Confinement modifies interactions of ultracold dipolar gases on optical lattices

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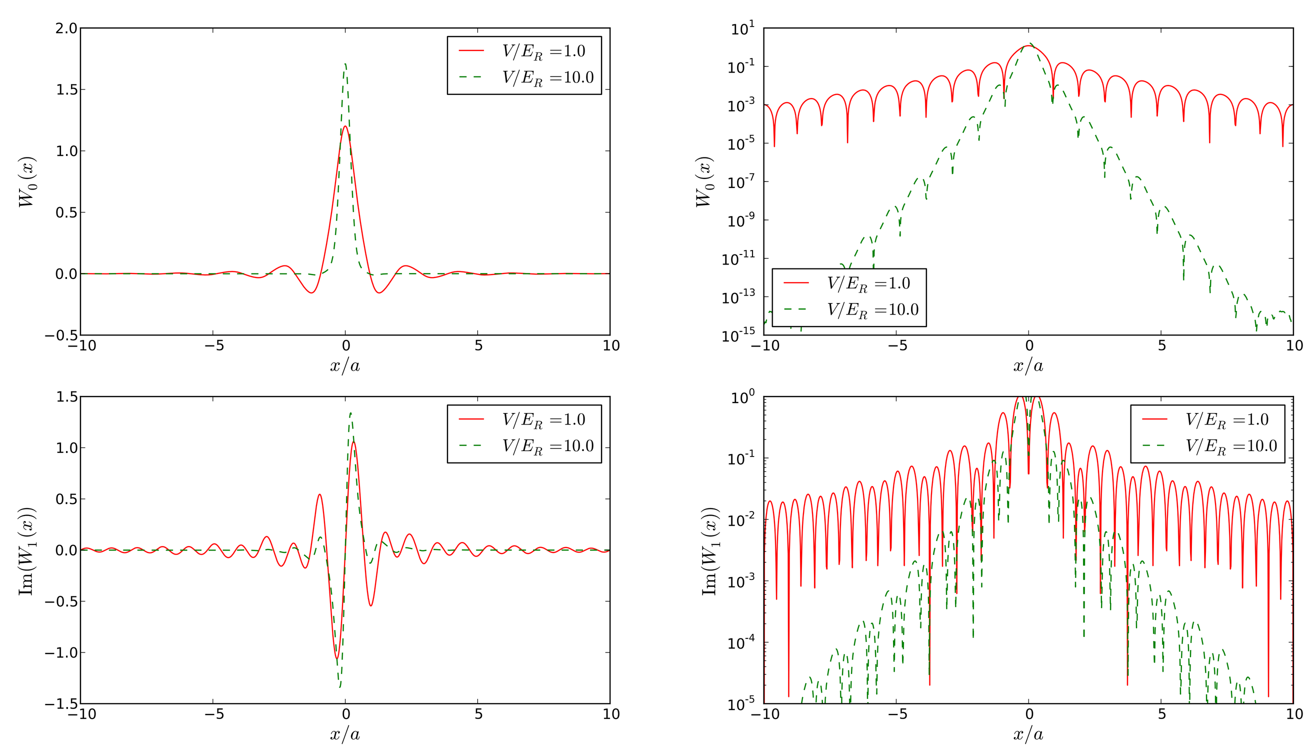
Motivation

- Several near-term dipolar gases in optical lattices (molecules!).
- Several theoretical proposals of many-body models.
- *All* assume effective dipolar interaction $\sim 1/r^3$.
- Main finding: Effective dipolar interaction is exponential at moderate range!
- d-wave symmetry⇒Modifications of interactions strongly dependent on imbalance in confinement
- Heavy tails of Wannier functions crucial, not widths.
- Implications for many-body physics, phase diagrams.

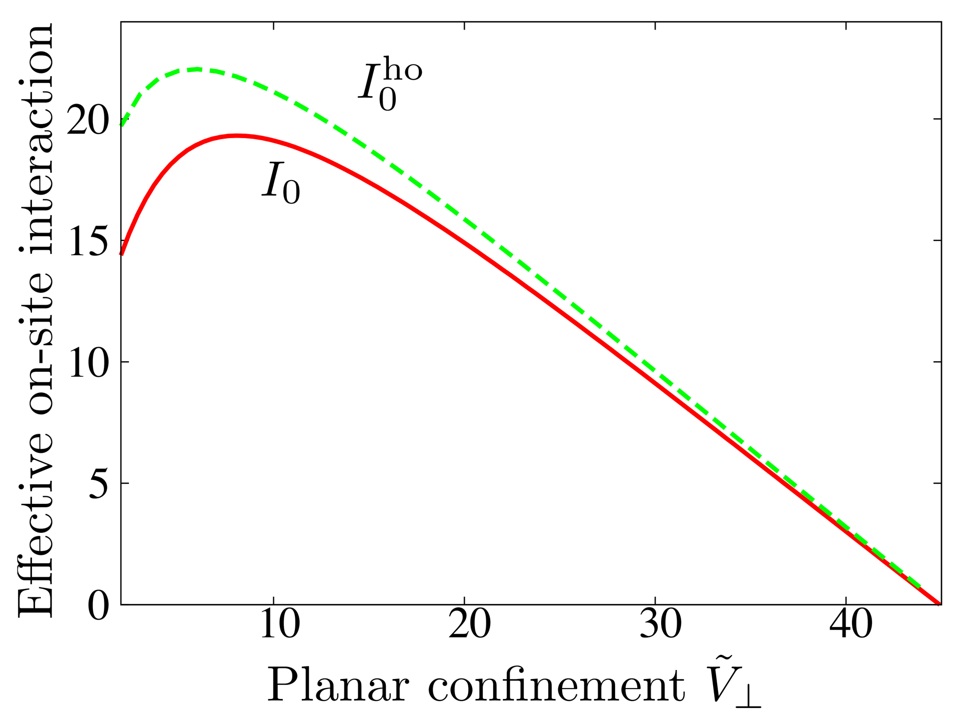
Wannier Functions

- $w_{\mathbf{i}}(\mathbf{r}) \equiv w(\mathbf{r}-\mathbf{r}_i) = L^{-1/2}\sum_{\mathbf{k}\in \mathrm{BZ}} e^{-i\mathbf{k}\cdot\mathbf{r}_i}\psi_{\mathbf{k}}(\mathbf{r})$
- Most localized orthonormal basis consistent with lattice symmetries.
- Exponentially decaying under very general conditions.
- Below: $V_{\mathrm{latt}}(x) = V\sin^2(\pi x/a)$, $E_R = \hbar^2\pi^2/2ma^2$



On-site comparison with harmonic oscillator

- Compare on-site interaction with dipolar energy in harmonic well.
- Consistency requires matching of local curvature $\ell_\nu = a/(\pi(V_\nu/E_R)^{1/4})$, $\nu = x, y, z$
- $I_0^{\mathrm{ho}} = \frac{\sqrt{2}}{\pi\bar{\ell}^3}\left[\frac{2}{3}+\beta^2-\frac{\beta}{1-\alpha^2}\cot^{-1}(\beta)\right]$, mean length $\bar{\ell} \equiv (\ell_z\ell_\perp^2)^{1/3}/a$, Confinement anisotropy $\alpha \equiv \ell_z/\ell_\perp$, $\beta \equiv \alpha(1-\alpha^2)^{-1/2}$.
- Vanishes for isotropic confinement→ spherical symmetry



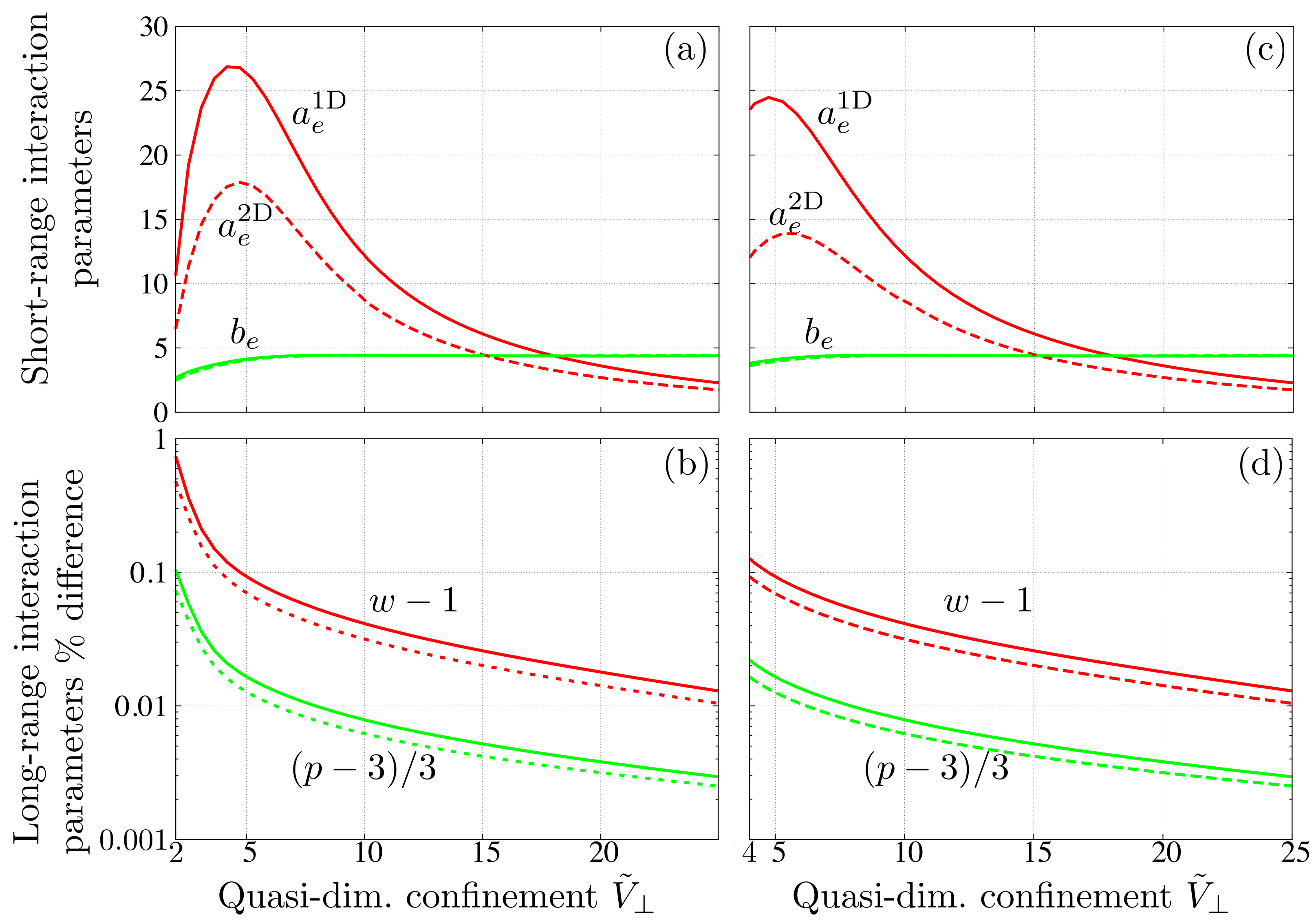
Numerical evaluation and results

- Second quantized interaction: $\hat{H}_{\mathrm{int}} = \frac{1}{2}\int d\mathbf{r}\int d\mathbf{r}'\,\hat{\psi}^\dagger(\mathbf{r})\hat{\psi}^\dagger(\mathbf{r}')V_{\mathrm{int}}(\mathbf{r}-\mathbf{r}')\hat{\psi}(\mathbf{r}')\hat{\psi}(\mathbf{r})$
- Expand $\hat{\psi}(\mathbf{r})$ in terms of Wannier functions → lattice model.
- Electric dipole-dipole in deep lattices $\hat{H}_{\mathrm{int}} = U[\frac{1}{2}\sum_{\mathbf{i}} I_0\hat{n}_{\mathbf{i}}(\hat{n}_{\mathbf{i}}-1)+\frac{1}{2}\sum_{\mathbf{i}\neq\mathbf{i}'} I_{\mathbf{i}',\mathbf{i}}\hat{n}_{\mathbf{i}}\hat{n}_{\mathbf{i}'}]$

$$a^3U \equiv [\hat{\mathbf{d}}_1\otimes\hat{\mathbf{d}}_2]_0^{(2)}\sqrt{3/2},\ I_0 \equiv a^3\mathcal{G}^{\mathrm{dd};0}_{\mathbf{0000}},\quad I_{\mathbf{i}',\mathbf{i}} \equiv a^3[\mathcal{G}^{\mathrm{dd};0}_{\mathbf{ii'i'i}} \pm \mathcal{G}^{\mathrm{dd};0}_{\mathbf{ii'ii'}}]$$

$$\mathcal{G}^{\mathrm{dd};0}_{\mathbf{i_1i_2i_2'i_1'}} = -2\int d\mathbf{r}\int d\mathbf{r}' w^\star_{\mathbf{i}_1}(\mathbf{r})\,w_{\mathbf{i}_1'}(\mathbf{r})\frac{C_0^{(2)}(\mathbf{r}-\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|^3}w^\star_{\mathbf{i}_2}(\mathbf{r}')\,w_{\mathbf{i}_2'}(\mathbf{r}')$$

- Evaluate integral numerically using convolution or Bloch expansion.
- Equally confined 3D lattice: same as in free space. $I_0 = 0$.
- Quasi-low D strongly dependent on confinement imbalance.
- Fit ansatz $I_j = a_e\exp(-b_e j)+wj^{-p}$, j is separation along x.
- Quasi-2D, $V_z = 45E_R$. Quasi-1D, $V_z = V_y = 45E_R$.



Implications for many-body physics

- Hard-core bosons with dipolar interactions: $\hat{H} = -t\sum_{\langle ij\rangle}\hat{a}_i^\dagger\hat{a}_j + U\sum_{i<j} I_{j-i}\hat{n}_i\hat{n}_j - \mu\sum_i\hat{n}_i$
- Transition from superfluid to crystalline phase with long range density order.
- Two dipolar realizations: Assuming $1/r^3$ (dashed line), computed (hatched, solid boundary).
- Dotted boundary→ rescaled to nearest-neighbor interaction