relevant for ETH experiments
Doublon decay in a compressible state

Excess energy $U$ is converted to kinetic energy of single atoms

Compressible state: Fermi liquid description

Doublon can decay into a pair of quasiparticles with many particle-hole pairs
Doublon decay in a compressible state

Perturbation theory to order $n=\frac{U}{6t}$
Decay probability

$$P \sim \left( \frac{t}{U} \right)^{\text{const} \cdot \frac{U}{6t}} \sim e^{-\text{const} \cdot \frac{U}{6t} \cdot \log\left(\frac{U}{t}\right)}$$

Doublon Propagator

Interacting “Single” Particles
To calculate the rate: consider processes which maximize the number of particle-hole excitations
Why understanding doublon decay rate is interesting

Important for adiabatic preparation of strongly correlated systems in optical lattices.

Response functions of strongly correlated systems at high frequencies. Important for numerical analysis.

Prototype of decay processes with emission of many interacting particles.
Example: resonance in nuclear physics: (i.e. delta-isobar)

Analogy to pump and probe experiments in condensed matter systems.
Doublon relaxation in organic Mott insulators ET-F$_2$TCNQ
One dimensional Mott insulator ET-F$_2$TCNQ

bis(ethylenedithio)tetrathiafulvalene difluorotetracyanoquinodimethane

\begin{align*}
\epsilon_2 \quad & \text{Phonon energy (eV)} \\
0.5 & 1 \\
1.5 & 2 \\
2.5 & 3 \\
\end{align*}

Mott-insulator state

t=0.1 eV

U=0.7 eV
Photoinduced metallic state

S. Wall et al. Nature Physics 7:114 (2011)

Photoexcitations

Conducting state by photo-doping

Surprisingly long relaxation time 840 fs

$\frac{\Delta R}{R} = 0$

Delay (fs)

$\frac{\Delta R}{R} = -0.1$

$\frac{\Delta R}{R} = -0.3$

$h/t = 40$ fs
Photoinduced metallic state

S. Wall et al. Nature Physics 7:114 (2011)

\[ \tau \sim \frac{2}{t} e^{1.6 \frac{U}{w}} \]

\( t = 0.1 \text{ eV} \)
\( w = 4t = 0.4 \text{ eV} \)
\( U = 0.7 \text{ eV} \)

\( \sim 1400 \text{ fs} \)

comparable to experimentally measured 840 ms
Exploring beyond simple Hubbard model with ultracold fermions
SU(N) Hubbard model with Ultracold Alkaline-Earth Atoms

Theory: A. Gorshkov, et al., Nature Physics 2010

**Ex:** $^{87}\text{Sr}$ ($I = 9/2$)

- $|e\rangle = ^3P_0$
- $|g\rangle = ^1S_0$

Experiments:
- realization of SU(6) fermions
- Takahashi et al. PRL (2010)
- Also J. Ye et al., Science (2011)

- Nuclear spin decoupled from electrons
- SU(N=2I+1) symmetry

→ SU(N) Hubbard models ⇒ valence-bond-solid & spin-liquid phases

- orbital degree of freedom ⇒ spin-orbital physics
- Kugel-Khomskii model [transition metal oxides with perovskite structure]
- SU(N) Kondo lattice model [for N=2, colossal magnetoresistance in manganese oxides and heavy fermion materials]
Nonequilibrium dynamics: expansion of interacting fermions in optical lattice

U. Schneider et al., Nature Physics 2012

New dynamical symmetry: identical slowdown of expansion for attractive and repulsive interactions
Competition between pairing and ferromagnetic instabilities in ultracold Fermi gases near Feshbach resonances

Phys. Rev. Lett. 2010


Motivated by experiments of G.-B. Jo et al., Science (2009)
Stoner model of ferromagnetism

Spontaneous spin polarization decreases interaction energy but increases kinetic energy of electrons

Mean-field criterion

\[ U N(0) = 1 \]

\( U \) – interaction strength
\( N(0) \) – density of states at Fermi level

Kanamori’s counter-argument: renormalization of \( U \).

\[
U_{\text{eff}} = \frac{U}{1 + U \chi_0} \sim \frac{U}{1 + \frac{U}{E_F}} < E_F
\]

then

\[
U_{\text{eff}} N(0) < 1
\]

Theoretical proposals for observing Stoner instability with cold gases:
Salasnich et. al. (2000); Sogo, Yabu (2002); Duine, MacDonald (2005); Conduit, Simons (2009); LeBlanck et al. (2009); ...

Recent work on hard sphere potentials: Pilati et al. (2010); Chang et al. (2010)
Experiments were done dynamically. What are implications of dynamics? Why spin domains could not be observed?

Earlier work by C. Salomon et al., 2003
Is it sufficient to consider effective model with repulsive interactions when analyzing experiments?

Feshbach physics beyond effective repulsive interaction
Feshbach resonance

Interactions between atoms are intrinsically attractive
Effective repulsion appears due to low energy bound states

Example:

\[ H = \frac{\hat{p}_1^2}{2m} + \frac{\hat{p}_2^2}{2m} + V_0 \xi^{-2} e^{-(\hat{x}_1 - \hat{x}_2)^2 / 2\xi^2} \]

\( V_0 \) tunable by the magnetic field
Can tune through bound state

scattering length
Feshbach resonance

Two particle bound state formed in vacuum

Stoner instability

BCS instability

Molecule formation and condensation

This talk: Prepare Fermi state of weakly interacting atoms.
Quench to the BEC side of Feshbach resonance.
System unstable to both molecule formation and Stoner ferromagnetism. Which instability dominates?
Pair formation
Two-particle scattering in vacuum

\[ |\Psi\rangle = \left( c_{k\uparrow}^{\dagger} c_{-k\downarrow}^{\dagger} + \sum_p \psi_p c_{p\uparrow}^{\dagger} c_{-p\downarrow}^{\dagger} \right) |0\rangle \]

Microscopic Hamiltonian

\[ \mathcal{H} = \sum_{p\sigma} \epsilon_p c_{p\sigma}^{\dagger} c_{p\sigma} + \frac{1}{V} \sum_{p,p'} V(p-p') c_{p\uparrow}^{\dagger} c_{-p\downarrow}^{\dagger} c_{-p'\downarrow} c_{p'\uparrow} \]

Schrödinger equation

\[ E |\Psi\rangle = \mathcal{H} |\Psi\rangle \]

\[ E\psi_p = 2\epsilon_p \psi_p + V(k-p) + \frac{1}{V} \sum_{p'} V(p-p') \psi_{p'} \]
**T-matrix**

\[ T_E(p, k) = (E - 2\epsilon_p)\psi_p \]

Lippman-Schwinger equation

\[ T_E(p, k) = V(p - k) + \frac{1}{V} \sum_{p'} V(p - p') \frac{T_E(p', k)}{E - 2\epsilon_{p'} + i0} \]

On-shell T-matrix. Universal low energy expression

\[ T_E = -\frac{m}{4\pi} \left( -\frac{1}{a} + r_em E - i \sqrt{mE} \right)^{-1} \]

For positive scattering length bound state at \( E = -\frac{1}{ma^2} \) appears as a pole in the T-matrix.
Cooperon

Two particle scattering in the presence of a Fermi sea

\[ | \Psi \rangle = \left( c_{k \uparrow} \dagger c_{-k \downarrow} \dagger + \sum_p \psi_p c_{p \uparrow} \dagger c_{-p \downarrow} \dagger \right) | FL \rangle = O \dagger | FL \rangle \]

Need to make sure that we do not include interaction effects on the Fermi liquid state in scattered state energy

\[ T(i \omega_n, q) = + + \ldots \]

\[ T(i \omega_n, q) = + \frac{i \omega_n}{2} + i \omega_1, \frac{q}{2} + p \]

\[ T(i \omega_n, q) = + \frac{i \omega_n}{2} - i \omega_1, \frac{q}{2} - p \]
Cooperon vs T-matrix

\[
T_E(p, k) = V(p - k) + \frac{1}{V} \sum_{p'} V(p - p') \frac{T_E(p', k)}{E - 2\epsilon_{p'} + i0}
\]

\[
C_E(p, k) = V(p - k) + \frac{1}{V} \sum_{p'} V(p - p') \frac{C_E(p', k) (1 - 2n_{p'})}{(E - 2(\epsilon_{p'} - \mu) + i0)}
\]

\[
C_E^{-1} = T_{E+2\mu}^{-1} + \int \frac{d^3 p}{(2\pi)^3} \frac{2n_p}{(E - 2(\epsilon_p - \mu))}
\]
Cooper channel response function

Linear response theory

\[ \mathcal{H} = \mathcal{H}_0 + \frac{1}{V} \sum_k \left( h^A_\omega \, e^{-i\omega t} \, c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger + \text{c.c.} \right) \]

Induced pairing field

\[ \Delta_\omega = \frac{1}{V} \sum_k \langle c_{-k\downarrow} c_{k\uparrow} \rangle_t \, e^{i\omega t} \]

Response function

\[ \chi^\Delta_\omega = \frac{\Delta_\omega}{h_\omega^A} = \frac{1}{V^2} \sum_{k,p} C_{\omega}(k,p) f_k f_p \]

Poles of the Cooper channel response function are given by \( C^\prime_\omega \)
Cooper channel response function

Linear response theory \[ \Delta_{q,\omega} = \chi_{q,\omega}^\Delta h_{q,\omega}^\Delta \]

Poles of the response function, \((\chi_{q,\omega_q}^\Delta)^{-1} = 0\), describe collective modes

Time dependent dynamics \[ \Delta_q(t) \sim e^{i\omega_q t} \]

When the mode frequency has negative imaginary part, the system is unstable

\[ \omega_q = -i\Gamma_q \]

\[ \Delta_q(t) \sim e^{\Gamma_q t} \]
Pairing instability regularized

\[
T_{E+2E_F-q^2/m}^{-1} + \int \frac{d^3k}{(2\pi)^3} \frac{n(\frac{q}{2} + k) + n(\frac{q}{2} - k)}{(E + 2E_F - \epsilon_{\frac{q}{2} + k} - \epsilon_{\frac{q}{2} - k})} = 0
\]

\[
T_E = \frac{m}{4\pi} \left( \frac{1}{a} + i\sqrt{mE} \right)^{-1}
\]

BCS side \( \Gamma \approx \frac{8}{e^2} E_F e^{-\pi/2 k_F a} \)

Instability rate coincides with the equilibrium gap (Abrikosov, Gorkov, Dzyaloshinski)

Instability to pairing even on the BEC side

Related work: Lamacraft, Marchetti, 2008
Pairing instability

Intuition: two body collisions do not lead to molecule formation on the BEC side of Feshbach resonance. Energy and momentum conservation laws can not be satisfied.

This argument applies in vacuum. Fermi sea prevents formation of real Feshbach molecules by Pauli blocking.

\[
|k| \leq \frac{1}{a_s} \quad \text{Molecule}
\]

\[
|k| \leq k_F \quad \text{Fermi sea}
\]
Pairing instability

Time dependent variational wavefunction

\[ | \Psi(t) \rangle = \prod_k \left( u_k(t) + v_k(t) \, c_{k\uparrow}^\dagger \, c_{-k\downarrow}^\dagger \right) | 0 \rangle \]

Time dependence of \( u_k(t) \) and \( v_k(t) \) due to \( \Delta_{BCS}(t) \)

For small \( \Delta_{BCS}(t) \):

\[ \frac{d}{dt} \log \Delta_{BCS} = \Delta \]
Pairing instability

Effects of finite temperature

From wide to narrow resonances

Three body recombination as in Shlyapnikov et al., 1996; Petrov, 2003; Esry 2005

Observed in recent experiments by Grimm’s group, arXiv:1112.0020
Magnetic instability
Stoner instability. Naïve theory

\[ \mathcal{H}_0 = \sum_{p\sigma} (\epsilon_p - \mu) c^\dagger_{p\sigma} c_{p\sigma} + U \int d^3 r \, n^\uparrow(r) n^\downarrow(r) \]

\[ U = 4\pi a_s / m \]

Linear response theory

\[ \mathcal{H} = \mathcal{H}_0 - (h^\alpha_{q\omega} e^{-i\omega t} S^\alpha_q + \text{c.c.}) \]

\[ S^\alpha_q = \frac{1}{2V} \sum_{p\sigma\sigma'} c^\dagger_{p+q\sigma} \sigma^\alpha_{\sigma\sigma'} c_{p\sigma'} \]

Spin response function

\[ \langle S^\alpha_{q\omega} \rangle = \chi^S_{q\omega} h^\alpha_{q\omega} \]

Spin collective modes are given by the poles of response function

\[ (\chi^S_{q\omega_q})^{-1} = 0 \]

Negative imaginary frequencies correspond to magnetic instability
RPA analysis for Stoner instability

\[ \mathcal{H}_{\text{eff}} = \sum \epsilon_p c_{p\sigma}^\dagger c_{p\sigma} - U \left( \langle S_{-q}^z (t) \rangle S_q^z + \langle S_q^z (t) \rangle S_{-q}^z \right) - (h_{q\omega}^\alpha e^{-i\omega t} S_{-q}^\alpha + \text{c.c.}) \]

Self-consistent equation on response function

\[ \langle S_{q\omega}^z \rangle = \chi_{q\omega}^0 (h_{q\omega}^\alpha + U \langle S_{q\omega}^z \rangle) \]

Spin susceptibility for non-interacting gas

\[ \chi_{q\omega}^0 = \int \frac{d^3p}{(2\pi)^3} \frac{n_{p+q} - n_p}{(\omega - (\epsilon_{p+q} - \epsilon_p))} \]

RPA expression for the spin response function

\[ \chi_{q\omega} = \frac{\chi_{q\omega}^0}{1 - U \chi_{q\omega}^0} \]
Quench dynamics across Stoner instability

Stoner criterion

\[ U_c = N(0)^{-1} \]

For \( U > U_c \) unstable collective modes

\[ \omega_q = -i\Gamma_q \]

\[ S^z_q(t) \sim e^{-i\omega_q t} \sim e^{\Gamma_q t} \]

Unstable modes determine characteristic lengthscale of magnetic domains
Stoner quench dynamics in D=3

Scaling near transition

\[ u = \frac{U}{U_c} - 1 \]

Growth rate of magnetic domains

\[ \Gamma_q \sim E_F u^{3/2} \]

Domain size

\[ \xi \sim \lambda_F u^{-1/2} \]

Unphysical divergence of the instability rate at unitarity

\[ \Gamma_{\text{max}} \]
Stoner instability is determined by two particle scattering amplitude.

Divergence in the scattering amplitude arises from bound state formation. Bound state is strongly affected by the Fermi sea.
Stoner instability

RPA spin susceptibility

\[ \Gamma_{q,k_1}(q, \omega) = 1 + \int \frac{d\hat{k}_2}{4\pi} \Gamma_{q,\omega}(\hat{k}_2) C(\hat{k}_1 + \hat{k}_2, \omega) I_{q,\omega}(\hat{k}_2) \]

Interaction = Cooperon

\[ C^{-1}(E, q) = \tau^{-1} \left( E + 2\epsilon_f - q^2 / 4m \right) + \int \frac{d^3k}{(2\pi)^3} n^F \left( \frac{q}{2} + k \right) + n^F \left( \frac{q}{2} - k \right) E - \epsilon_{\frac{q}{2} + k} - \epsilon_{\frac{q}{2} - k} \]
Stoner instability

Pairing instability always dominates over pairing

If ferromagnetic domains form, they form at large $q$
Tests of the Stoner magnetism

Spin fluctuations relative to noninteracting fermions

Only short range correlations and no domain formation

Extremely fast molecule formation rate at short times

Atoms loss rate is 13% of $E_F$ on resonance (averaged over trap)

C. Sanner et al., arXiv:1108.2017
Lecture 2: Ultracold fermions

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Future directions in ultracold atoms

Nonequilibrium quantum many-body dynamics

Long intrinsic time scales
- Interaction energy and bandwidth $\sim 1\text{kHz}$
- System parameters can be changed over this time scale

Decoupling from external environment
- Long coherence times

Can achieve highly non equilibrium quantum many-body states

$$H_i \rightarrow H_f$$

$$|\Psi(t)\rangle = e^{-iH_ft} |\Psi_i\rangle$$
Emergent phenomena in dynamics of classical systems

Universality in quantum many-body systems in equilibrium

Solitons in nonlinear wave propagation

Bernard cells in the presence of T gradient

Broken symmetries

Fermi liquid state

Do we have emergent universal phenomena in nonequilibrium dynamics of many-body quantum systems?
Hubbard model at half filling

Paramagnetic Mott phase:
- one fermion per site
- charge fluctuations suppressed
- no spin order

$T \sim U$

BCS-type theory applies

$T_N \propto t e^{-\sqrt{\frac{t}{U}}}$

Heisenberg model applies

$T_N \sim \frac{t^2}{U}$
Hubbard model at half filling

\[ T_N \propto t e^{-\sqrt{\frac{t}{U}}} \]

\[ T \sim U \]

Current experiments

BCS-type theory applies

Heisenberg model applies

\[ T_N \sim \frac{t^2}{U} \]