tunneling theory of few interacting atoms in a trap

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cold atoms in the few-body limit

$^{87}$Rb, Bloch group

bosons

$^{6}$Li, Jochim group

fermions

(yesterday talk)


motivation

control key parameters of clean correlated system

ideal lab for few-fermion physics

comparison with exact theoretical models

building block of many-body systems
few-fermion vs bulk physics

bulk: kinetic energy + interaction
homogeneous (cf. many fermions at trap center)

few particles in a trap: quantum confinement
inhomogeneous

analogies with atoms, nuclei, quantum dots

tunneling spectroscopy, shell structure, Hund’s rule, pairing for few fermions
outline

- tunneling spectroscopy in interacting cold atoms & condensed-matter nano-objects: *quasiparticle theory*

- repulsive interactions between $^6\text{Li}$ atoms

- wave function imaging in interacting quantum dots

- pairing for a few $^6\text{Li}$ atoms & pair tunneling
tunneling spectroscopy à la Heidelberg

prepare a $^6$Li atom in the trap ground state

talk by G. Zuern yesterday
tunneling spectroscopy à la Heidelberg

switch off the potential barrier
tunneling spectroscopy à la Heidelberg

the atom escapes...
tunneling spectroscopy à la Heidelberg

after hold time \( t \), switch on the barrier
tunneling spectroscopy à la Heidelberg

...second possibility
tunneling spectroscopy à la Heidelberg

after hold time $t$
tunneling spectroscopy à la Heidelberg

the atom remains in the trap
tunneling spectroscopy à la Heidelberg

\[ P(1) + P(2) = 1 \text{ at any } t \]

(a) check if atom in the trap
(b) repeat many times
(c) vary hold time \( t \)
(d) iterate
measure decay time $\tau$

$$N_{WKB}(t) = N_0 e^{-t/\tau}$$
many fermions: energy spectroscopy

two-species fermions
no interaction
many fermions: energy spectroscopy

decay as resonance
many fermions: energy spectroscopy

dominant decay channel at Fermi energy
...what if atoms interact?
...what if atoms interact?

\[ g = 0 \]

Heidelberg setup

\[ V_{\text{int}} = g \delta(x_1 - x_2) \]
...what if atoms interact?

$g \neq 0$

$\varepsilon_1 \rightarrow \varepsilon = \text{chemical potential}$
interaction blockade

measure chemical potential

\[ \varepsilon(N) = E_0(N) - E_0(N - 1) \]

equivalent to addition energy in quantum dots and ionization potential in atoms and molecule

prediction: Kapelle, Reimann & coworkers [PRL 99, 010402 (2007)]

exp confirmation (bosons): Bloch group [PRL 101, 090404 (2008)]

compute \( \tau \) using \( \varepsilon \) in WKB formula (mean-field theory)?
two interacting atoms (Zuern et al., PRL 2012)

\[ V_{\text{int}} = g \, \delta(x_1 - x_2) \]
two interacting atoms (Zuern et al., PRL 2012)
two interacting atoms (Zuern et al., PRL 2012)

\[ V_{\text{int}} = g \delta(x_1 - x_2) \]

after T. Busch et al. (1998)
mean-field theory fails

M. Rontani, PRL 108, 115302 (2012)
Scanning Tunneling Spectroscopy

single molecule
well-isolated nano-objects
quantized energy levels
Coulomb blockade

short nanotube
wave function imaging
quantum dot
STS in electrically insulated molecules

Repp et al., PRL 94, 026803 (2005)

P. Liljeroth et al., Nano Lett. 10, 2475 (2010).
A. Bellec et al., Nano Lett. 9, 144 (2009).
STS in electrically insulated molecules

\[ E_F \]

\[ \text{tip} \]

\[ \text{vacuum} \]

\[ N \]

\[ \text{molecule} \]

\[ \text{tunnel barrier} \]

\[ \text{backgate} \]

\[ \text{NaCl layer} \]

\[ \text{pentacene} \]

\[ \text{metallic substrate} \]
STS in electrically insulated molecules

apply tip-gate bias voltage
STS in electrically insulated molecules

PRL 94, 026803 (2005)

peak in $dl / dV$
from $N$ to $N - 1$
STS in electrically insulated molecules

peak in $\frac{dl}{dV}$ from $N$ to $N+1$

$E_F$

$N$

$tips$

tunnel barrier

molecule

$PRL \ 94, \ 026803 \ (2005)$
mean-field theory

d$I/dV(r) \approx \sum_{\alpha} |\psi_\alpha(r)|^2 \delta(\varepsilon_\alpha - E_F)

energy-resolved local density of states (LDOS) = single-particle level

Tersoff & Hamann 1985
mean-field theory

\[ \frac{dI}{dV} \approx |\psi_{\text{HOMO}}(\mathbf{r})|^2 \]
mean-field theory

\[ \frac{dI}{dV} \approx |\psi_{\text{LUMO}}(\mathbf{r})|^2 \]
ambiguities of mean-field theory

- $N$ or $N + 1$ to compute self-consistent orbitals?
what is actually measured in tunneling experiments in the presence of many-body interactions?

generic question

wave function $\psi^N$ is NOT a single electron configuration $\phi^N$: $\psi^N = \sum C^N_i \phi^N_i$ or $N + 1$ to compute self-consistent orbitals?

ambiguities of mean-field theory
Bardeen’s viewpoint (1961): many-body matrix element connecting states with $N$ and $N-1$ fermions in the trap / molecule / Quantum Dot

\[ \frac{1}{\tau} \frac{dI}{dV} \propto \frac{2\pi}{\hbar} |M|^2 \ n(E_f) \]

$T = 0$

density of final states
resonant many-body states of the whole system

\[ \{ k^* \}, N \rangle \]

\[ \{ k \}, N - 1 \rangle \]

\[ N \]
$\mathbf{M} \propto \langle \{k\}, N - 1 \left| \hat{\mathcal{M}} \right| \{k^*\}, N \rangle,$

\[
\hat{\mathcal{M}} = \frac{\hbar^2}{2m^*} \int \left[ \hat{\Psi}^+ \frac{\partial \hat{\Psi}}{\partial z} - \frac{\partial \hat{\Psi}^+}{\partial z} \hat{\Psi} \right] \delta(z_{\text{bar}} - z) d\tau
\]

\[
\hat{\Psi}(\mathbf{r}) = \sum_\alpha \phi_\alpha(\mathbf{r}) \hat{c}_\alpha + \sum_k \chi_k(\mathbf{r}) \hat{c}_k
\]

field operator

single-particle QD state  single-particle continuum state
\[ \mathbf{M} \propto \langle \{k\}, N - 1 | \hat{\mathcal{M}} | \{k^*\}, N \rangle, \]

\[ \hat{\mathcal{M}} = \frac{\hbar^2}{2m^*} \int \left[ \hat{\Psi}^+ \frac{\partial \hat{\Psi}}{\partial z} - \frac{\partial \hat{\Psi}^+}{\partial z} \hat{\Psi} \right] \delta(z_{\text{bar}} - z) \, d\tau \]

\[ \hat{\Psi}(\mathbf{r}) = \sum_{\alpha} \phi_{\alpha}(\mathbf{r}) \hat{c}_\alpha + \sum_k \chi_k(\mathbf{r}) \hat{c}_k \]

field operator

single-particle QD state  single-particle continuum state

\[ \frac{dI}{dV} \approx \left| \varphi_{QP}(\mathbf{r}) \right|^2 \delta(E_F - E_N + E_{N-1}) \]

Rontani and Molinari PRB 2005

\[ 1 / \tau \approx \left| \left[ \varphi^*_{QP}(x) \frac{d\chi_{\varepsilon}(x)}{dx} - \chi_{\varepsilon}(x) \frac{d\varphi^*_{QP}(x)}{dx} \right]_{x=x_{\text{bar}}} \right|^2 \]

Rontani PRL 2012
key quantity

\[ \varphi_{QP}(\mathbf{r}) = \langle \Psi_{N-1} | \hat{\Psi}(\mathbf{r}) | \Psi_N \rangle \]

hole “quasiparticle” wave function

Rontani and Molinari PRB 2005

in practice:

\[ \varphi_{QP}(\mathbf{r}) = \sum_{i,j} c_i^{N-1*} c_j^N \psi_{\alpha(i,j)}(\mathbf{r}) \]

expansion coefficients:

\[ \Psi_N = \sum c_j^N \Phi_j^N \]

single-particle orbital
outline

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• repulsive interactions between $^6$Li atoms

• wave function imaging in interacting quantum dots

• pairing for a few $^6$Li atoms & pair tunneling
mean-field theory fails

M. Rontani, PRL 108, 115302 (2012)
quasiparticle wave function theory
quasiparticle
wave function
theory
evidence for ‘fermionization’

M. Rontani, PRL 108, 115302 (2012)
Evidence for ‘fermionization’

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\[ g = 0 + \]

\[ g = \infty \]

\[ g = 0 - \]
change of spectral weight

\[ \frac{1}{\tau} \approx \frac{A_{QP}}{\tau_0} \]

\( \tau_0 = \text{WKB mean-field} \)

\( A_{QP} = \text{norm} \)
\[ g = 0^+ \]

\[ g = \infty \]

\[ g = 0^- \]

Initial

\[ \frac{1}{\sqrt{2}} \]

\[ -\frac{1}{\sqrt{2}} \]

Final

\[ \frac{1}{\sqrt{2}} \]

\[ -\frac{1}{\sqrt{2}} \]
so far

- quasiparticle theory for decay time of $^6$Li atoms works

- $1/\tau = (1/\tau_0) \times \text{(many-body factor)}$

- measure chemical potential and spectral weight
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quantum confinement in nanostructures

simplest case: quantum well

2D confinement

3D

2D

1D

0D

bulk

quantum well

quantum wire quantum dot
experiment: InAs quantum dots

STM images

strong anisotropy

Nano Lett. 7, 2071 (2007)
STGS spectroscopy

Nano Lett. 7, 2071 (2007)

Voltage (V)

(dI/dV)/(I/V)

Center
side
WL

A: s state
B: \( p_y \) state
C: \( p_y \) state
D: \( d \) state

first guess: \( N = 0 \rightarrow N = 1 \) ground- and excited-states
Hamiltonian

envelope function approximation,
semiconductor effective parameters

\[ H = \sum_{i=1}^{N} \left( -\frac{\hbar^2}{2m^*} \nabla_i^2 + \frac{m^*}{2} \left( \omega_0^2 x_i^2 + \omega_0^2 y_i^2 \right) \right) + \frac{e^2}{2\kappa_r} \sum_{i \neq j} \frac{1}{|\vec{r}_i - \vec{r}_j|} \]

single-particle term

many-body term

compute the wavefunction as a superposition of Slater determinants

\[ |\Phi_i^N\rangle = c_{l\sigma}^{\dagger}c_{m\sigma}^{\dagger} \cdots |0\rangle \]

\[ |\Psi_N\rangle = \sum_i c_i^{N} |\Phi_i^N\rangle \]


compute \( \varphi_{QD}(r) \)

full configuration interaction
ground & excited states
correlation in a circular QD

\[ H = \sum_{i=1}^{N} \left( -\frac{\hbar^2}{2m^*} \nabla_i^2 + \frac{m^* \omega_0^2}{2} (x_i^2 + y_i^2) \right) \]

single-particle term

\[ + \frac{e^2}{2\kappa_r} \sum_{i \neq j} \frac{1}{|\vec{r}_i - \vec{r}_j|} \]

many-body term

\[ \approx \Delta \varepsilon \]

\[ \approx \sqrt{\Delta \varepsilon} \]

large \( \Delta \varepsilon \)

mean-field theory holds

small \( \Delta \varepsilon \)

correlation effects
$N = 0 \rightarrow N = 1$

simulating the STS image

$$\frac{dI}{dV} \propto |\varphi_{\text{QD}}(\mathbf{r})|^2 = |\psi_{1s}(\mathbf{r})|^2$$

lengths in units of $l_{\text{QD}}$
$N = 1 \rightarrow N = 2$

$dI / dV \propto \left| \varphi_{\text{QD}}(r) \right|^2 = \left| \psi_{1s}(r) \right|^2$

$\Delta \varepsilon \rightarrow \infty$

no correlation

lengths in units of $l_{\text{QD}}$
\[ N = 1 \rightarrow N = 2 \]

\[ dI / dV \propto |\phi_{QD}(r)|^2 \]

\[ \Delta \varepsilon = 100 \text{ meV} \]

lengths in units of \( l_{QD} \)
\[ N = 1 \rightarrow N = 2 \]

\[ dI / dV \propto |\varphi_{\text{QD}}(\mathbf{r})|^2 \]

\[ \Delta \varepsilon = 50 \text{ meV} \]
$N = 1 \rightarrow N = 2$

\[ dI / dV \propto |\varphi_{\text{QD}}(\mathbf{r})|^2 \]

\[ \Delta \varepsilon = 10 \text{ meV} \]

lengths in units of $l_{\text{QD}}$
$N = 1 \rightarrow N = 2$

\[ \frac{dI}{dV} \propto |\varphi_{\text{QD}}(r)|^2 \]

\[ \Delta \varepsilon = 5 \text{ meV} \]

lengths in units of $l_{\text{QD}}$
\[ N = 1 \rightarrow N = 2 \]

\[ \frac{dI}{dV} \propto |\varphi_{\text{QD}}(\mathbf{r})|^2 \]

\[ \Delta\varepsilon = 1 \text{ meV} \]

Lengths in units of \( l_{\text{QD}} \)
\( N = 1 \rightarrow N = 2 \)

\[
dI / dV \propto |\varphi_{QD}(\mathbf{r})|^2
\]

\( \Delta \varepsilon = 0.5 \text{ meV} \)

lengths in units of \( l_{QD} \)
\[ N = 1 \rightarrow N = 2 \]

\[ \frac{dI}{dV} \propto |\varphi_{\text{QD}}(\mathbf{r})|^2 \]

\[ \Delta \varepsilon = 0.1 \text{ meV} \]

Lengths in units of \( l_{\text{QD}} \)
$N = 1 \rightarrow N = 2$

\[
dI / dV \propto |\varphi_{\text{QD}}(r)|^2
\]

$\Delta \varepsilon = 0.05 \text{ meV}$

lengths in units of $l_{\text{QD}}$
\[ N = 1 \rightarrow N = 2 \]

\[ \frac{dI}{dV} \propto \left| \varphi_{\text{QD}}(\mathbf{r}) \right|^2 \]

\[ \Delta \varepsilon = 0.01 \text{ meV} \]

lengths in units of \( l_{\text{QD}} \)
effect of anisotropy
$N = 1 \rightarrow N = 2$

effect of anisotropy

$$dI / dV \propto |\varphi_{\text{QD}}(r)|^2$$

$$\omega_{0x} / \omega_{0y} = 1$$

lengths in units of $l_{\text{QD}}$
$N = 1 \rightarrow N = 2$

effect of anisotropy

$$\frac{dI}{dV} \propto \left| \varphi_{QD}(r) \right|^2$$

$$\frac{\omega_{0x}}{\omega_{0y}} = 1.21$$

lengths in units of $l_{QD}$
$N = 1 \rightarrow N = 2$

**effect of anisotropy**

\[
\frac{dI}{dV} \propto |\varphi_{QD}(r)|^2
\]

\[
\omega_{0x} / \omega_{0y} = 1.69
\]

lengths in units of $l_{QD}$
$N = 1 \rightarrow N = 2$

effect of anisotropy

d$I / dV \propto |\varphi_{\text{QD}}(\mathbf{r})|^2$

$\omega_{0x} / \omega_{0y} = 2.25$

lengths in units of $l_{\text{QD}}$
predictions

STS image distortion driven by:

- confinement strength
- dot anisotropy
- dielectric environment
theo-exp comparison
theo-exp comparison

\[\text{exp} \quad 0 \rightarrow 1\]

- D
- C
- B
- A

\[280 \quad 370 \quad 460 \quad \text{meV}\]

\[0.8 \quad 1.0 \quad 1.2 \quad V\]

\[d_y \quad p_y \quad s\]

\[\star \quad \star\]

\[\star = \text{theo-exp matching}\]
theo-exp comparison

 exp

 A   B   C   D
 0.8  1.0  1.2

 280  370  460 meV

 0→1

 1→2

 ε

 δ

 γ

 β

 d_y

 p_y

 s

 β

 γ

 δ

 ε

 ★★ = theo-exp matching
theo-exp comparison

\[ \text{exp} \]

\[ \text{d}_y \]

\[ \text{p}_y \]

\[ \text{s} \]

\[ \beta \]

\[ \gamma \]

\[ \delta \]

\[ \varepsilon \]

\[ \star \star = \text{theo-exp matching} \]
theo-exp comparison

Nano Lett. 7, 2071 (2007)
is the C state really due to double charging?

\[ \Gamma_{in} \ll \Gamma_{out} \]

1 e\(^{-}\) in the dot

low \( I_{stab} \)

\[ \Gamma_{in} \gg \Gamma_{out} \]

2 e\(^{-}\) in the dot

high \( I_{stab} \)

Nano Lett. 7, 2071 (2007)
origin of the C-state image?
the origin of the C-state image

76 %

\[ + \]

11 %

6 %

wave function (a.u.)

\[ S \]

\[ C \text{ state} \]

\[ d \]
wires and carbon nanotubes

Wigner localization observed in carbon nanotubes
S. Pecker et al., Nature Phys. 2013
conclusions

- theo and exp of quasiparticle wave function imaging
- sensitivity to correlation effects
outline

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evidence of pairing in 1D

exp = G. Zuern et al., PRL 2013
correlated pair tunneling

$1/(g)$ vs $g$ (units of $\hbar \omega_0/\hbar \omega_0^2 2^{1/2}$)

exp = G. Zuern et al., PRL 2013
International School on Physics of Indirect Excitons

Ettore Majorana Center, Erice (IT) | July 26—August 1, 2014
Marie Curie ITN INDEX Summer School

http://web.nano.cnr.it/ispie2014/
Lecturers
J. Baumberg: Polaritons
L. Butov: Indirect excitons
M. Dyakonov: Spin physics of excitons
L. Keldysh*: Fundamentals of excitons
L. Levitov: Exciton physics in bilayers and graphene
A. Pinczuk: Optics of two-dimensional electron gases quantum Hall bilayers
D. Ritchie: Electrically formed electron-hole systems

Speakers
K. Bolotin: TBA
F. Dubin: Dark excitons
A. Holleitner: Few-exciton physics
V. Pellegrini: TBA
L. Pfeiffer: Semiconductor bilayers
M. Polini: TBA
L. Ponomarenko: Transport in bilayer graphene
M. Rontani: Anomalous magnetization of carbon nanotubes as excitonic insulators
P. Savvidis: TBA
C. Tejedor: TBA
M. Vladimirova: Spin dynamics in coupled quantum wells

2 hours + 1 hour discussion / exercise