Quantum Impurities

A Challenge for Quantum Simulation with Ultracold Atoms

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- Harvard University / ITAMP -

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Collaborators

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ultracold quantum gases

atoms trapped by laser in harmonic confinement



condensed matter system with well controlled Hamiltonian

e.g.

$$H = \sum_{\mathbf{p}} \epsilon_{\mathbf{p}} \hat{c}_{\mathbf{p}}^{\dagger} \hat{c}_{\mathbf{p}} + g \sum_{\mathbf{k}, \mathbf{k}', \mathbf{q}} \hat{c}_{\mathbf{k}'-\mathbf{q}}^{\dagger} \hat{c}_{\mathbf{k}} \hat{c}_{\mathbf{k}'}$$
Invertice strength type blocks of the strength type blocks of the

- ➡ interaction strength tunable
- → experimental accessible:
 - density
 - transport coefficients (viscosity, spin diffusion...)
 - responses, correlations



ultracold quantum gases

cold atoms as quantum simulators

optical lattices / single-site detection:

Mott-Insulator to Superfluid transition

MOTT-SUPERFLUID TRANSITION



SHERSON ET AL., NATURE 467 (2010)



QUANTUM GAS MICROSCOPE



BAKR ET AL. SCIENCE 329 (2010) IMAGE: CUAWEB.MIT.EDU - GREINER GROUP

ultracold quantum gases

cold atoms as quantum simulators

optical lattices / single-site detection:

Mott-Insulator to Superfluid transition

Feshbach resonances:

unitary Fermi gas / BEC-BCS crossover

▶ ...







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- ▶ appear in many flavors in condensed matter physics
- relatively simple system from many-body perspective: allow to advance theory in 'controlled way'
- system on the verge from few- to many-body physics

 impurity physics appears also naturally in: quantum optics, quantum dots, NV centers, atomic clocks, cavity QED...



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- decoherence of Rabi oscillations
- level shifts
- line broadening



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finite interactions:

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- level shifts
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- level shifts
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Theoretical challenge: Calculate properties of impurity (strongly) coupled to environment





 novel functional renormalization group method for non-perturbative RG flows of spectral functions RS, ENSS, PRA 83 (2011)



Mainly studied experimentally: THEORY REPUISIVE BRANCH PHYSICS: CUI, ZHAI, PRA 81 (2010), RS, ENSS, PRA 83 (2011), MASSIGNAN, BRUUN, EPJD 65 (2011) Review: Massignan, Zaccanti, Bruun Rep. Proc. Phys. 77, 034401 (2014) Fermi polaron [in continuum] ideal Fermi gas Image: Continuum] Image: Continuum] Image: Continuum] Image: Continuum] Image: Continuum]

- novel functional renormalization group method for non-perturbative RG flows of spectral functions RS, ENSS, PRA 83 (2011)
 - regime of weak attractive interactions
 - energy shift of coherent level



- novel functional renormalization group method for non-perturbative RG flows of spectral functions RS, ENSS, PRA 83 (2011)
 - regime of weak attractive interactions
 - energy shift of coherent level
 - 2) regime of strong attractive interactions



Mainly studied experimentally:

Fermi polaron [in continuum] THEORY REPULSIVE BRANCH PHYSICS: CUI, ZHAI, PRA 81 (2010), RS, ENSS, PRA 83 (2011), MASSIGNAN, BRUUN, EPJD 65 (2011) REVIEW: MASSIGNAN, ZACCANTI, BRUUN REP. PROG. PHYS. 77, 034401 (2014)



Question: What is the spectrum of the impurity?

- novel functional renormalization group method for non-perturbative RG flows of spectral functions RS, ENSS, PRA 83 (2011)
 - regime of weak attractive interactions
 - energy shift of coherent level
 - 2) regime of strong attractive interactions
 - *emergent* effective repulsive interactions
 - single state has split into two branches
 - repulsive branch: ferromagnetic transition cf. work by Tin-Lun Ho, and Massignan, YU, Bruun, PRL 110 (2013)



Experimental observation

our proposal: inverse radio-frequency [rf] spectroscopy RS, ENSS, PRA 83 (2011)

doi:10.1038/nature11065

THREE SPATIAL DIMENSIONS

LETTER KOHSTALL ET AL., NATURE 485 (2012)

Metastability and coherence of repulsive polarons in a strongly interacting Fermi mixture

C. Kohstall^{1,2}, M. Zaccanti¹, M. Jag^{1,2}, A. Trenkwalder¹, P. Massignan³, G. M. Bruun⁴, F. Schreck¹ & R. Grimm^{1,2}







experiment





KOHSTALL ET AL., NATURE 485 (2012)

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experiment





KOHSTALL ET AL., NATURE 485 (2012)



Wednesday, October 29, 14

Our recent work: The Bose Polaron



what happens if medium is Bose gas?

⇒ Bose polaron

A cond-mat motivation: The Froehlich polaron

a paradigm condensed matter model:





Wednesday, October 29, 14

Fröhlich Hamiltonian Fröhlich, Adv. Phys. 3, 325 (1954)

$$\hat{H} = \sum_{\mathbf{p}} \omega_p \hat{b}_{\mathbf{p}}^{\dagger} \hat{b}_{\mathbf{p}} + \sum_{\mathbf{p}} \epsilon_{\mathbf{p}} \hat{c}_{\mathbf{p}}^{\dagger} \hat{c}_{\mathbf{p}} + \sum_{\mathbf{q},\mathbf{p}} \alpha_q \, \hat{c}_{\mathbf{p}+\mathbf{q}}^{\dagger} \hat{c}_{\mathbf{p}} (\hat{b}_{-\mathbf{q}}^{\dagger} + \hat{b}_{\mathbf{q}})$$

- impurity dressed by phonon cloud becomes the 'Fröhlich polaron'
- ▶ enhanced effective mass, renormalized energy SEE E.G. MILLER ET AL. PHYS. REV. 127 ('62)





Fröhlich Hamiltonian Fröhlich, Adv. Phys. 3, 325 (1954)

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perturbation theory:
$$m^* = \frac{m}{1 - \alpha/6}$$
 $\xrightarrow[\alpha > 0]{\alpha > 0}$ self-localization?





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perturbation theory:
$$m^* = \frac{m}{1 - \alpha/6}$$
 $\xrightarrow{\alpha > 0}_{\text{large}}$ self-localization?
strong interactions: variational wave function
LANDAU, PEKAR, JETP 18 (1948); FEYNMAN, COHEN, PHYS. REV. 102 (1956)

- describes localized particle
- yields energy smaller than pert. theory at strong coupling, further evidence of self-localization

Fröhlich Hamiltonian Fröhlich, Adv. Phys. 3, 325 (1954)

$$\hat{H} = \sum_{\mathbf{p}} \omega_p \hat{b}_{\mathbf{p}}^{\dagger} \hat{b}_{\mathbf{p}} + \sum_{\mathbf{p}} \epsilon_{\mathbf{p}} \hat{c}_{\mathbf{p}}^{\dagger} \hat{c}_{\mathbf{p}} + \sum_{\mathbf{q},\mathbf{p}} \alpha_q \, \hat{c}_{\mathbf{p}+\mathbf{q}}^{\dagger} \hat{c}_{\mathbf{p}} (\hat{b}_{-\mathbf{q}}^{\dagger} + \hat{b}_{\mathbf{q}})$$

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perturbation theory:
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 $\rightarrow 0$ $\rightarrow 0$ self-localization?• strong interactions: variational wave function
LANDAU, PEKAR, JETP 18 (1948); FEYNMAN, COHEN, PHYS. REV. 102 (1956) $exp(-\frac{1}{2}g^*y^*) - \frac{1}{2}g^*y^* - \frac{1}{2}g^$

The Bose polaron with ultracold atoms

impurity in Bose gas: Bose polaron

e.g. take strongly imbalanced mixture of ultracold atoms (F. GENERAL CASE: B. LIU, J.HU INT. J. MOD. PHYS, 26 (2012)

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weakly interacting BEC: Bogoliubov approximation for BEC

$$\label{eq:phi} \begin{split} \varphi(\mathbf{x},t) = \sqrt{n_B} + \phi(\mathbf{x},t) \\ & \bigstar \\ \text{mean-field} \qquad \textbf{fluctuations} \end{split}$$

The Bose polaron with ultracold atoms

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e.g. take strongly imbalanced mixture of ultracold atoms (F. GENERAL CASE: B. LIU, J.HU INT. J. MOD. PHYS, 26 (2012)

$$S = \int d^{4}x \varphi^{*}(x) \left(\partial_{\tau} - \frac{1}{2m_{B}} \nabla^{2} - \mu_{B}\right) \varphi(x) + \frac{g_{B}}{2} [\varphi(x)^{*} \varphi(x)]^{2} \qquad \text{bosons} \\ \text{impurity} \\ + \psi^{*}(x) \left(\partial_{\tau} - \frac{1}{2m_{I}} \nabla^{2} - \mu_{I}\right) \psi(x) + g_{IB} \psi(x)^{*} \psi(x) \varphi(x)^{*} \varphi(x) \qquad \text{impurity} \\ \text{weakly interacting BEC: Bogoliubov approximation for BEC} \\ \varphi(\mathbf{x}, t) = \sqrt{n_{B}} + \phi(\mathbf{x}, t) \\ \mathbf{x}_{\text{mean-field}} \qquad \mathbf{x}_{\text{fluctuations}} \\ \text{at weak coupling: Fröhlich Hamiltonian} \\ S_{\text{eff}} = S_{\text{kin}}^{\text{Bos}} + S_{\text{kin}}^{\text{Imp}} + g_{IB} \int_{x} n_{B}(\mathbf{r}) |\psi(\mathbf{r})|^{2} + g_{IB} \int \left\{ \sqrt{n_{B}} \psi^{*}_{\mathbf{k}+\mathbf{q}} \psi_{\mathbf{k}} (\phi_{\mathbf{q}} + \phi^{*}_{-\mathbf{q}}) \right\} \\ \mathbf{MF energy shift} \qquad \text{"Fröhlich term"} \\ \text{ELECTON IN BEC: PFau GROUP [STUTIGATI] - BALEWSKI ET AL., NATURE 502 (2013)} \\ \end{array}$$

 $S_{\rm eff} = S_{\rm kin}^{\rm Bos} + S_{\rm kin}^{\rm Imp} + g_{IB}$

 $\sqrt{n_B}\psi_x^*\psi_x(\phi_x+\phi_x^*)+n_B\psi_x^*\psi_x$ "Fröhlich terms"

 $g_{IB} = \frac{2\pi\hbar^2}{m_r} a_{IB}$

strong effective phonon-impurity interaction wanted

...

HEISELBERG ET AL., PRL 85 (2000) CUCCHIENTTI, TIMMERMANS, PRL 96 (2006) KALAS, BLUME, PRA 73 (2006) WANG, PRL 96 (2006) ENSS, ZWERGER, EPJB 68 (2009) TEMPERE, OBERTHALER ET AL., PRB 80 (2009) CASTEELS ET AL., PRA 83,84,86 (2011) CASTEELS, CAUTEREN, TEMPERE, DEVREESE, LASER PHYS. 21 (2011) CASTEELS, TEMPERE, DEVREESE, PRA 84 (2011) CASTEELS, TEMPERE, DEVREESE, PRA 86 (2012) DASENBROOK, KOMNIK, PRB 87 (2013) BLINOVA, BOSHIER, TIMMERMANS, PRA 88 (2013) SHASHI, GRUSDT, ABANIN, DEMLER, PRA 89, 053617 (2014) GRUSDT, SHCHADILOVA, RUBTSOV, DEMLER, 1410.2203 (2014)



$$S_{\text{eff}} = S_{\text{kin}}^{\text{Bos}} + S_{\text{kin}}^{\text{Imp}} + g_{IB} \int \left\{ \sqrt{n_B} \psi_x^* \psi_x (\phi_x + \phi_x^*) + n_B \psi_x^* \psi_x \qquad g_{IB} = \frac{2\pi\hbar^2}{m_r} a_{IB} \right\}$$

"Fröhlich terms"

How to achieve large, positive scattering length a_{IB} ?

1. way: large microscopic repulsion



not sufficient:



$$S_{\text{eff}} = S_{\text{kin}}^{\text{Bos}} + S_{\text{kin}}^{\text{Imp}} + \underbrace{g_{IB}}_{H} \int \left\{ \sqrt{n_B} \psi_x^* \psi_x (\phi_x + \phi_x^*) + n_B \psi_x^* \psi_x \right\} \qquad g_{IB} = \frac{2\pi \hbar^2}{m_r} a_{IB}$$

How to achieve large, positive scattering length a_{IB} ?
1. way: large microscopic repulsion
$$\underbrace{V(r)}_{a_{IB}} \quad f_0 \quad f_1 \quad f_1 \quad f_2 \quad f_1 \quad f_2 \quad f_2 \quad f_1 \quad f_2 \quad f_2 \quad f_1 \quad f_2 \quad f_2 \quad f_2 \quad f_1 \quad f_2 \quad f_2 \quad f_2 \quad f_2 \quad f_2 \quad f_2 \quad f_1 \quad f_2 \quad f_2 \quad f_2 \quad f_2 \quad f_2 \quad f_2 \quad f_1 \quad f_2 \quad f_2$$

a continuum E $back B = \frac{\hbar^2}{ma^2}$ $back B = \frac{\hbar^2}{ma^2}$

increasing attraction

2. way: use resonance [here shape resonance, cold atoms: typ. Feshbach resonance]



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1. microscopic attraction needed





 $g_{IB} \neq \frac{2\pi\hbar^2}{m_r} a_{IB}$ 'mean-field replacement' invalid!



1. microscopic attraction needed



- 2. pairing fluctuations become relevant
 - → MF approach & Fröhlich Hamiltonian becomes invalid

in RG language: Froehlich: weak coupling RG fixed point cold atoms at Feshbach resonance: strong coupling RG fixed point similar RG analysis for Bose-Fermi Mixture: B. Liu, J. Hu Int. J. Mod. Phys, 26 (2012)

Our work: Bose polaron from a truly attractive model

simple quantum field-theory approach

assume homogeneous, weakly interacting BEC

RATH, RS, PRA 88 (2013)

$$\varphi(\mathbf{x},t) = \rho_0^{1/2} + \phi(\mathbf{x},t)$$

$$\mathbf{x} \quad \mathbf{x}$$
 mean-field fluctuations

Bogoliubov approximation for bosons: keep all terms up to quadratic in ϕ , ϕ^*

$$S_{\text{eff}} = \int_{\omega, p} \left\{ \frac{1}{2} \begin{pmatrix} \phi_p^* \\ \phi_{-p} \end{pmatrix} \begin{pmatrix} -\left[G_{\phi}^{(0)}(-p)\right]^{-1} & g_{\phi\phi}\rho_0 \\ g_{\phi\phi}\rho_0 & -\left[G_{\phi}^{(0)}(p)\right]^{-1} \end{pmatrix} \begin{pmatrix} \phi_p \\ \phi_{-p}^* \end{pmatrix} + \psi_p^* \left(-i\omega + \frac{p^2}{2m_{\psi}} - \mu_{\psi}\right) \psi_p \right\} \\ + \tilde{g}_{\phi\psi} \int_x \left[\psi_x^* \psi_x \phi_x^* \phi_x \right] + \sqrt{\rho_0} \psi_x^* \psi_x (\phi_x + \phi_x^*) + \rho_0 \psi_x^* \psi_x \right]$$

Unlike previous approaches, we keep **pairing fluctuations**

"Fröhlich terms"

The Question



do cold atoms forget underlying microscopic physics?

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do cold atoms forget underlying microscopic physics?

Quantity to address this question in quantum field theory:

Spectral function (gives access to radio-frequency response etc...)

$$\mathcal{A}(\omega, \boldsymbol{p}) = -2 \operatorname{Im} G^{\mathrm{R}}(\omega, \boldsymbol{p})$$

T-matrix approximation



prerequisite: recover exact two-body solution [unlike previous works]

resummed perturbation theory



Result for momentum resolved spectral function



unlike condmat: two coherent quasi-particle excitations!

almost "standard" repulsive polaron a > 0

- ▶ at positive energy
- enhanced effective mass
- finite lifetime!
- Iargely reduced quasi-particle weight





Result for momentum resolved spectral function



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"new" attractive polaron $\forall a$

- actual ground state at negative energies!
- cannot be found in Fröhlich approaches
- interacts attractively with BEC
- enhanced effective mass



Result for momentum resolved spectral function



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 $1/a_{IB}$

attractive polaron



stable ground state at all scattering lengths

OBSERVED AT WEAK COUPLING PFAU GROUP [STUTTGART]: BALEWSKI ET AL., NATURE 502 (2013)







So far: Non-selfconsistent T-matrix approach



single boson taken out of condensate

BEC impurity

So far: Non-selfconsistent T-matrix approach



single boson taken out of condensate



equivalent to simple variational wave function

$$\begin{split} |\psi_0\rangle &= \sqrt{Z} \hat{c}_0^{\dagger} |\text{BEC}\rangle + \sum_{\mathbf{k}} \mathcal{A}(\mathbf{k}) \hat{c}_{-\mathbf{k}}^{\dagger} \hat{b}_{\mathbf{k}}^{\dagger} |\text{BEC}\rangle \\ & \uparrow \\ & \uparrow \\ & \text{impurity} \\ & \text{boson excited out of } \\ & \text{condensate} \\ \end{split}$$

 captures very simple 'entanglement' between BEC and impurity

recently studied in: LI AND DAS SARMA, ARXIV:1404.4054

Selfconsistent T-matrix approach



 solved numerically using algorithm developed for *functional renormalization group approach* for RG flow of full spectral functions
 RS, ENSS, PRA 83 (2011)

Selfconsistent T-matrix approach



- solved numerically using algorithm developed for *functional renormalization group approach* for RG flow of full spectral functions
 RS, ENSS, PRA 83 (2011)
- accounts for infinitely many virtual excitations of bosons out of the coherent condensate state

Non-selfconsistent:

single boson taken out of condensate



infinite number of bosons
 taken out of condensate way beyond product wave

functions for BEC

Self-consistent T-matrix - Results





Wednesday, October 29, 14

Self-consistent T-matrix - Results



Challenge

- Efimov effect + statistics: Bose-Fermi mixtures unstable due to enhanced three-body recombination
 SEE E.G. RS, RATH, ZWERGER, EJB 85 (2012)
 EFIMOV IN SPIN-ORBIT BOSONS: SHI, CUI, ZHAI PRL 112 (2014)
- possible BEC deformation due to large interactions



E.G. ${}^{40}\text{K}/{}^{41}\text{K}$ mixture at B=543 G

SEE MIT GROUP: WU ET AL. PRA 84 (2012)

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- maps out impurity spectral function
 - similar procedure proposed and used for fermions



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Summary

- Using a field theoretical approach we studied impurity in ultracold BEC close to Feshbach resonance
- Spectrum exhibits two distinct quasi-particle branches
 - attractive polaron
 - ➡ repulsive (Fröhlich) polaron

- We predict finite lifetime of repulsive polaron: Quantum simulation of Fröhlich model challenging with ultracold atoms
- We propose experimental procedure to measure polaron properties via radiofrequency spectroscopy





- Our theory describes the polaron right after the drive to the final state Here the repulsive polaron is in a highly excited, non-equilibrium state
- ▶ What happens on time scales longer than those of RF experiments?



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dynamical competition between molecule formation & Froehlich self-localization & bubble formation

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2 interplay few & many-body physics

▶ Fate of Efimov physics in the realm of the polaron problem?

Detailed study of impurity-molecule crossover



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Thank you!

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