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Fermi-polaron-like effects in a one-dimensional (1D) optical lattice

M J Leskinen, O H T Nummi, F Massel and P Törmä[1]
Department of Applied Physics, PO Box 5100, 02015 Aalto University, Finland
E-mail: paivi.torma@tkk.fi

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Abstract. We study a highly imbalanced Fermi gas in a one-dimensional (1D) optical lattice from the polaronic point of view. The time-evolving block decimation algorithm is used to calculate the ground state and dynamics of the system. We find polaronic behaviour qualitatively similar to that in the recent experiment by Schirotzek *et al* (2009 *Phys. Rev. Lett.* **102** 230402), where radio-frequency (rf) spectroscopy was used to observe polarons in 3D space. In the weakly interacting limit, our exact results are in excellent agreement with a polaron ansatz, and in the strongly interacting limit, the results match with an approximative solution of the Bethe ansatz (BA), suggesting crossover from a quasiparticle to a charge-density excitation regime.

Contents

[1] Author to whom any correspondence should be addressed.

1. Introduction

Impurity problems are essential in determining the low-temperature properties of condensed matter systems. A well-known example is an electron moving in a crystal lattice and interacting with its surrounding ions [2]. This creates lattice polarization and deformation, which are carried with the electron through the material. Interactions with the ions create an effective potential for the electron and try to slow it down, which can be modelled as the effective mass of the electron. Another famous impurity problem is the Kondo effect [3], where the scattering of conduction electrons with magnetic impurities gives rise to electrical resistivity. Ultracold atom gases provide an excellent ground for the study of impurity problems owing to the controllability of the system parameters. For instance, two-component gases can be realized by using two different hyperfine spin states of alkali atoms. The population imbalance can be controlled by transferring particles between the two hyperfine states with radiofrequency (rf) pulses. The inter-component interaction can be tuned by Feshbach resonances [4].

Along with their theoretical description in ultracold bosonic gases (see e.g. [5, 6]), polarons were recently observed in an ultracold atomic Fermi gas [1, 7]. In [1], rf spectroscopy was used to measure a sharp quasiparticle peak solely for the minority component in the highly imbalanced gas of ^{6}Li atoms. Theoretically, various approaches, such as Monte Carlo studies [8, 9], T-matrix approaches [10]–[12] and variational ansatz [10, 13, 14], have been used to model the phenomenon. A variational ansatz by F Chevy [13] has explained the qualitative features of the experiment. In [14], a variational ansatz describing also the Bose–Einstein condensate (BEC) side of the Feshbach resonance, including molecular formation, was proposed, and the ground state properties matched well with the Monte Carlo studies [8].

In one-dimensional (1D) optical lattices, exact methods provide straightforward approaches for highly polarized gases [15]–[19]. In this paper, we use an exact numerical method to investigate highly imbalanced Fermi gases from the polaronic point of view. We study both the ground state properties and the dynamics, and make a comparison to two different approximative solutions. In the weakly interacting limit, the results are compared to the polaron ansatz of [13], and in the strongly interacting limit, the results are compared to an approximative solution of the Bethe ansatz (BA). In both limits, excellent agreement between the exact and approximative solutions is found. However, although we analyse the numerical results using a polaron ansatz, we do not necessarily claim the existence of a polaron in a 1D system: well-defined polaronic quasiparticles may not exist due to the 1D nature of the system. We discuss the implications of our results for 3D systems.

In section 2, we consider ground state properties of highly imbalanced gases. In section 3, we study the rf response of the ground states. In section 4, the limitations of our model as well as the connection to higher dimensional systems are discussed. In section 5, we present the conclusions.

2. Exact simulations

For atoms in an optical lattice, the physics is well captured by the Fermi–Hubbard model,

$$\hat{H}_0 = -J \sum_{\langle i,\, j\rangle\sigma} \hat{c}^{\dagger}_{i\sigma}\hat{c}_{j\sigma} + U \sum_{i} \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}, \tag{1}$$

where J is the hopping energy, U is the on-site interaction strength between different spin components $\sigma \in \{\uparrow, \downarrow\}$, $\hat{c}_{i\sigma}$ ($\hat{c}^{\dagger}_{i\sigma}$) annihilate (create) a fermion for a site i with spin σ and $\hat{n}_{i\sigma} = \hat{c}^{\dagger}_{i\sigma}\hat{c}_{i\sigma}$. Here we consider only attractive interactions $U < 0$. In the recent experiments in [1, 7] in highly polarized gases, qualitative features have been explained with the variational ansatz [13]

$$|\Psi\rangle = \varphi_0\, \hat{c}^{\dagger}_{0\downarrow}\, |FS\rangle_{\uparrow}\, |\emptyset\rangle_{\downarrow} \tag{2}$$

$$+ \sum_{q<k_{\mathrm{F}}^{\uparrow}, k>k_{\mathrm{F}}^{\uparrow}} \varphi_{kq}\, \hat{c}^{\dagger}_{k\uparrow}\, \hat{c}_{q\uparrow}\, \hat{c}^{\dagger}_{q-k\downarrow}\, |FS\rangle_{\uparrow}\, |\emptyset\rangle_{\downarrow}, \tag{3}$$

where $|FS\rangle$ refers to a filled Fermi sea, $|\emptyset\rangle$ to the vacuum state and $k_{\mathrm{F}}^{\uparrow}$ is a Fermi momentum for spin $\uparrow$ particles. In the first term, the minority particle lies at the bottom of the band and the majority atoms form the Fermi sea. In the second term, the minority atom is scattered out from the lowest momentum state and the filled Fermi sea of majority particles is broken to particle–hole excitations. The variational coefficients φ_0 and φ_{kq} are found by minimizing the energy. The energy difference between the interacting and non-interacting ground states is often named as the polaron energy $E_{\mathrm{p}} = E_g - E_g^{\text{non-int}}$ because this energy difference corresponds to the energy needed to add a single impurity. Note that, with our definition, $E_{\mathrm{p}} < 0$ for attractive interaction strengths. The quantity $Z = |\varphi_0|^2$ is a measure of the quasiparticle weight of the polaron.

In order to see how well the ansatz describes the system, we have calculated the exact ground state using the time-evolving block decimation (TEBD) algorithm [20], which allows us to determine several observables. The polaron energy is the expectation value $E_{\mathrm{p}} = \langle g|\hat{H}_0|g\rangle - E_g^{\text{non-int}}$ and the quasiparticle weight is the square of the innerproduct $Z = |\langle g \mid g^{\text{non-int}}\rangle|^2$, where $|g\rangle$ and $|g^{\text{non-int}}\rangle$ are ground states for the interaction strengths $U < 0$ and $U = 0$, respectively, both with the same particle numbers. In figure 1 the polaron energy E_{p} and in figure 2 the quasiparticle weight for the ansatz and exact numerics are shown. For small interaction strengths $U \lesssim 5J$, the results are in good agreement but start to deviate for strong attractions.

In 3D free space the breakdown of the ansatz (3) in the BEC limit has been shown experimentally [1] and described theoretically [14]. In the limit $1/(k_{\mathrm{F}}a) \ll 1$, the emergence of molecular states is expected. However, in a 1D optical lattice, molecules are not formed even for strong, attractive interactions $-U \gg 1$.

M Punk *et al* [14] provided an ansatz for the molecular regime. In their ansatz, the dominant contribution comes from the term

$$\sum_{k>k_{\mathrm{F}}^{\uparrow}} \phi_k c^{\dagger}_{\downarrow -k} c^{\dagger}_{\uparrow k} c_{\uparrow 0} |FS\rangle_{\uparrow}\, |\emptyset\rangle_{\downarrow}, \tag{4}$$

where ϕ_k are variational coefficients. The summation is now restricted to momenta above the Fermi momentum $k_{\mathrm{F}}^{\uparrow}$ of majority particles. The momentum distributions for the minority and majority components in our case are shown in figure 3. The momentum distribution for minority components is extremely small above the Fermi momentum $k_{\mathrm{F}}^{\uparrow}$, and therefore the ansatz for the molecular regime in highly polarized gases does not improve the ansatz (3) in 1D lattices. However, we are able to explain our results in the strongly interacting limit quantitatively with the BA. In the limit $-U/J \to \infty$, the BA solution can be approximatively mapped to spinless

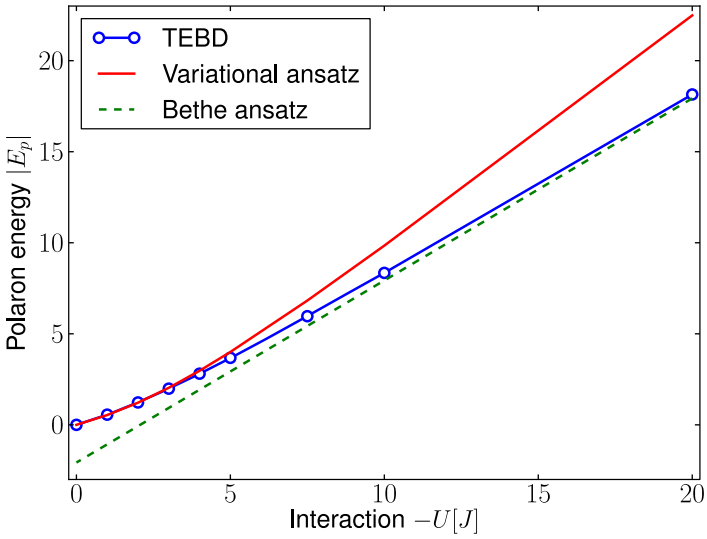

Figure 1. The polaron energy E_p as a function of the interaction strength $(-U)$. The weakly interacting regime is well described by the ansatz of equation (3) (red solid line) and the strongly interacting limit with the BA with $-U/J \to \infty$ (green dashed line). The number of sites is $N_\mathrm{L} = 40$ and the atom numbers are $N_\uparrow = 20$, $N_\downarrow = 1$.

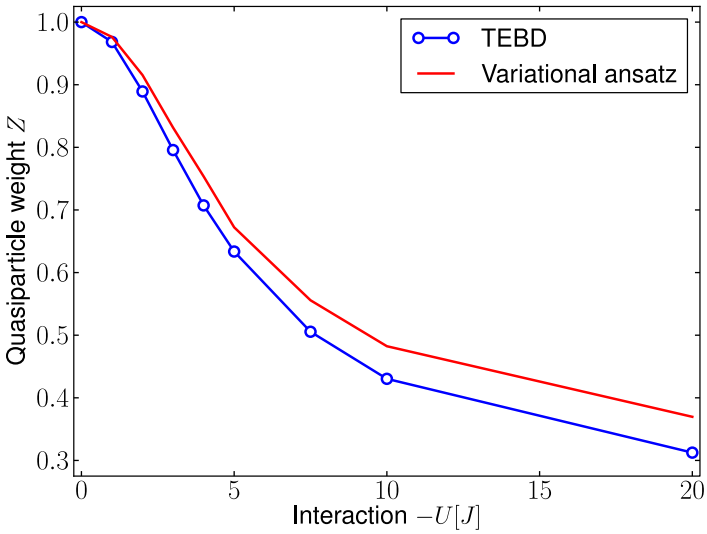

Figure 2. The quasiparticle weight $Z = |\varphi_0|^2$ as a function of the interaction strength $-U$. Parameters are as in figure 1.

fermions [21]. The energy becomes (see the appendix)

$$E = U - 2J \sum_{i=1}^{N_\uparrow - N_\downarrow} \cos(k_j), \tag{5}$$

$$k_j = \frac{\pi j}{N_\mathrm{L} + 1}. \tag{6}$$

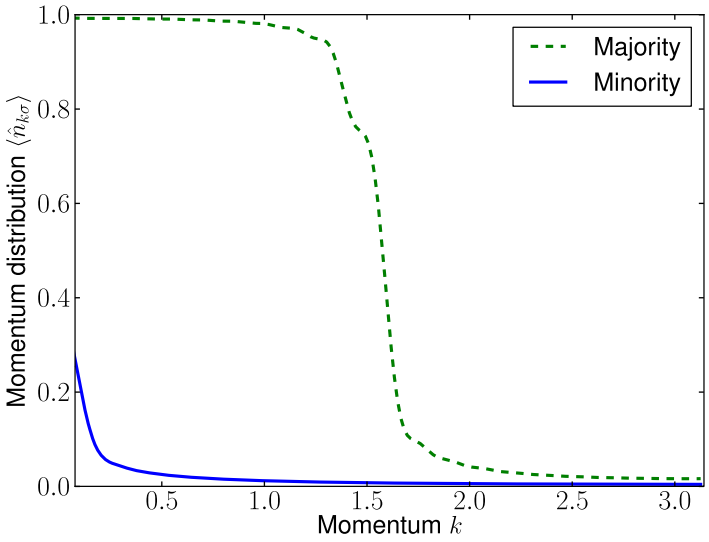

Figure 3. Momentum distributions $\langle \hat{n}_{k,\sigma} \rangle = \langle \hat{c}^{\dagger}_{k\sigma} \hat{c}_{k\sigma} \rangle$ for the interaction strength $U = -10$. The number of lattice sites is $N_{\mathrm{L}} = 40$ and the atom numbers are $N_{\uparrow} = 20$, $N_{\downarrow} = 1$. The pairing emerges between atoms close to the two Fermi surfaces; no pairing between k and $-k$ above $k_{\mathrm{F}}^{\uparrow}$ is present.

For $N_{\uparrow} = 20$, $N_{\downarrow} = 1$ and $N_{\mathrm{L}} = 40$, the polaron energy results from the calculation

$$E_{\mathrm{p}} = E(U, N_{\uparrow}, N_{\downarrow}) - E^{\text{non-int}}(U = 0, N_{\uparrow}, N_{\downarrow}) \tag{7}$$

$$= U - 2J \sum_{j=1}^{19} \cos(k_j) \tag{8}$$

$$- \left(-2J \sum_{j=1}^{20} \cos(k_j) - 2J \cos(k_1) \right) \tag{9}$$

$$= U + 2J \cos(k_1) + 2J \cos(k_{20}) \approx U + 2.07J, \tag{10}$$

where $E(U, N_{\uparrow}, N_{\downarrow})$ ($E^{\text{non-int}}(U = 0, N_{\uparrow}, N_{\downarrow})$ is the energy for the system with interaction strength U ($U = 0$) and particle numbers $N_{\uparrow}, N_{\downarrow}$ ($N_{\uparrow}, N_{\downarrow}$). The BA result is shown in figure 1 with the exact result. In the strongly interacting limit $-U \gtrsim 7J$, the BA solution is in good agreement with the exact solution.

3. Radiofrequency (rf) spectroscopy

In the experiment [1], rf spectroscopy was performed on the minority and majority spin components. In rf spectroscopy, one of the spin components, $\uparrow$ or $\downarrow$, is coupled to a third spin state, denoted by 3, which is not populated and sufficiently weakly interacting with the initial states. Theoretically, the rf field is well described in the rotating wave approximation by the Hamiltonian

$$\hat{H}^{\sigma}_{\mathrm{rf}}(t) = \Omega \sum_{j} (\mathrm{e}^{-\mathrm{i}\delta t} \hat{c}^{\dagger}_{j\sigma} \hat{c}_{j3} + \mathrm{e}^{\mathrm{i}\delta t} \hat{c}^{\dagger}_{j3} \hat{c}_{j\sigma}), \tag{11}$$

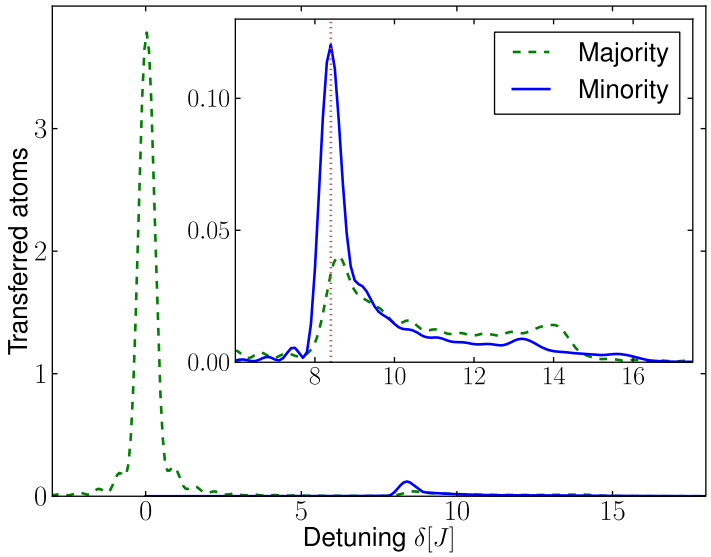

Figure 4. Minority and majority spectrum for $U = -10$. The inset is a zoom of higher detunings where a quasiparticle peak emerges. The vertical line is the polaron energy E_p calculated from the exact ground state. The number of spin components are $N_\uparrow = 20$, $N_\downarrow = 1$ and the number of lattice sites is $N_L = 40$. Spectra for other interactions are qualitatively similar.

where the sum is over the lattice sites, Ω is the coupling strength and δ is the detuning of the rf field from the σ–3 transfer frequency.

From the variational ansatz (3), we have straight access to the rf spectra through the Fermi golden rule

$$I_\downarrow \propto \sum_f |\langle f|\hat{H}_{\mathrm{rf}}^{\downarrow}|g\rangle|^2\, \delta^{(1d)}(\delta - E_f + E_g) \tag{12}$$

$$= |\varphi_0|^2\, \delta^{(1d)}(\delta - |E_p|) + \Gamma^{\mathrm{inc}}(\varphi_{kq}, \delta), \tag{13}$$

where the summation is over all states with energies E_f, $|g\rangle$ is the ground state and E_g its energy [1]. The first term gives rise to a narrow peak at the polaron energy and behind that is a broad tail resulting from the term $\Gamma^{\mathrm{inc}}(\varphi_{kq}, \delta)$ describing the incoherent part. Qualitatively, the measured spectra [1] matched with the variational ansatz for the attractive interaction strengths and close to the unitary limit. However, in the BEC side $1/(k_F a) \ll 1$, the minority and the majority spectra overlapped completely, which signalled molecular pairing. The TEBD algorithm allows us to calculate the full time-evolution of the system, and therefore we can evaluate the relation between the rf spectra and the polaron-like state. To obtain the spectra, we first calculate the ground state of the Fermi–Hubbard Hamiltonian (1) and then the dynamics by operating on the ground state with the time-evolution operator $\exp(-\mathrm{i}\hat{H}t)$ consisting of the Hubbard Hamiltonian and the rf field,

$$\hat{H} = \hat{H}_0 + \hat{H}_{\mathrm{rf}}^{\sigma}. \tag{14}$$

The spectra for the minority and majority components calculated using exact numerics are shown in figure 4. In the majority spectrum, the main contribution is at zero detuning because

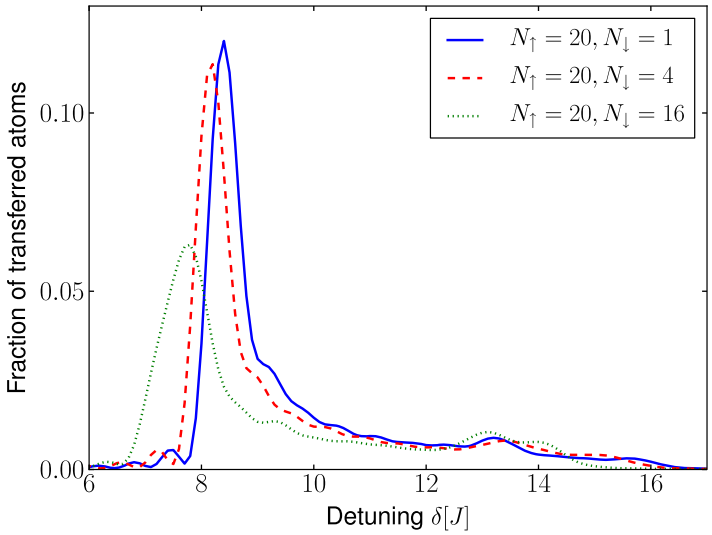

Figure 5. Minority component spectra for various imbalances. The interaction strength is $U = -10J$.

of the unpaired atoms, but some atoms are transferred also when $\delta \sim 8 - 14J$. The minority spectra are highly peaked at $\delta = 8.4J$, and the peak position is exactly at the polaron energy E_p, which is calculated from the exact ground state and is very well approximated by equation (10). At larger detunings, a long tail emerges but is cut due to the restriction of momenta in an optical lattice to $k \in [-\pi, \pi]$.

In equation (13), the particle–hole excitations give rise to the incoherent part of the spectra

$$\Gamma^{\mathrm{inc}}(\varphi_{kq}, \delta) = |\varphi_{kq}|^2\, \delta^{(1d)}(\delta - \epsilon_{q-k} - \epsilon_k + \epsilon_q + \epsilon_0 - |E_\mathrm{p}|), \tag{15}$$

where $\epsilon_k = -2J\cos(k)$ is the dispersion relation for non-interacting particles in a lattice. The minimum detuning that contributes to the minority spectrum is for $q = k$ and gives $\delta_{\min} = E_\mathrm{p}$. The maximum detuning arises when the system has the hole in the bottom of the Fermi sea $q = 0$ and the excitation lies at the van Hove singularity $p = \pi$, i.e. $\delta_{\max} = \epsilon_{-\pi} + \epsilon_\pi - \epsilon_0 + E_\mathrm{p} - \epsilon_0 = E_\mathrm{p} + 8J$. Now, the width of the spectrum is $\delta_{\max} - \delta_{\min} = 8J$. This is in good agreement with the exact spectra.

In figure 5, we have varied the polarization. The spectra look similar for large spin imbalance $N_\downarrow/N_\uparrow \lesssim 0.2$ but for small spin imbalance the spectra get broadened and are shifted to lower detunings. Let us analyse the peak positions with the BA. The Fermi golden rule states that the peak position comes from the energy difference between the ground state and the final state. For the ground state with $N_\uparrow = 20$ and $N_\downarrow = 2$, the final state for the Fermi golden rule analysis has the particle numbers $N_\uparrow = 20$, $N_\downarrow = 1$ and $N_3 = 1$. Therefore, the energy difference becomes

$$\Delta E = E_\mathrm{G} - E_\mathrm{F} \tag{16}$$

$$= 2U - 2J \sum_{i=1}^{18} \cos(k_i) \tag{17}$$

$$-\left(U-2J\sum_{i=1}^{19}\cos(k_i)-2J\cos(k_{\text{final}})\right) \tag{18}$$

$$=U+2J\cos(k_{19})+2J\cos(k_{\text{final}}). \tag{19}$$

The lowest contribution to the spectrum arises when $k_{\text{final}}=k_1$, which implies

$$|E_{\text{p}}|-|\Delta E|=2J\cos(k_{19})-2J\cos(k_{20})\approx 0.15. \tag{20}$$

The energy difference $|\Delta E|$ is smaller than the polaron energy $|E_{\text{p}}|$ (energy difference in the case of a single minority component), and therefore the spectrum shifts to lower detunings when polarization is increased. Furthermore, we can make quantitative comparison of this BA result to the exact numerics. The distance between the two peaks in the rf spectrum for the cases $N_\downarrow=1$ and 2 is about 0.1, which is in good agreement with the BA result $|E_{\text{p}}|-|\Delta E|=0.15$.

4. Discussion

We have shown that, in a highly imbalanced Fermi gas, the ground state exhibits polaronic-like behaviour. The quasiparticle nature of this excitation, which can be deduced from the non-zero quasiparticle weight of the polaron, is confirmed by rf-spectroscopy analysis. Two considerations are, however, in order. The first concerns the dynamical properties of the quasiparticle. From our analysis, it is not possible to prove the stability of the polaronic-like particle propagation through the cloud of majority atoms. The polaron weight might split up into particle–hole excitations. The rf spectroscopy, measuring the single-particle spectral function, does not describe collective properties. A non-zero value for quasiparticle residue would correspond to dynamical stability of the quasiparticle,

$$\lim_{t\to\infty}|G_\downarrow(\mathbf{k}=0,t)|\neq 0. \tag{21}$$

The second consideration relates to the quasiparticle description of the polaron. On general grounds it is well established that 1D systems exhibit a 'collectivization' of the excitation, the typical example being the spin–charge separation in the *balanced* Fermi–Hubbard Hamiltonian. However, it has been shown that, in the case of an *imbalanced* gas, the spin-charge separation is violated [15, 16, 18, 19]. We expect that the validity of the ansatz given in equation (3), and hence the validity of the polaron quasiparticle description even in the 1D case, in the limit of weak interaction, can be pictured as the extreme limit of the violation of the spin–charge separation.

5. Conclusions

We have investigated the ground state properties and the rf spectrum of a highly imbalanced Fermi gas in a 1D optical lattice. The exact numerical results can be explained in terms of the variational ansatz given in equation (3) and of the BA equation (in the limit of $-U/J\to\infty$) for $-U\lesssim 5J$ and $-U\gtrsim 7J$, respectively. Our results suggest the possibility of existence of a polaronic quasiparticle. Further analysis is, however, required to investigate its dynamical properties. Moreover, we would like to point out that the setup proposed here is well within the reach of current experimental capabilities. Our analysis provides exact numerical results for comparison with future experiments, as well as an effective physical interpretation of both the weak and the strong interaction limits.

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Appendix

Equation (6) can be obtained considering the BA solution for the open-boundary conditions (OBC) Fermi–Hubbard model in the limit $U/J \to \infty$. Analogously to the calculations performed in [21], it is possible to prove that the excitations of the system, for a repulsive interaction, can be described in terms of $N = N_\uparrow + N_\downarrow$ spinless fermions with energy and momenta given respectively by

$$\begin{aligned} E &= -2J \sum_{j=1}^{N} \cos k_j, \\ k_j &= \frac{\pi}{L+1} I_j, \quad I_j \in \mathbb{N}, \quad j = [1 \dots N]. \end{aligned} \tag{A.1}$$

The expression for k_j in equation (A.1) is derived from the BA equations of [22]. The BA equations for $N_\uparrow$ up, $N_\downarrow$ down electrons on N_L sites can be written as

$$2Lk_j = 2\pi I_j - 2k_j - \sum_{\beta=1}^{N_\uparrow} \left[\Phi\left(2\frac{\sin(k_j) - \lambda_\beta}{u}\right) \right. \tag{A.2}$$

$$\left. + \Phi\left(2\frac{\sin(k_j) + \lambda_\beta}{u}\right) \right] \tag{A.3}$$

and

$$\sum_{j=1}^{N_\uparrow + N_\downarrow} \left[\Phi\left(2\frac{\lambda_\alpha - \sin(k_j)}{u}\right) + \Phi\left(2\frac{\lambda_\alpha + \sin(k_j)}{u}\right) \right] \tag{A.4}$$

$$= 2\pi J_\alpha + \sum_{\beta=1(\beta\neq\alpha)} \left[\Phi\left(\frac{\lambda_\alpha - \lambda_\beta}{u}\right) + \Phi\left(\frac{\lambda_\alpha + \lambda_\beta}{u}\right) \right], \tag{A.5}$$

where $j = 1, \dots, N_\uparrow + N_\downarrow$, $\alpha = 1, \dots, N_\downarrow$, I_j , $J_\alpha \in \mathbb{N}$, $U/J = u$, $\Phi(x) = 2\tan^{-1}(2x)$ and λ_α are the spin velocities.

The distribution of I_j should correspond to a condition where the energy is minimized. For a balanced gas at half filling, the energy minimization condition is given by $I_j = [1 \dots L]$, leading to $E = -2J \sum_{j=1}^{L} \cos k_j = 0$, $p = \sum_{j=1}^{L} k_j$.

If we take into account the mapping $U \to -U$ and that, in the limit $U/J \to \infty$, the total number of pairs is equal to $N_\downarrow$, the single-site basis states can be mapped according to the following scheme,

$$|\uparrow\downarrow\rangle \leftrightarrow |\downarrow\rangle, \quad |\emptyset\rangle \leftrightarrow |\uparrow\rangle, \tag{A.6}$$

leading to $N = N_{\mathrm{L}} - (N_{\downarrow} - N_{\uparrow})$, and hence

$$E = -2J \sum_{j=1}^{N_{\mathrm{L}}-(N_{\downarrow}-N_{\uparrow})} \cos k_j, \tag{A.7}$$

which, taking into account the fact that $\sum_{j=1}^{N_{\mathrm{L}}} \cos k_j = 0$, can be written as

$$E = -2J \sum_{j=1}^{N_{\uparrow}-N_{\downarrow}} \cos k_j. \tag{A.8}$$

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