Strongly interacting fermions in optical lattices: from few to many particles

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Cooper Pairing

For attractive interaction, Many-Body instability

Binding energy, $T_C \sim e^{-\pi/2k_F|a_s|}$ Radius $\sim e^{\pi/2k_F|a_s|}$



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Motivation

Bring together two of the most successful tools for ultracold gases: Feshbach resonances and optical lattices





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Fundamentally: how do fermions pair to form bosons?

How do we optimize making diatomic molecules from atoms? Can we devise tractable models for many-body physics near unitarity?

Feshbach resonances



Two-channel model: s-wave scattering length $a_s = -\frac{\mu g^2}{2\pi\hbar^2\nu}$ Effective range $r_B = \frac{\pi\hbar^4}{\mu^2 g^2}$ Scattering amplitude $f(\mathbf{k}) = -\frac{1}{1/a_s + ik + r_b k^2}$



Feshbach resonances



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Lattice physics

$$V_{\text{latt}}\left(\mathbf{r}\right) = V \sum_{i=x,y,z} \sin^2\left(\pi i/a\right)$$

- Lattice potential is non-separable
- Couples center-of-mass and relative coordinates
- Band structure "structures continuum"
- New length and energy scales

Scale	Typical values
Lattice spacing $a \pmod{a}$	550
Temperature T (nK)	~100
Recoil energy $\hbar^2 \pi^2 / 2ma^2$ (kHz)	25 (⁴⁰ K), 170 (⁶ Li)
Lowest band tunneling $t(E_R)$	~ 0.01
Band gap (E_R)	~ 5
Effective range r_B (nm)	$\lesssim 1$
Interchannel coupling $g/E_R a^{3/2}$	$\gtrsim 16$

Optical lattices



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Usual assumptions

- Replace interaction with free-space pseudopotential
- Restrict to the lowest band
- Requires low energy, small s-wave scattering length

 $a_s \ll a$

 $U\left(\mathbf{r}\right) = \frac{4\pi\hbar^{2}a_{s}}{m}\delta\left(\mathbf{r}\right)$

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Hubbard model

Simplest model of interacting lattice fermions

$$\hat{H} = -t \sum_{\langle i,j \rangle} \sum_{\sigma \in \{\uparrow,\downarrow\}} \left[\hat{a}_{i,\sigma}^{\dagger} \hat{a}_{j,\sigma} + \text{h.c.} \right] + U \sum_{i} \hat{n}_{i,\uparrow} \hat{n}_{i,\downarrow}$$



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Hubbard parameters

Improved ansatz

- Lattice pseudopotential set by lattice scattering properties
- Includes all bands via the lattice scattering amplitude
- Also allows for renormalization of two-particle theory

$$\lambda_{\text{Hubb.}} = \frac{U}{1 - UG(E)}$$

$$\lim_{E \to 0} \lambda_{\text{Hubb.}} = \lim_{E \to 0} \lambda_{\text{exact}}$$

$$U = \frac{1}{G(0) + 1/\lambda_{\text{exact}}}$$

$$M = \frac{U}{G(0) + 1/\lambda_{\text{exact}}}$$

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Single vs. two-channel models

Why does it fail?

- Lacks complete momentum dependence of scattering amplitude
- Actual effective potential in two-channel model:

$$U_{\mathbf{k},\mathbf{k}'} = \mathcal{P}\frac{g_{\mathbf{k}}g_{\mathbf{k}'}}{2\epsilon_{\mathbf{k}} - E}$$
$$E = \nu_0 - \mathcal{P}\sum_{\mathbf{k}} \frac{g_{\mathbf{k}}^2}{2\epsilon_{\mathbf{k}} - E}$$

Single channel model lacks residual momentum dependence as coupling becomes pointlike

Solution: Use a two-channel many-body lattice model!

Fermi-Bose Hubbard Hamiltonian

$$\hat{H} = \hat{H}_f + \hat{H}_b + \hat{H}_{fb}$$

Multiband Fermi-Hubbard Hamiltonian

$$\hat{H}_{f} = -\sum_{m} t_{m}^{f} \sum_{\langle i,j \rangle} \sum_{\sigma \in \{\uparrow,\downarrow\}} \left(\hat{f}_{i,\sigma;m}^{\dagger} \hat{f}_{j,\sigma;m} + \text{h.c.} \right) - \sum_{m,m'} \left| U_{m,m'}^{f} \right| \sum_{i} \hat{n}_{i,\uparrow;m}^{f} \hat{n}_{i,\downarrow;m'}^{f} - \sum_{i,\sigma,m} \left(\mu_{f} - E_{m}^{f} \right) \hat{n}_{i,\sigma;m}^{f}$$

Multiband Bose-Hubbard Hamiltonian

$$\hat{H}_{b} = -\sum_{m} t_{m}^{b} \sum_{\langle i,j \rangle} \left(\hat{b}_{i;m}^{\dagger} \hat{b}_{j;m} + \text{h.c.} \right) + \sum_{m,m'} \frac{U_{m,m'}^{b}}{2} \sum_{i} \left[\hat{n}_{i;m}^{b} \left(\hat{n}_{i;m'}^{b} - \delta_{m,m'} \right) \right] - \sum_{i,\sigma,m} \left(\mu_{b} - E_{m}^{b} \right) \hat{n}_{i;m}^{b}$$

$$Bose-Fermi \ coupling$$

$$\hat{H}_{fb} = \sum_{i,s,m,m'} g_{s}^{mm'} \left(\hat{b}_{i;s}^{\dagger} \hat{f}_{i,\uparrow;m} \hat{f}_{i,\downarrow;m'} + \text{h.c.} \right) + \sum_{i,m,m',\sigma} V_{mm'} \hat{n}_{i;m'}^{b} \hat{n}_{i,\sigma;m}^{f}$$

Correct but awful!

- i, j site indices
- In principle infinite summation over fermionic and molecular bands
- Not amenable to treatment by modern methods

m, m' band indices

 σ "spin" indices

- Effective range is small-high energy physics is very short range
- Long wavelength physics captured by lowest band fermions
- At low density, high energy physics is two-body physics
- Recouple at many-particle level



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$$\begin{split} \hat{H}_{o} | \mathbf{K}, \mathbf{q}; \mathbf{n}, \mathbf{m} \rangle &= E_{\mathbf{nm}}^{\mathbf{K}} \left(\mathbf{q} \right) | \mathbf{K}, \mathbf{q}; \mathbf{n}, \mathbf{m} \rangle \\ \hat{H}_{c} | \mathbf{K}; \mathbf{s} \rangle &= E_{\mathbf{sK}}^{(b)} | \mathbf{K}; \mathbf{s} \rangle \\ \hat{\Upsilon}_{\mathbf{s}}^{\mathbf{K}} &= \langle \mathbf{K}; \mathbf{s} | \psi_{c} \rangle \end{split}$$



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Open Channel Closed Channel Project into lattice basis $\left[E - \nu - \hat{H}_c\right] |\psi_c\rangle = \hat{g} \frac{1}{E - \hat{H}_0 + i\eta} \hat{g} |\psi_c\rangle$ Energy Band index $\hat{H}_{o}|\mathbf{K},\mathbf{q};\mathbf{n},\mathbf{m}\rangle = E_{\mathbf{nm}}^{\mathbf{K}}(\mathbf{q})|\mathbf{K},\mathbf{q};\mathbf{n},\mathbf{m}\rangle$ Band index (\mathbf{n}, \mathbf{m}) $\hat{H}_c |\mathbf{K}; \mathbf{s}\rangle = E_{\mathbf{s}\mathbf{K}}^{(b)} |\mathbf{K}; \mathbf{s}\rangle$ $g_{\mathbf{nms}}$ $\Upsilon_{\mathbf{s}}^{\mathbf{K}} = \langle \mathbf{K}; \mathbf{s} | \psi_c \rangle$ $\nu_{\mathbf{s}}$ $\hat{g} = g \alpha_{\Lambda} (\mathbf{r})$ Total quasimomentum \mathbf{K} CM quasimomentum \mathbf{K} $\lim_{\Lambda \to \infty} \alpha_{\Lambda} \left(\mathbf{r} \right) = \delta \left(\mathbf{r} \right)$

 $h_{\mathbf{sK}}^{\mathbf{nm}}\left(\mathbf{q}\right) = \langle \mathbf{K}; \mathbf{s} | \hat{g} | \mathbf{K}, \mathbf{q}; \mathbf{n}, \mathbf{m} \rangle$

$$\begin{bmatrix} E_{\mathbf{K}} - \nu - E_{\mathbf{sK}}^{(b)} \end{bmatrix} \Upsilon_{\mathbf{s}}^{\mathbf{K}} = \frac{g^2}{v} \sum_{\mathbf{t}} \chi_{\mathbf{st}}^{\mathbf{K}} (E_{\mathbf{K}}) \Upsilon_{\mathbf{t}}^{\mathbf{K}}$$
$$\chi_{\mathbf{st}}^{\mathbf{K}} (E_{\mathbf{K}}) = \sum_{\mathbf{nm}} \int \frac{d\mathbf{q}}{v_{\mathrm{BZ}}} \frac{h_{\mathbf{sK}}^{\mathbf{nm}} (\mathbf{q}) h_{\mathbf{tK}}^{\mathbf{nm}} (\mathbf{q})}{E_{\mathbf{K}} - E_{\mathbf{nm}}^{\mathbf{K}} (\mathbf{q}) + i\eta}$$

Regularization

$$\begin{bmatrix} E_{\mathbf{K}} - \nu - E_{\mathbf{s}\mathbf{K}}^{(b)} \end{bmatrix} \Upsilon_{\mathbf{s}}^{\mathbf{K}} = \frac{g^2}{v} \sum_{\mathbf{t}} \chi_{\mathbf{s}\mathbf{t}}^{\mathbf{K}} (E_{\mathbf{K}}) \Upsilon_{\mathbf{t}}^{\mathbf{K}}$$
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- Renormalization is χ without the optical lattice
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$$\left[E_{\mathbf{K}} - \bar{\nu} - E_{\mathbf{sK}}^{(b)}\right] \Upsilon_{\mathbf{s}}^{\mathbf{K}} = \frac{g^2}{v} \sum_{\mathbf{t}} \left[\chi_{\mathbf{st}}^{\mathbf{K}} \left(E_{\mathbf{K}}\right) - \bar{\chi}_{\mathbf{st}}^{\mathbf{K}}\right] \Upsilon_{\mathbf{t}}^{\mathbf{K}}$$



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$$a_s = -mg^2/4\pi\hbar^2\nu, \quad E_R = \hbar^2\pi^2/2ma^2$$

$$\Rightarrow \left(8a_s E_R/\pi a \right) \left[\chi^{\mathbf{K}} \left(E_{\mathbf{K}} \right) - \bar{\chi}^{\mathbf{K}} \right] \Upsilon^{\mathbf{K}} - \Upsilon^{K} = 0$$

Nonlinear eigenvalue problem!



Results for K=0



"Band structures" for general quasimomentum



"Band structures" for general quasimomentum



Projection $\begin{bmatrix} E_{\mathbf{K}} - \bar{\nu} - E_{\mathbf{s}\mathbf{K}}^{(b)} \end{bmatrix} \Upsilon_{\mathbf{s}}^{\mathbf{K}} = \frac{g^2}{v} \sum_{\mathbf{t}} \left[\tilde{\chi}_{\mathbf{st}}^{\mathbf{K}} \left(E_{\mathbf{K}} \right) - \bar{\chi}_{\mathbf{st}}^{\mathbf{K}} \right] \Upsilon_{\mathbf{t}}^{\mathbf{K}}$ $\tilde{\chi}_{\mathbf{st}}^{\mathbf{K}} \left(E_{\mathbf{K}} \right) = \sum_{\mathbf{nm} \neq (\mathbf{1}, \mathbf{1})} \int \frac{d\mathbf{q}}{v_{\mathrm{BZ}}} \frac{h_{\mathbf{sK}}^{\mathbf{nm}} \left(\mathbf{q} \right) h_{\mathbf{tK}}^{\mathbf{nm}} \left(\mathbf{q} \right)}{E_{\mathbf{K}} - E_{\mathbf{nm}}^{\mathbf{K}} \left(\mathbf{q} \right) + i\eta}$ 2)Partition into low and high energy spaces Open Channel Closed Channel High energy Low energy

$\begin{aligned} & \left[E_{\mathbf{K}} - \bar{\nu} - E_{\mathbf{sK}}^{(b)} \right] \Upsilon_{\mathbf{s}}^{\mathbf{K}} = \frac{g^2}{v} \sum_{\mathbf{t}} \left[\tilde{\chi}_{\mathbf{st}}^{\mathbf{K}} \left(E_{\mathbf{K}} \right) - \bar{\chi}_{\mathbf{st}}^{\mathbf{K}} \right] \Upsilon_{\mathbf{t}}^{\mathbf{K}} \\ & \tilde{\chi}_{\mathbf{st}}^{\mathbf{K}} \left(E_{\mathbf{K}} \right) = \sum_{\mathbf{nm} \neq (\mathbf{1}, \mathbf{1})} \int \frac{d\mathbf{q}}{v_{\mathrm{BZ}}} \frac{h_{\mathbf{sK}}^{\mathbf{nm}} \left(\mathbf{q} \right) h_{\mathbf{tK}}^{\mathbf{nm}} \left(\mathbf{q} \right)}{E_{\mathbf{K}} - E_{\mathbf{nm}}^{\mathbf{K}} \left(\mathbf{q} \right) + i\eta} \end{aligned}$

- Compute χ without contributions from lowest open channel band
- Renormalization is same as full two-body problem
- Scattering length obtained is the true two-body scattering length
- Same scaling analysis in cutoff applies
- Together with dynamical lowest band fermions, correctly reproduces all scattering states in the lowest band and nearby bound states
- If higher scattering bands are relevant, project them out and include dynamically
- Energetic range of model can be extended arbitrarily



Projection



)



$$\begin{aligned} \hat{H}_{\text{eff}} &= -t_f \sum_{\sigma \in \{\uparrow,\downarrow\}} \sum_{\langle i,j \rangle} \hat{a}_{i\sigma}^{\dagger} \hat{a}_{j\sigma} + E_0 \sum_{\sigma \in \{\uparrow,\downarrow\}} \sum_i \hat{n}_{i\sigma}^{(f)} - \sum_{\alpha \in \mathcal{M}} \sum_{i,j} t_{i,j}^{\alpha} \hat{d}_{i,\alpha}^{\dagger} \hat{d}_{j,\alpha} + \sum_{\alpha \in \mathcal{M}} \sum_i \hat{n}_{i\alpha}^{(b)} \\ &+ \sum_{\alpha \in \mathcal{M}} \sum_{ijk} g_{i-j,i-k}^{\alpha} \left[\hat{d}_{i,\alpha}^{\dagger} \hat{a}_{j,\uparrow} \hat{a}_{k,\downarrow} + \text{h.c.} \right] \end{aligned}$$



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$$\hat{H}_{\text{eff}} = -t_f \sum_{\sigma \in \{\uparrow,\downarrow\}} \sum_{\langle i,j \rangle} \hat{a}_{i\sigma}^{\dagger} \hat{a}_{j\sigma} + E_0 \sum_{\sigma \in \{\uparrow,\downarrow\}} \sum_i \hat{n}_{i\sigma}^{(f)} - \left[\sum_{\alpha \in \mathcal{M}} \sum_{i,j} t_{i,j}^{\alpha} \hat{d}_{i,\alpha}^{\dagger} \hat{d}_{j,\alpha}\right] + \sum_{\alpha \in \mathcal{M}} \sum_i \hat{n}_{i\alpha}^{(b)} + \sum_{\alpha \in \mathcal{M}} \sum_{i,j} t_{i,j}^{\alpha} \hat{d}_{i,\alpha}^{\dagger} \hat{d}_{j,\alpha} + \sum_{\alpha \in \mathcal{M}} \sum_{i,j} \hat{n}_{i\alpha}^{(f)} \hat{d}_{i,\alpha}^{\dagger} \hat{d}_{j,\gamma} \hat{d}_{i,\alpha} + \text{h.c.} \right]$$

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$$\hat{H}_{\text{eff}} = -t_f \sum_{\sigma \in \{\uparrow,\downarrow\}} \sum_{\langle i,j\rangle} \hat{a}_{i\sigma}^{\dagger} \hat{a}_{j\sigma} + E_0 \sum_{\sigma \in \{\uparrow,\downarrow\}} \sum_i \hat{n}_{i\sigma}^{(f)} - \sum_{\alpha \in \mathcal{M}} \sum_{i,j} t_{i,j}^{\alpha} \hat{d}_{i,\alpha}^{\dagger} \hat{d}_{j,\alpha} + \sum_{\alpha \in \mathcal{M}} \sum_i \hat{n}_{i\alpha}^{(b)} + \sum_{\alpha \in \mathcal{M}} \sum_{i,j} t_{i,j}^{\alpha} \hat{d}_{i,\alpha}^{\dagger} \hat{d}_{j,\alpha} + \sum_{\alpha \in \mathcal{M}} \sum_{i,j} \hat{n}_{i\alpha}^{(f)} \hat{d}_{i,\alpha}^{\dagger} \hat{d}_{j,\gamma} \hat{d}_{i,\alpha} + \text{h.c.} \right]$$

$$\hat{H}_{\text{eff}} = -t_f \sum_{\sigma \in \{\uparrow,\downarrow\}} \sum_{\langle i,j\rangle} \hat{a}_{i\sigma}^{\dagger} \hat{a}_{j\sigma} + E_0 \sum_{\sigma \in \{\uparrow,\downarrow\}} \sum_i \hat{n}_{i\sigma}^{(f)} - \sum_{\alpha \in \mathcal{M}} \sum_{i,j} t_{i,j}^{\alpha} \hat{d}_{i,\alpha}^{\dagger} \hat{d}_{j,\alpha} + \sum_{\alpha \in \mathcal{M}} \sum_i \hat{n}_{i\alpha}^{(b)} + \sum_{\alpha \in \mathcal{M}} \sum_{i,j} q_{i-j,i-k}^{\alpha} \left[\hat{d}_{i,\alpha}^{\dagger} \hat{a}_{j,\uparrow} \hat{a}_{k,\downarrow} + \text{h.c.} \right]$$

20

$$\hat{H}_{\text{eff}} = -t_f \sum_{\sigma \in \{\uparrow,\downarrow\}} \sum_{\langle i,j \rangle} \hat{a}_{i\sigma}^{\dagger} \hat{a}_{j\sigma} + E_0 \sum_{\sigma \in \{\uparrow,\downarrow\}} \sum_i \hat{n}_{i\sigma}^{(f)} - \sum_{\alpha \in \mathcal{M}} \sum_{i,j} t_{i,j}^{\alpha} \hat{d}_{i,\alpha}^{\dagger} \hat{d}_{j,\alpha} + \sum_{\alpha \in \mathcal{M}} \sum_i \hat{n}_{i\alpha}^{(b)} + \sum_{\alpha \in \mathcal{M}} \sum_{ijk} g_{i-j,i-k}^{\alpha} \left[\hat{d}_{i,\alpha}^{\dagger} \hat{a}_{j,\uparrow} \hat{a}_{k,\downarrow} + \text{h.c.} \right]$$

$$\begin{aligned} \hat{H}_{\text{eff}} &= -t_f \sum_{\sigma \in \{\uparrow,\downarrow\}} \sum_{\langle i,j \rangle} \hat{a}_{i\sigma}^{\dagger} \hat{a}_{j\sigma} + E_0 \sum_{\sigma \in \{\uparrow,\downarrow\}} \sum_i \hat{n}_{i\sigma}^{(f)} - \sum_{\alpha \in \mathcal{M}} \sum_{i,j} t_{i,j}^{\alpha} \hat{d}_{i,\alpha}^{\dagger} \hat{d}_{j,\alpha} + \sum_{\alpha \in \mathcal{M}} \sum_i \hat{n}_{i\alpha}^{(b)} \\ &+ \sum_{\alpha \in \mathcal{M}} \sum_{ijk} g_{i-j,i-k}^{\alpha} \left[\hat{d}_{i,\alpha}^{\dagger} \hat{a}_{j,\uparrow} \hat{a}_{k,\downarrow} + \text{h.c.} \right] \end{aligned}$$

The Fermi resonance Hamiltonian $\hat{H}_{\text{eff}} = -t_f \sum_{\sigma \in \{\uparrow,\downarrow\}} \sum_{\langle i,j \rangle} \hat{a}_{i\sigma}^{\dagger} \hat{a}_{j\sigma} + E_0 \sum_{\sigma \in \{\uparrow,\downarrow\}} \sum_i \hat{n}_{i\sigma}^{(f)} - \sum_{\alpha \in \mathcal{M}} \sum_{i,j} t_{i,j}^{\alpha} \hat{d}_{i,\alpha}^{\dagger} \hat{d}_{j,\alpha} + \sum_{\alpha \in \mathcal{M}} \bar{\nu}_{\alpha} \sum_i \hat{n}_{i\alpha}^{(b)}$ $\sum \sum g_{i-j,i-k}^{\alpha} \left[\hat{d}_{i,\alpha}^{\dagger} \hat{a}_{j,\uparrow} \hat{a}_{k,\downarrow} + \text{h.c.} \right]$ $\alpha \in \mathcal{M} \ ijk$ 10 | (b) $|g_{000,000}|/E_R$ (a) $|\bar{\nu}|/E_R$ $g_{000,000}$ $g_{000,100}$ 1 $g_{100,000}$ $g_{200,000}$ $|t_{000,100}|/E_{R_{e}}$ 0.1 $t_{000,200}/E_R$ $|g_{100,000}|/E_R$ $|t_{000,110}|/E_R$ $|g_{200,000}|/E_R$ $|t_{000,111}|/E_R|$ 0.01 $|g_{000,100}|/E_R$ -2 a_s/a a_s/a

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 $|t_{000,111}|/E_R|$

 a_s/a

 $|g_{200,000}|/E_R$

 $|g_{000,100}|/E_R$

-2

 a_s/a

0.01

The Fermi resonance Hamiltonian $\hat{H}_{\text{eff}} = -t_f \sum_{\sigma \in \{\uparrow,\downarrow\}} \sum_{\langle i,j \rangle} \hat{a}_{i\sigma}^{\dagger} \hat{a}_{j\sigma} + E_0 \sum_{\sigma \in \{\uparrow,\downarrow\}} \sum_i \hat{n}_{i\sigma}^{(f)} - \sum_{\alpha \in \mathcal{M}} \sum_{i,j} t_{i,j}^{\alpha} \hat{d}_{i,\alpha}^{\dagger} \hat{d}_{j,\alpha} + \sum_{\alpha \in \mathcal{M}} \sum_i \hat{n}_{i\alpha}^{(b)}$ $\sum \sum g_{i-j,i-k}^{\alpha} \left[\hat{d}_{i,\alpha}^{\dagger} \hat{a}_{j,\uparrow} \hat{a}_{k,\downarrow} + \text{h.c.} \right]$ $\alpha \in \mathcal{M} \ ijk$ 10 | (b) $|g_{000,000}|/E_R$ (a) $|\bar{\nu}|/E_R$ $g_{000,000}$ $g_{000,100}$ 1 $g_{100,000}$ $g_{200,000}$ $|t_{000,100}|/E_R$ 0.1 $t_{000,200}/E_R$ $|g_{100,000}|/E_R$ $|t_{000,110}|/E_R$ $|g_{200,000}|/E_R$ $|t_{000,111}|/E_R$ 0.01 $|g_{000,100}|/E_R$ -2 a_s/a a_s/a

Extensions and Conclusions

Extensions

- Multichannel resonances-basis expanded to include a channel index
- Higher-I pairing/ more general two-body potential
- Arbitrary single particle potentials

Conclusions

- Investigated BEC-BCS crossover in a lattice at the two-body level
- Derived effective few-band model for low-energy, low filling limit
- Significant qualitative and quantitative differences with models derived using separable potential approximations
- All parameters microscopically attainable

Thank You!

Narrow resonances

