Polarons in cold atomic gases: a brief introduction

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Quantum Few- to Many-body Physics in Ultracold Atoms WIPM

## Outline

- What is polaron?
  - Condensed-matter background
  - Polarons in cold atoms: general picture
  - Early experiments
- How to characterize polarons in cold atomic gases
  - Chevy's ansatz
  - T-matrix formalism
- An example: polaron in alkaline-earth(-like) atoms
- Outlook

# What is polaron?

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• Quasiparticle excitation describing a single impurity moving in its environment (in a general sense)

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- Quasiparticle excitation describing a single impurity moving in its environment (in a general sense)
- Landau (localized electrons) and Pekar (phonon clouds) (1933-1951)
- The Fröhlich polaron (1950s)



- Phonons not affected by a single electron
- Brillouin-Wigner perturbation theory

$$E_p = E_0 + \frac{p^2}{2m^*} + O(p^4)$$

• Large (Fröhlich) vs. small polarons (Landau)



## In cold atoms

## • Pairing in polarized Fermi gases



M. W. Zwierlein et al. Science 311, 492 (2006)



G. B. Partridge et al. Science 311, 503 (2006)

- Large-polarization limit: polaron physics
- Interaction tunable through Feshbach resonance

# Feshbach resonance (*s*-wave interaction)



- Multi-channel resonant scattering
- The scattering length diverges as the threshold of an 'open' channel coincides with a bound state energy of a 'closed' channel
- Strong-  $(a \rightarrow 0^+)$  and weak-interaction  $(a \rightarrow 0^-)$  limits

#### Introduction

Fate of impurity: limiting cases and those inbetween

- Weak-interaction limit: free impurity
- Strong-interaction limit: impurity-atom dimer



From Phys. Rev. Lett. 102, 230402 (2009)

- Inbetween: polaronic branch and dimeronic branch
- Transition occurs between polaronic quasiparticles and many-body bound states
- Predicted by diagrammatic QMC calculations

N. Prokof'ev and B. Svistunov, Phys. Rev. B 77, 020408(R) (2008)

#### Introduction

# Early experiments on polaron-molecule transition I





- rf-spectroscopy measurement
- Weakly interacting quasiparticle
- Polaron-molecule transition
- Consistent with QMC

A. Schirotzek, C.-H. Wu, A. Sommer, M. W. Zwierlein, Phys. Rev. Lett. 102, 230402 (2009)

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#### Introduction

# Early experiments on polaron-molecule transition II



C. Kohstall, et al., Nature 485, 615 (2012)



M. Koschorreck, et al., Nature 485, 619 (2012)

- Attractive and repulsive polarons in 3D and 2D
- Repulsive polaron: a metastable quasiparticle
- Molecule-hole continuum
- Consistent with calculations based on perturbation theory

### Detection schemes





R. Schimdt, M. Knap, D. A. Ivanov, J.-S. You, M. Cetina, E. Demler, Rep. Prog. Phys. 81, 024401 (2018)

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Standard rf spectroscopy

How to characterize polarons theoretically?

- Variational approach: Chevy's ansatz F. Chevy, Phys. Rev. A 74, 063628 (2006)
- T-matrix approach
  - R. Combescot, A. Recati, C. Lobo, F. Chevy, Phys. Rev. Lett. 98, 180402 (2007) M. Punk, W. Zwerger Phys. Rev. Lett. 99, 170404 (2007)
- 1/N expansion
   M. Veillette *e al.*, Phys. Rev. A 78, 033614 (2008)
- Fixed-node QMC

C. Lobo, A. Recati, S. Giorgini, S. Stringari, Phys. Rev. Lett. 97, 200403 (2006)

## Diagrammatic QMC

N. V. Prokof'ev, B. V. Svistunov, Phys. Rev. B 77, 020408(R) (2008)

Other

R. Schimdt, et al., Rep. Prog. Phys. 81, 024401 (2018)

Chevy's ansatz (polarons in a polarized two-component Fermi gas)

• Polaron ansatz wave function

$$|\Psi\rangle_{\mathbf{Q}} = \left(\psi_{\mathbf{Q}}b_{\mathbf{Q}}^{\dagger} + \sum_{q < k_F, k > k_F} \psi_{\mathbf{k}\mathbf{q}}b_{\mathbf{Q}-\mathbf{k}+\mathbf{q}}^{\dagger}a_{\mathbf{k}}^{\dagger}a_{\mathbf{q}}\right)|\mathrm{FS}\rangle_{N}$$

Hamiltonian

$$H = \sum_{\mathbf{k}} \epsilon_k b_{\mathbf{k}}^{\dagger} b_{\mathbf{k}} + \sum_{\mathbf{k}} \epsilon_k a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}} + U \sum_{\mathbf{k}, \mathbf{k}', \mathbf{q}} a_{\mathbf{k}}^{\dagger} b_{\mathbf{k}'}^{\dagger} b_{\mathbf{k}'+\mathbf{q}} a_{\mathbf{k}'-\mathbf{q}}$$

- Minimize  $\langle \Psi | H | \Psi \rangle_{\mathbf{Q}}$  or  $H | \Psi \rangle_{\mathbf{Q}} = E_P | \Psi \rangle_{\mathbf{Q}}$  (truncation)
- More particle-hole excitations possible
- Renormalization of bare interaction U with  $U_0 = 4\pi \hbar^2 a_s/m$

$$\frac{1}{U} = \frac{1}{U_0} - \sum_{\mathbf{k}} \frac{1}{2\epsilon_k}$$

Equations for the coefficients (assuming Q = 0)

$$U\psi_0(\sum_{qk_F}\psi_{\mathbf{kq}} = E_P\psi_0$$
$$(\epsilon_k - \epsilon_q + \epsilon_{\mathbf{q}-\mathbf{k}})\psi_{\mathbf{kq}} + U\psi_0 + U\sum_{k>k_F}\psi_{\mathbf{kq}} = E_P\psi_{\mathbf{kq}}$$

Therefore we have

$$\left(\frac{1}{U} - \sum_{\mathbf{k}} \frac{1}{A_{\mathbf{k}\mathbf{q}}}\right) A_{\mathbf{q}} - \frac{1}{E_P} \sum_{\mathbf{q}} A_{\mathbf{q}} = 0, \text{ with } \begin{cases} A_{\mathbf{k}\mathbf{q}} = E_P - (\epsilon_k - \epsilon_q + \epsilon_{\mathbf{q}-\mathbf{k}}) \\ A_{\mathbf{q}} = U\psi_0 + U \sum_{\mathbf{k}} \psi_{\mathbf{k}\mathbf{q}} \end{cases}$$

Closed equation

$$E_P = \sum_{q < k_F} \frac{1}{\frac{1}{U} - \sum_{k > k_F} \frac{1}{E_P - \epsilon_k + \epsilon_q - \epsilon_{\mathbf{q}-\mathbf{k}}}}$$

Molecular wave function

$$|M\rangle_{\mathbf{Q}} = \sum_{k>k_F} \phi_{\mathbf{k}} b^{\dagger}_{\mathbf{Q}-\mathbf{k}} a^{\dagger}_{\mathbf{k}} |\mathrm{FS}\rangle_{N-1} + \sum_{k,k'>k_F} \phi_{\mathbf{k}\mathbf{k'q}} b^{\dagger}_{\mathbf{Q}-\mathbf{k}-\mathbf{k'+q}} a^{\dagger}_{\mathbf{k}} a^{\dagger}_{\mathbf{k'}} a_{\mathbf{q}} |\mathrm{FS}\rangle_{N-1}$$

Equations for the coefficients (assuming Q = 0)

$$\begin{split} A_{\mathbf{k}}\phi_{\mathbf{k}} &= U\phi_{\mathbf{k}}(\sum_{q < k_{F}}) + U\sum_{k' > k_{F}}\phi_{\mathbf{k}'} + U\sum_{k' > k_{F}, q < k_{F}}\phi_{\mathbf{k}\mathbf{k}'\mathbf{q}} - U\sum_{k' > k_{F}, q < k_{F}}\phi_{\mathbf{k}'\mathbf{k}\mathbf{q}} \\ A_{\mathbf{k}\mathbf{k}'\mathbf{q}}\phi_{\mathbf{k}\mathbf{k}'\mathbf{q}} &= U\sum_{k'' > k_{F}}\phi_{\mathbf{k}''\mathbf{k}'\mathbf{q}} + U\sum_{k'' > k_{F}}\phi_{\mathbf{k}\mathbf{k}''\mathbf{q}} + U\phi_{\mathbf{k}} \end{split}$$

With

$$A_{\mathbf{k}} = E_M - 2\epsilon_k$$
$$A_{\mathbf{k}\mathbf{k}'\mathbf{q}} = E_M - \epsilon_{\mathbf{q}-\mathbf{k}-\mathbf{k}'} - \epsilon_k - \epsilon_{k'}$$

Note: i)  $\phi_{\mathbf{k}\mathbf{k}'\mathbf{q}} = -\phi_{\mathbf{k}'\mathbf{k}\mathbf{q}}$ ; ii)  $E_M$  relative to the energy of  $|FS\rangle_{N-1}$ .

# Defining

$$G_{\mathbf{kq}} = \phi_{\mathbf{k}} + 2\sum_{\mathbf{k}'} \phi_{\mathbf{kk'q}},$$

## we have

$$\begin{split} \left(\frac{1}{U} - \sum_{k' > k_F} \frac{1}{A_{\mathbf{k}\mathbf{k}'\mathbf{q}}}\right) G_{\mathbf{k}\mathbf{q}} + \sum_{k'' > k_F} \frac{G_{\mathbf{k}''\mathbf{q}}}{A_{\mathbf{k}\mathbf{k}''\mathbf{q}}} \\ - \sum_{q' < k_F} \frac{G_{\mathbf{k}\mathbf{q}'}}{A_{\mathbf{k}}} - \sum_{k'' > k_F} \left(\frac{1}{U} - \sum_{k''' > k_F} \frac{1}{A_{\mathbf{k}'''}}\right) \frac{\sum_{q' < k_F} G_{\mathbf{k}''\mathbf{q}'}}{A_{\mathbf{k}}A_{\mathbf{k}''}} = 0. \end{split}$$

Simpler case: the bare molecular state

$$\frac{1}{U} = \sum_{k > k_F} \frac{1}{A_{\mathbf{k}}}.$$

# Comparison of results (3D)



- Compare  $E_M E_F$  with  $E_P$  ( $E_b = -\hbar^2/ma_s^2$  subtracted)
- Crossing at  $(k_F a_s)_c^{-1} = 0.84$  vs 0.90 (diagrammatic QMC)

M. Punk, P. T. Dumitrescu, W. Zwerger, Phys. Rev. A 80, 053605 (2009)

# Comparison of results (2D)



- Polaron-molecule transition exists in 2D
- Polaron with single (two) particle-hole pair(s)

M. M. Parish, Phys. Rev. A 83, 051603(R) (2011)

M. M. Parish, J. Levinsen, Phys. Rev. A 87, 033616 (2013)

M. Koschorreck et al., Nature 485, 619 (2012)

Convergence of results on the single particle-hole level



Converge quickly at the lowest orders of particle-hole excitations

• Destructive interference between higher-order terms

R. Combescot, S. Giraud, Phys. Rev. Lett. 101, 050404 (2008)

T-matrix approach (polaron single-hole level)

$$G_{\downarrow}^{-1}(\mathbf{p},\omega) = \omega + i0^{+} - \epsilon_{p\downarrow} - \Sigma(\mathbf{p},\omega)$$
$$\Sigma(\mathbf{p},\omega) = \Sigma^{(1)}(\mathbf{p},\omega) + \Sigma^{(2)}(\mathbf{p},\omega) + \dots$$
$$E_{P} = \operatorname{Re}\left[\Sigma(\mathbf{p}=0,E_{P})\right]$$



- Equivalent to the variational approach
- Better extendability, e.g., capable of analyzing losses

R. Combescot, A. Recati, C. Lobo, F. Chevy, Phys. Rev. Lett. 98, 180402 (2007) G. M. Bruun and P. Massignan, Phys. Rev. Lett. 105, 020403 (2010)

General features in the spectral funcion

$$A_{\downarrow}(\mathbf{p}, E) = -2\mathrm{Im} \frac{1}{E + i0^{+} - \epsilon_{\mathbf{p}\downarrow} - \Sigma(\mathbf{p}, E)}$$



- Attractive and repulsive polaron
- Broadening and decay channels
- Molecule-hole continuum

P. Massignan, G. Bruun, Eur. Phys. J. D 65, 83 (2011)

Polaron decay rate, impurity residue and effective mass

• Pole expansion (for well-defined quasiparticles)

$$G_{\downarrow}(\mathbf{p},\omega) \approx \frac{Z_P}{\omega - E_P - \frac{p^2}{2m^*} + i\frac{\Gamma_P}{2}}$$

• Impurity residue

$$Z_P = \{1 - \mathsf{Re}\left[\partial_{\omega}\Sigma(0, E_P)\right]\}^{-1}$$

Effective mass

$$\frac{m}{m^*} = Z_P \left\{ 1 + \operatorname{\mathsf{Re}}\left[\partial_{\epsilon_p} \Sigma(0, E_P)\right] \right\}$$

Polaron decay rate

$$\Gamma_P = -2Z_P \mathrm{Im}\left[\Sigma(0, E_P)\right]$$

## Decay of polarons and molecules



- Additional p-h pair due to energy-momentum conservation
- Other decay channels possible: repulsive to attractive polaron, repulsive polaron to bare impurity
- Diagrams for molecular state

G. M. Bruun and P. Massignan, Phys. Rev. Lett. 105, 020403 (2010)

# Alkaline-earth(-like) atoms

- Sr, Yb, Ca, etc.
- Two valence electrons: a rich level structure
- Even vs. odd isotopes

An example:



- Clock-state manifolds
- Versatile control

## Orbital Feshbach resonance



Two-body interaction channels at short range

$$|\pm\rangle = \frac{1}{2}(|ge\rangle \pm |eg\rangle) \otimes (|\downarrow\uparrow\rangle \mp |\uparrow\downarrow\rangle)$$

R. Zhang, Y. Cheng, H. Zhai, P. Zhang, Phys. Rev. Lett. 115, 135301 (2015)

G. Pagano et al., Phys. Rev. Lett. 115, 265301 (2015)

M. Höfer et al., Phys. Rev. Lett. 115, 265302 (2015)

## Polaron problem in alkaline-earth(-like) atoms



- Inter-orbital spin-exchange interaction
- Excitation of scattering states in the closed channel
- Effect of external magnetic field

J.-G. Chen, T.-S. Deng, WY, W. Zhang, Phys. Rev. A 94, 053627 (2016) T.-S. Deng, Z.-C. Lu, Y.-R. Shi, J.-G. Chen, W. Zhang, WY, Phys. Rev. A 97, 013635 (2018)

Hamiltonian

$$H_{0} = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} (a_{g,\mathbf{j}\mathbf{k}}^{\dagger} a_{g,\mathbf{j}\mathbf{k}} + a_{e,\uparrow,\mathbf{k}}^{\dagger} a_{e,\uparrow,\mathbf{k}}) + \sum_{\mathbf{k}} (\epsilon_{\mathbf{k}} + \frac{\delta}{2}) (a_{e,\mathbf{j}\mathbf{k}}^{\dagger} a_{e,\mathbf{j}\mathbf{k}} + a_{g,\uparrow\mathbf{k}}^{\dagger} a_{g,\uparrow\mathbf{k}}), \qquad \stackrel{|e|\downarrow\rangle}{\underbrace{\frac{\delta}{2}}}$$

$$H_{\text{int}} = \frac{g_{+}}{2} \sum_{\mathbf{q}} A_{+}^{\dagger}(\mathbf{q}) A_{+}(\mathbf{q}) + \frac{g_{-}}{2} \sum_{\mathbf{q}} A_{-}^{\dagger}(\mathbf{q}) A_{-}(\mathbf{q}),$$

with

$$A_{\pm}(\mathbf{q}) = \sum_{\mathbf{k}} (a_{e,\downarrow,\mathbf{k}} a_{g,\uparrow,\mathbf{q}-\mathbf{k}} \mp a_{e,\uparrow,\mathbf{k}} a_{g,\downarrow,\mathbf{q}-\mathbf{k}})$$

## The overall picture in terms of spectral function



 $A(0,E) = -2 \operatorname{Im} G_{e\uparrow}(0,E)$   $g_0 = \frac{g_+ + g_-}{2}, \quad g_1 = \frac{g_- - g_+}{2}$ 

J. Xu, R. Zhang, Y. Cheng, P. Zhang, R. Qi, H. Zhai Phys. Rev. A 94, 033609 (2016) T.-S. Deng, Z.-C. Lu, Y.-R. Shi, J.-G. Chen, W. Zhang, WY, Phys. Rev. A 97, 013635 (2018)

Ground-state of the impurity system: attractive polaron vs molecule

$$\begin{split} |P\rangle_{\mathbf{Q}} &= \gamma a_{e,\uparrow\mathbf{Q}}^{\dagger} |g_{\downarrow}\rangle_{N} + \sum_{\substack{|\mathbf{k}| > k_{F} \\ |\mathbf{q}| < k_{F}}} \alpha_{\mathbf{k}\mathbf{q}} a_{e,\uparrow\mathbf{Q}+\mathbf{q}-\mathbf{k}}^{\dagger} a_{g,\downarrow\mathbf{k}}^{\dagger} a_{g,\downarrow\mathbf{q}} |g_{\downarrow}\rangle_{N} \\ &+ \sum_{\substack{|\mathbf{q}| < k_{F} \\ |\mathbf{q}| < k_{F}}} \beta_{\mathbf{k}\mathbf{q}} a_{e,\downarrow\mathbf{Q}+\mathbf{q}-\mathbf{k}}^{\dagger} a_{g,\uparrow\mathbf{k}}^{\dagger} a_{g,\downarrow\mathbf{q}} |g_{\downarrow}\rangle_{N}, \\ |M\rangle_{\mathbf{Q}} &= \sum_{\substack{|\mathbf{k}| > k_{F}}} \alpha_{\mathbf{k}} a_{e,\uparrow\mathbf{Q}-\mathbf{k}}^{\dagger} a_{g,\downarrow\mathbf{k}}^{\dagger} |g\downarrow\rangle_{N-1} + \sum_{\mathbf{k}} \beta_{\mathbf{k}} a_{e,\downarrow\mathbf{Q}-\mathbf{k}}^{\dagger} a_{g,\uparrow\mathbf{k}}^{\dagger} |g\downarrow\rangle_{N-1}. \end{split}$$

• Schrödinger's equation

$$(H_0 + H_{\rm int})|\alpha\rangle = (E_\alpha + E_{\rm FS})|\alpha\rangle, \quad \alpha = P, M$$

with  $E_{\rm FS}$  the energy of the Fermi sea with N atoms.

Polaron energy and polaron-molecule transition



- Polaron-molecule transition in the attractive branch
- Variation of weights in the polaron wave function

## Repulsive polaron: residue and effective mass



Understanding the kinks

$$T^{oo}(\mathbf{q},\omega) = \frac{\frac{1}{2}(g_+ + g_-) - g_+ g_- \chi^c}{1 - \frac{1}{2}(g_+ + g_-)(\chi^o + \chi^c) + g_+ g_- \chi^o \chi^c}$$
$$\chi^c(\mathbf{q},\omega) = \sum_{\mathbf{k}} \frac{1}{\omega + i0^+ - \epsilon_{\mathbf{k}} - \epsilon_{\mathbf{q}-\mathbf{k}} - \delta}$$
$$\chi^o(\mathbf{q},\omega) = \sum_{|\mathbf{k}| > k_F} \frac{1}{\omega + i0^+ - \epsilon_{\mathbf{k}} - \epsilon_{\mathbf{q}-\mathbf{k}}}$$

- Location of kinks:  $\delta = E_+$ ,  $\delta = E_+ + \frac{E_F}{2}$
- Contribution of the imaginary part of  $\chi^c(\mathbf{q},\omega)$  to  $\Sigma(\mathbf{q},E)$

## Understanding pair propagators





## Impact on the decay of repulsive polaron



$$\Sigma(0, E) = \int \frac{d\mathbf{q}}{(2\pi)^3} \int \frac{d\omega}{2\pi} G^0_{g\downarrow}(\mathbf{q}, \omega) T^{oo}(\mathbf{q}, E + \omega)$$
$$\Gamma = -2Z_+[\mathrm{Im}\Sigma(0, E_+)]$$

• Decay into the bare impurity state in the attractive branch

F. Scazza et al., Phys. Rev. Lett. 118, 083602 (2017)

Phase separation and itinerant ferromagnetism

- Stoner's itinerant ferromagnetism: polarization + repulsive interaction → ferromagnetism
- Experimental evidence? (in alkali atoms)

G.-B. Jo et al., Science 325, 1521 (2009)

C. Sanner et al., Phys. Rev. Lett. 107, 175302 (2011)

G. Valtolina et al., Nat. Phys. 13, 704 (2017)

In alkaline-earth-(like) aotms?

Criterion?

- Phase separation vs. polaron state: energetic considerations
- Long-lived polaron excitations:  $\Gamma \ll E_F$

P. Massignan, Z. Yu, G. M. Bruun, Phys. Rev. Lett. 110, 230401 (2013)

# Phase diagram



- OFR non-universal
- A favorable parameter window for probing ferromagnetism

# Outlook

Variants of the polaron problem

Polaron in a Bose-Einstein condensate
 Pitaevskii, Blume, Timmermans, Jaksch, Devereese, Li, Demler, Cui, Zhai...

Exp: Jin, Arlt...

- Polaron in a Fermi superfluid
   Nishida, Cui, Yi
- Polaron in spin-orbit coupled Fermi gas Cui, Zhang, Yi
- Rotating impurities: angulon

Lemeshko,...

A probe to many-body system, a bridge between few and many...



M. Lemeshko, PRL (2017)