Momentum occupation number bounds for interacting fermions

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We derive rigorous bounds on the average momentum occupation numbers \( \langle n_{k\sigma} \rangle \) in the Hubbard and Kondo models in the ground state and at non-zero temperature \( (T > 0) \) in the grand canonical ensemble. For the Hubbard model with \( T > 0 \) our bound proves that, when interaction strength \( \ll k_B T \ll \mathrm{Fermi} \) energy, \( \langle n_{k\sigma} \rangle \) is guaranteed to be close to its value in a low temperature free fermion system. For the Kondo model with any \( T > 0 \) our bound proves that \( \langle n_{k\sigma} \rangle \) tends to its non-interacting value in the infinite volume limit. In the ground state case our bounds instead show that \( \langle n_{k\sigma} \rangle \) approaches its non-interacting value as \( k \) moves away from a certain surface in momentum space. For the Hubbard model at half-filling on a bipartite lattice, this surface coincides with the non-interacting Fermi surface. In the Supplemental Material we extend our results to some generalized versions of the Hubbard and Kondo models. Our proofs use the Fermi statistics of the particles in a fundamental way.

Introduction: Under certain conditions, gapless free fermion systems are expected to be stable to interactions, in the sense that certain properties of the interacting system resemble those of the free system. This expectation is the basis for Landau’s Fermi liquid theory [1], and it can be justified in some cases using a Renormalization Group approach [2–4]. Perhaps the most famous result along these lines is Luttinger’s theorem (LT), which states that the volume enclosed by the Fermi surface in an interacting system [5] is equal to the volume enclosed by the Fermi surface in the corresponding free system [6–8]. While this result is interesting, most derivations of it rely on unproven assumptions, and so it cannot be expected to hold in generic models of interacting fermions.

Luttinger’s original work relied on perturbation theory, and so his result may not hold if perturbation theory is not absolutely convergent [9]. Most recent works on LT take a different approach but make other assumptions, for example that the system is a Fermi liquid at low energies [10–16]. There are a few rigorous results on LT in one-dimensional (1D) systems [17] and in some 2D systems that lack inversion symmetry [18][19]. However, there are also several counterexamples to the original statement of LT [20–24].

It is useful to think of LT as a stability result that states that the momentum space picture in an interacting system resembles the picture in the corresponding free system. In this work we prove stability results along these lines for the Hubbard and Kondo models in their ground state and at non-zero temperature. Specifically, we derive rigorous bounds on the deviation of the average momentum occupation numbers \( \langle n_{k\sigma} \rangle \) from their non-interacting values. Our focus on \( \langle n_{k\sigma} \rangle \) is inspired by Luttinger’s original work [7], where he showed (again, using perturbation theory) that \( \langle n_{k\sigma} \rangle \) has a discontinuity at the location of the interacting Fermi surface. This discontinuity was also rigorously proven to exist in some 2D models without inversion symmetry [18].

Our rigorous bounds on the \( \langle n_{k\sigma} \rangle \) allow us to prove the following results. For the Hubbard model at non-zero temperature our bound proves the existence of a parameter regime of the form \( (\epsilon_F = \text{Fermi energy}) \) in which \( \langle n_{k\sigma} \rangle \) is guaranteed to be close to its value in a low temperature free fermion system. For the Kondo model at any non-zero temperature our bound proves that \( \langle n_{k\sigma} \rangle \) tends to its non-interacting value in the infinite volume limit. In the ground state case our results show that \( \langle n_{k\sigma} \rangle \) approaches its non-interacting value of 0 or 1 as \( k \) moves away from a certain surface in momentum space. For the Hubbard model at half-filling on a bipartite lattice, this surface coincides with the non-interacting Fermi surface. In the ground state and \( T > 0 \) cases our results for the Kondo model are much stronger, and this is because the interaction in the Kondo model only involves a single lattice site. In the Supplemental Material (SM) we extend these results to generalized versions of the Hubbard and Kondo models.

For the Hubbard model our stability results are strongest in the case with \( T > 0 \), and it is useful to discuss the reason for this. The key physical idea involved is that the system is most likely to “look” like a low temperature free fermion system when \( k_B T \ll \epsilon_F \) but \( T \) is still above the transition temperature for any low temperature instabilities (e.g., a superconducting transition or the Kohn-Luttinger instability [25, 26]). This idea was strongly emphasized in a fascinating series of works in the mathematical physics literature that established stability [27] of free fermions to interactions in 2D systems at low but non-zero temperatures [28–36]. Our results on the Hubbard model demonstrate the power of this idea in yet another concrete setting.

Hubbard and Kondo models: We consider Hubbard and Kondo models on a Bravais lattice \( \Lambda \). Both models feature spinful fermions, and we denote by \( c_{x\sigma} \) and \( c_{x\sigma}^\dagger \) the annihilation and creation operators for a fermion of spin \( \sigma \in \{\uparrow, \downarrow\} \) on a site \( x \in \Lambda \). These operators obey the standard anticommutation relations \( \{c_{x\sigma}, c_{y\tau}^\dagger\} = 0 \) and \( \{c_{x\sigma}, c_{y\tau}\} = δ_{xy}δ_{\sigma\tau} \). We also define the Fourier-transformed fermions \( c_{k\sigma} \) by \( c_{k\sigma} = |\Lambda|^{-\frac{1}{2}} \sum_{x} c_{x\sigma} e^{-ik\cdot x} \), where \( k \) is a wave vector in the first Brillouin zone of \( \Lambda \), and \( |\Lambda| \) is the total number of sites in the lattice. We define the number operators in real space and reciprocal space by \( n_{x\sigma} = c_{x\sigma}^\dagger c_{x\sigma} \) and \( n_{k\sigma} = c_{k\sigma}^\dagger c_{k\sigma} \). The total number operator is \( N = \sum_{\sigma} N_\sigma \), where \( N_\sigma = \sum_{x} n_{x\sigma} = \sum_{k} n_{k\sigma} \) is the number operator for
spin $\sigma$. Finally, the Kondo model features an additional impurity spin of magnitude $s$, with $s \in \{1/2, 1, 3/2, \ldots\}$. This spin is represented by the vector operator $\vec{S} = (S^x, S^y, S^z)$ whose components satisfy the usual relations $[S^x, S^y] = iS^z$ (plus cyclic permutations) and $\vec{S} \cdot \vec{S} = s(s + 1)$.

The Hamiltonians for our models take the form

$$H_{\text{Hubbard}} = \sum_{\mathbf{k}, \sigma} (\epsilon_{\mathbf{k}} - \mu) n_{\mathbf{k}\sigma} + u \sum_{\mathbf{x}} n_{\mathbf{x}\uparrow} n_{\mathbf{x}\downarrow},$$

$$H_{\text{Kondo}} = \sum_{\mathbf{k}, \sigma} (\epsilon_{\mathbf{k}} - \mu) n_{\mathbf{k}\sigma} + J \vec{S} \cdot \left( \sum_{\mathbf{r}, \tau} c_{\mathbf{r}\tau}^\dagger \vec{c}_{\mathbf{r}\tau} \frac{\sigma_{\tau\tau'}}{2} \right),$$

where the different quantities appearing here are as follows. First, $\mu$ is the chemical potential. Next, the energy dispersion $\epsilon_{\mathbf{k}}$ is the Fourier transform of (the negative of) a translation invariant hopping matrix $t_{\mathbf{x},\mathbf{y}}$. We assume that $t_{\mathbf{x},\mathbf{y}}$ satisfies $t_{\mathbf{x},\mathbf{x}} = 0$ and $t_{\mathbf{x},\mathbf{y}} = t_{\mathbf{y},\mathbf{x}} = t_{\mathbf{x}+\mathbf{r},\mathbf{y}+\mathbf{r}}$ for any $\mathbf{r} \in \Lambda$, and then $\epsilon_{\mathbf{k}} := -t \sum_{\mathbf{r}} t_{\mathbf{x}+\mathbf{r},\mathbf{y}} \epsilon_{\mathbf{k}-\mathbf{r}}$ (which is independent of $\mathbf{x}$ by translation invariance). For example, with nearest-neighbor hopping of strength $t/2$ on the (hyper)cubic lattice in $D$ dimensions, we have $\epsilon_{\mathbf{k}} = -t \sum_{j=1}^{D} \cos(k_j)$, where the $k_j$ are the components of $\mathbf{k}$. Next, $H_{\text{Hubbard}}$ features an on-site Hubbard interaction of strength $u$, where $u > 0$ ($u < 0$) for repulsive (attractive) interactions. Finally, $H_{\text{Kondo}}$ features a Heisenberg interaction between the impurity spin and the spin of the fermion at $\mathbf{x} = 0$ (here, $\vec{\sigma} = (\sigma^x, \sigma^y, \sigma^z)$ is the vector of Pauli matrices, $\sigma^x_{\tau\tau'}$ is the $\tau$ matrix element of $\sigma^x$, etc.). This interaction has a strength $J$ and is antiferromagnetic (ferromagnetic) for $J > 0$ ($J < 0$).

Our main results concern the expectation values $\langle n_{\mathbf{k}\sigma} \rangle$ in the ground state of these models and in the thermal state at inverse temperature $\beta = (k_B T)^{-1}$. In both cases we work in the grand canonical ensemble. In the ground state case this means that we work with the lowest energy state of the Hamiltonian over all possible fermion number sectors. In the non-zero temperature case this means that we trace over the entire Fock space of the spin-up and spin-down fermions (in the Kondo case we also trace over the Hilbert space of the impurity spin).

We use $|\psi\rangle$ to denote the grand canonical ground state or a particular ground state if there is a ground state degeneracy. The expectation value of any operator $\mathcal{O}$ in the ground state is defined by $\langle \mathcal{O} \rangle := \langle \psi | \mathcal{O} | \psi \rangle$. In the ground state case and at non-zero temperature by $\langle \mathcal{O} \rangle := \text{Tr} \left( e^{-\beta H} \right) / Z$, where $Z = \text{Tr} \left( e^{-\beta H} \right)$. For the Hubbard model the ground state can always be chosen to have a definite number of fermions of each spin [37]. We denote these fermion numbers by $N_{\mathbf{r}}$ and the corresponding filling fractions by $\rho_{\mathbf{r}}$, i.e., $N_{\mathbf{r}} = N_{\mathbf{r}} |\psi\rangle$ and $\rho_{\mathbf{r}} = N_{\mathbf{r}} / |\Lambda|$. With this notation, we are now ready to present our results.

**Theorem 1 (non-zero temperature):** Let $f_{\mathbf{k}}$ denote the Fermi-Dirac distribution with chemical potential $\mu$, $f_{\mathbf{k}} = (e^{(\epsilon_{\mathbf{k}} - \mu)/T} + 1)^{-1}$. For any $\beta < \infty$, the momentum occupation numbers $\langle n_{\mathbf{k}\sigma} \rangle$ for the models in Eq. (1) obey

$$-\delta f_{\mathbf{k}} \leq \langle n_{\mathbf{k}\sigma} \rangle - f_{\mathbf{k}} \leq \delta (1 - f_{\mathbf{k}}),$$

where the constant $\delta$ is given by

$$\delta = \begin{cases} \frac{\beta |u|}{\beta |3J|/2} & \text{Hubbard model} \\ \frac{\beta |J|s}{2\sqrt{|\Lambda|}} & \text{Kondo model} \end{cases}.$$

**Discussion:** The momentum occupation numbers for the free model $H_0 = \sum_{\mathbf{k}, \sigma} (\epsilon_{\mathbf{k}} - \mu) n_{\mathbf{k}\sigma}$ are given exactly by the Fermi-Dirac distribution $f_{\mathbf{k}}$. Therefore, Theorem 1 shows that, when $\beta \ll 1$, the momentum occupation numbers for the interacting system are very close to those of the free model $H_0$. In the Kondo case we also have $\delta \to 0$ in the infinite volume limit $|\Lambda| \to \infty$, so for that model $\langle n_{\mathbf{k}\sigma} \rangle - f_{\mathbf{k}}$ as $|\Lambda| \to \infty$ at any non-zero temperature.

Let us now consider the Hubbard model. In that case $\delta \ll 1$ will hold at high temperatures, but the most interesting aspect of Theorem 1 is that it reveals the existence of a regime where the $\langle n_{\mathbf{k}\sigma} \rangle$ resemble the occupation numbers of a free fermion system at low temperature. To see this, recall that the free system described by $H_0$ is said to be at low temperature if $k_B T \ll \epsilon_F$, where $\epsilon_F := \left| \epsilon_0 - \mu \right|$ is the Fermi energy and $\epsilon_0$ is the value of the dispersion at the origin ($\mathbf{k} = 0$) of the Brillouin zone. Then Theorem 1 implies that the $\langle n_{\mathbf{k}\sigma} \rangle$ resemble the momentum occupation numbers of a low temperature free fermion system if $u, T$, and $\epsilon_F$ obey $|u| \ll k_B T \ll \epsilon_F$.

**Theorem 2 (Hubbard, ground state):** In any ground state of $H_{\text{Hubbard}}$ the momentum occupation numbers $\langle n_{\mathbf{k}\sigma} \rangle$ obey

$$\langle n_{\mathbf{k}\sigma} \rangle \leq \frac{|u| \sqrt{\rho_{\mathbf{k}}} }{\epsilon_{\mathbf{k}} - \mu + u \rho_{\mathbf{k}}} , \quad \text{if } \epsilon_{\mathbf{k}} - \mu + u \rho_{\mathbf{k}} > 0 \quad (4a)$$

$$1 - \langle n_{\mathbf{k}\sigma} \rangle \leq \frac{|u| \sqrt{\rho_{\mathbf{k}}} }{\epsilon_{\mathbf{k}} - \mu + u \rho_{\mathbf{k}}} , \quad \text{if } \epsilon_{\mathbf{k}} - \mu + u \rho_{\mathbf{k}} < 0 ,$$

where $\rho_{\mathbf{k}}$ is the opposite of $\sigma$ (e.g., $\uparrow = \downarrow$).

**Discussion:** These bounds show that $\langle n_{\mathbf{k}\sigma} \rangle$ approaches its non-interacting value of 0 or 1 as $\mathbf{k}$ moves away from the surface in reciprocal space defined by $\epsilon_{\mathbf{k}} - \mu + u \rho_{\mathbf{k}} = 0$ (note that the non-interacting Fermi surface is defined by $\epsilon_{\mathbf{k}} - \mu = 0$). There is also a small region around this surface where these bounds are no longer effective because the denominator becomes smaller than the numerator as $k$ approaches this surface. The size of this region is determined by the interaction strength $u$ and the densities $\rho_{\mathbf{k}}$. Finally, this bound has an interesting property in the case of half-filling on a bipartite lattice [38], where $\mu = u/2$ and $\rho_{\mathbf{k}} = 1/2$ [39, 40]. In this case $\epsilon_{\mathbf{k}} - \mu + u \rho_{\mathbf{k}} = 0$ and so the surface defined by $\epsilon_{\mathbf{k}} - \mu = 0$ coincides with the non-interacting Fermi surface at half-filling, which is just defined by $\epsilon_{\mathbf{k}} = 0$.

**Theorem 3 (Kondo, ground state):** In any ground state of $H_{\text{Kondo}}$ the momentum occupation numbers $\langle n_{\mathbf{k}\sigma} \rangle$ obey

$$\langle n_{\mathbf{k}\sigma} \rangle \leq \frac{3}{2\sqrt{|\Lambda|}} \frac{|J|s}{|\epsilon_{\mathbf{k}} - \mu|} , \quad \text{if } \epsilon_{\mathbf{k}} - \mu > 0 \quad (5a)$$

$$1 - \langle n_{\mathbf{k}\sigma} \rangle \leq \frac{3}{2\sqrt{|\Lambda|}} \frac{|J|s}{|\epsilon_{\mathbf{k}} - \mu|} , \quad \text{if } \epsilon_{\mathbf{k}} - \mu < 0 . \quad (5b)$$
**Discussion:** A related result was obtained in Theorem 2 of Ref. 41 for a different family of quantum impurity models. In comparing with our Theorem 2, this bound has an extra factor of $\sqrt{|\Lambda|}$, and so it is much more powerful than our result for the Hubbard model. In particular, for any $k$ that is far enough from the non-interacting Fermi surface to satisfy an inequality of the form

$$|\epsilon_k - \mu| \geq A|\Lambda|^{-p}, \quad p < 1/2,$$

where $A$ is a constant with units of energy, we find that $\langle n_k \rangle$ tends to its non-interacting value of 0 or 1 in the infinite-volume limit. The only values of $k$ that do not satisfy a bound like (6) are contained within a small region around the non-interacting Fermi surface, and the width of this region vanishes in the limit $|\Lambda| \to \infty$.

**Plan for the rest of the main text:** In the rest of the main text we present the proof of Theorem 1 for the Hubbard model. We prove our other results in the SM. The key to proving Theorem 1 is a basic bound that we state in Lemma 1 below. We now state Lemma 1 and then use it to prove Theorem 1. We then present the proof of Lemma 1 itself.

**Lemma 1:** Let $|\phi\rangle$ be any normalized state in the Fock space of the spin-up and spin-down fermions, and let $U = \sum_\mathcal{E} n_{\mathcal{E}} c_{\mathcal{E}}^\dagger c_{\mathcal{E}}$ be the Hubbard interaction. Then for any $k$ and $\sigma$ the expectation value $\langle \phi | c_{k \sigma}^\dagger U_{\mathcal{E}} c_{k \sigma} | \phi \rangle$ obeys

$$|\langle \phi | c_{k \sigma}^\dagger U_{\mathcal{E}} c_{k \sigma} | \phi \rangle| \leq |u|,$$

and an identical bound holds for $|\langle \phi | c_{k \sigma}^\dagger U_{\mathcal{E}} c_{k \sigma} | \phi \rangle|$.

**Remark:** The same bound holds for the thermal expectation value $\langle c_{k \sigma}^\dagger U_{\mathcal{E}} c_{k \sigma} \rangle$. To see it, let $|\ell\rangle$ and $E_\ell$ be a complete set of eigenvectors and eigenvalues of $H_{\text{Hubbard}}$. Then we have

$$|\langle c_{k \sigma}^\dagger U_{\mathcal{E}} c_{k \sigma} \rangle| = \left| \frac{1}{Z} \sum_\ell \langle \ell | c_{k \sigma}^\dagger U_{\mathcal{E}} c_{k \sigma} | \ell \rangle e^{-\beta E_\ell} \right|$$

$$\leq \frac{1}{Z} \sum_\ell \left| \langle \ell | c_{k \sigma}^\dagger U_{\mathcal{E}} c_{k \sigma} | \ell \rangle \right| e^{-\beta E_\ell}$$

$$\leq |u|,$$

where the last line follows from $Z = \sum_x e^{-\beta E_x}$.

**Proof of Theorem 1 (Hubbard case):** The first step is to use the thermodynamic inequality

$$\frac{1}{2} \beta \langle \mathcal{O}^\dagger [H, \mathcal{O}] - [H, \mathcal{O}^\dagger] \mathcal{O} \rangle \geq \Phi(\langle \mathcal{O}^\dagger \mathcal{O} \rangle, \langle \mathcal{O} \mathcal{O}^\dagger \rangle),$$

where $\mathcal{O}$ can be any operator and $\Phi(u, v)$ is the function of two real variables defined by

$$\Phi(u, v) := u \ln(u) - u \ln(v).$$

This inequality is a local version of the **Gibbs variational principle**, and it can be derived as in Lemma 6 of Ref. 42.

We use this inequality twice: first with $\mathcal{O} = c_{k \sigma}^\dagger c_{k \sigma}$, and then with $\mathcal{O} = c_{k \sigma}^\dagger$. In the first case we find that

$$-\beta (\epsilon_k - \mu) \langle n_{k \sigma} \rangle + \frac{1}{2} \beta \langle c_{k \sigma}^\dagger U_{\mathcal{E}} c_{k \sigma} \rangle - \langle U_{\mathcal{E}} c_{k \sigma}^\dagger c_{k \sigma} \rangle \geq \Phi(\langle n_{k \sigma} \rangle, 1 - \langle n_{k \sigma} \rangle).$$

In the second case we find that

$$\beta (\epsilon_k - \mu) (1 - \langle n_{k \sigma} \rangle) + \frac{1}{2} \beta \langle c_{k \sigma}^\dagger U_{\mathcal{E}} c_{k \sigma} \rangle - \langle U_{\mathcal{E}} c_{k \sigma}^\dagger c_{k \sigma} \rangle \geq \Phi(1 - \langle n_{k \sigma} \rangle, \langle n_{k \sigma} \rangle).$$

Next, we use Lemma 1 to obtain upper bounds on the terms involving $U$ in these inequalities. For example, in (11) we can use

$$\frac{1}{2} \langle c_{k \sigma}^\dagger U_{\mathcal{E}} c_{k \sigma} \rangle - \langle U_{\mathcal{E}} c_{k \sigma}^\dagger c_{k \sigma} \rangle \leq \langle c_{k \sigma}^\dagger U_{\mathcal{E}} c_{k \sigma} \rangle \leq |u|.$$

**After applying Lemma 1 our two inequalities take the form**

$$-\beta (\epsilon_k - \mu) \langle n_{k \sigma} \rangle + \delta \geq \Phi(\langle n_{k \sigma} \rangle, 1 - \langle n_{k \sigma} \rangle)$$

$$\beta (\epsilon_k - \mu) (1 - \langle n_{k \sigma} \rangle) + \delta \geq \Phi(1 - \langle n_{k \sigma} \rangle, \langle n_{k \sigma} \rangle),$$

where $\delta = \beta |u|$ as before.

To complete the proof we need to use inequalities (14) to obtain upper and lower bounds on the difference $\langle n_{k \sigma} \rangle - f_k$. To do this we use the fact that $\Phi(1, x)$ and $\Phi(x, 1)$ are both convex functions of $x$ for $x \in (0, 1)$. A convex function $f(x)$ obeys the bound $f(x) \geq f(x_0) + f'(x_0)(x - x_0)$ for any $x_0 \neq x$, where $f'(x) = df(x)/dx$. We now apply this bound to the inequalities in Eq. (14), taking $x = \langle n_{k \sigma} \rangle$ and $x_0 = f_k$.

For the first inequality in Eq. (14) we have $f(x) = \Phi(1, x - x)$, and so $f'(x_0) = 1 - \beta (\epsilon_k - \mu) + e^{-\beta (\epsilon_k - \mu)}$. We then find, after some algebra, that

$$\langle n_{k \sigma} \rangle - f_k \leq \delta (1 - f_k).$$

For the second inequality in Eq. (14) we instead have $f(x) = \Phi(x, 1 - x)$, and in that case we find that

$$\langle n_{k \sigma} \rangle - f_k \geq -\delta f_k.$$

These two inequalities complete the proof of Theorem 1.

**Proof of Lemma 1:** We will prove the bound in Eq. (7) for the case of spin-up. The proofs for the other bounds in Lemma 1 are nearly identical. We start by defining new fermion operators $\tilde{c}_{k \sigma}$ that obey all the usual anticommutation relations except that $\tilde{c}_{k \sigma}$ now commutes with $\tilde{c}_{y \alpha}$ and $\tilde{c}_{x \beta}$ for all $x$ and $y$. These operators are defined as $\tilde{c}_{x \beta} = c_{x \beta}^\dagger$ and $\tilde{c}_{x \beta} = (-1)^{N_{x \beta}} c_{x \beta}^\dagger$. In terms of these we also define the number operators $\tilde{n}_{x \sigma} = c_{x \sigma}^\dagger c_{x \sigma}$, which are equal to the original operators $n_{x \sigma}$. We also define Fourier-transformed operators $\tilde{c}_{k \sigma}$ and their number operators $\tilde{n}_{k \sigma} = c_{k \sigma}^\dagger c_{k \sigma} = n_{k \sigma}$ exactly as before. The Hubbard model has the interesting property that it takes the same form when expressed in terms of these new operators. In addition, we can now view $H_{\text{Hubbard}}$ as acting on the tensor product $\mathcal{F}_x \otimes \mathcal{F}_y$ of the Fock spaces $\mathcal{F}_x$ and $\mathcal{F}_y$ for the new spin-up and spin-down fermions $\tilde{c}_{x \beta}$ and $\tilde{c}_{x \beta}$. We will use this tensor product structure shortly.

To bound $|\langle \phi | c_{k \sigma}^\dagger U_{\mathcal{E}} c_{k \sigma} | \phi \rangle|$, we start with the explicit formula

$$c_{k \sigma}^\dagger U_{\mathcal{E}} c_{k \sigma} = -\frac{\bar{u}}{|\Lambda|} \sum_{x, q} \tilde{c}_{k \sigma}^\dagger \tilde{c}_{q \tau} \tilde{n}_{x \xi} e^{-i(k - q) \cdot x}.$$
At this point it is useful to explain why it is slightly subtle to obtain a $|\Lambda|$-independent bound on $|\langle \phi | c_{k \uparrow}^\dagger U, c_{k \uparrow} | \phi \rangle|$. We can see from Eq. (17) that this quantity has one factor of $|\Lambda|$ in the denominator, but two sums over $|\Lambda|$ terms each (the sums over $x$ and $q$), and the absolute value of the summand $|\langle \phi | c_{k \downarrow}^\dagger \tilde{c}_q \tilde{c}_q \tilde{c}_{q \uparrow} | \phi \rangle e^{-i(k-q)\cdot x}|$ is (naively) of order 1. From this simple analysis it seems like we will end up with a bound on this quantity of order $|\Lambda|$. This analysis is incorrect because it does not take into account cancellations that follow from Fermi statistics.

To proceed, we expand $|\phi\rangle$ in a way that uses the tensor product structure of the Hilbert space when we work in terms of the new fermion operators $\tilde{c}_{x \sigma}$. Let $\{|\alpha\rangle\}$ be a real space occupation number basis for $\tilde{F}_\uparrow$, and let $\{|\alpha\rangle\}$ be the same for $\tilde{F}_\downarrow$. To be more precise, each state $|\alpha\rangle$ is determined by $|\Lambda|$ different numbers $a_x \in \{0, 1\}$ that satisfy $\sum_x a_x \leq |\Lambda|$, and $|\alpha\rangle$ takes the form $|\alpha\rangle = \prod_x (\tilde{c}_{x \uparrow}^\dagger)^{a_x} |0\rangle$, where $|0\rangle$ is the Fock vacuum for $\tilde{F}_\uparrow$ and where the order of the product is not important here. The states $|\alpha\rangle$ for $\tilde{F}_\uparrow$ take a similar form.

Using these basis states, we expand $|\phi\rangle$ as

$$|\phi\rangle = \sum_{\alpha, \alpha'} W_{\alpha \alpha'} |\alpha\rangle \otimes |\alpha'\rangle,$$

where $W_{\alpha \alpha'}$ is a matrix of coefficients (this step is inspired by Ref. 39). Since $|\phi\rangle$ is normalized, the coefficients $W_{\alpha \alpha'}$ obey the sum rule $\sum_{\alpha, \alpha'} W_{\alpha \alpha'}^2 = 1$. Since $\tilde{n}_{x \downarrow}$ is diagonal in the $|\alpha\rangle$ basis, we now find that

$$\langle \phi | c_{k \uparrow}^\dagger U, c_{k \uparrow} | \phi \rangle = -\frac{u}{|\Lambda|} \sum_{x, q} e^{-i(k-q)\cdot x} \sum_{\alpha} \langle \chi_\alpha | \tilde{c}_{k \uparrow}^\dagger \tilde{c}_q | \chi_\alpha \rangle \langle \chi_\alpha | \tilde{n}_{x \downarrow} | \chi_\alpha \rangle ,$$

where we defined the states $|\chi_\alpha\rangle \in \tilde{F}_\uparrow$ by

$$|\chi_\alpha\rangle := \sum_{\alpha} W_{\alpha \alpha'} |\alpha\rangle .$$

These states are not normalized. Instead, their norms satisfy the sum rule

$$\sum_{\alpha} \langle \chi_\alpha | \chi_\alpha \rangle = 1.$$

If we also define the coefficients $A_{kq}^{(\alpha)}$ and $M_{kq}^{(\alpha)}$ by

$$A_{kq}^{(\alpha)} := \sum_{x} \langle \chi_\alpha | \tilde{n}_{x \downarrow} | \alpha \rangle e^{-i(k-q)\cdot x} ,$$

$$M_{kq}^{(\alpha)} := \langle \chi_\alpha | \tilde{c}_{k \uparrow}^\dagger \tilde{c}_q | \chi_\alpha \rangle ,$$

then at this point we have

$$\langle \phi | c_{k \uparrow}^\dagger U, c_{k \uparrow} | \phi \rangle = -\frac{1}{|\Lambda|} \sum_{\alpha, \alpha'} \sum_{q} A_{kq}^{(\alpha)} M_{kq}^{(\alpha)} ,$$

where we have exchanged the order of the sums.

We now use the triangle inequality on the outer sum over $\alpha$ to obtain

$$|\langle \phi | c_{k \uparrow}^\dagger U, c_{k \uparrow} | \phi \rangle| \leq \frac{1}{|\Lambda|} \sum_{\alpha, \alpha'} \sum_{q} A_{kq}^{(\alpha)} M_{kq}^{(\alpha)} .$$

(24)

We then bound the inner sum over $q$ using the Cauchy-Schwarz inequality,

$$\sum_{q} A_{kq}^{(\alpha)} M_{kq}^{(\alpha)} \leq \sqrt{\left( \sum_{q} A_{kq}^{(\alpha)} \right)^2 \left( \sum_{q} M_{kq}^{(\alpha)} \right)^2} .$$

(25)

Next, we have

$$\sum_{q} A_{kq}^{(\alpha)} \leq u^2 |\Lambda| \sum_{x} \langle \chi_\alpha | \tilde{n}_{x \downarrow} | \alpha \rangle^2 \leq (u|\Lambda|)^2 ,$$

(26)

where the first equality is just the Plancherel theorem. The last step is to bound the sum involving $M_{kq}^{(\alpha)}$. To do that, we need a few facts about fermion density matrices.

**Fermion density matrices and operator norms:** Consider a set of fermion creation and annihilation operators $c_i, c_i^\dagger$ obeying the usual relations $\{c_i, c_j\} = 0$ and $\{c_i, c_j^\dagger\} = \delta_{ij}$, where the indices $i$ and $j$ take values in some finite index set $I$. For any state $|\chi\rangle$ in the Fock space of these operators, we can define a Hermitian matrix $M$ whose matrix elements are given by $M_{ij} := \langle \chi | c_i^\dagger c_j | \chi \rangle$. This matrix is the single-particle reduced density matrix for the fermions in the state $|\chi\rangle$. An important result about $M$ is that, if $\lambda$ is any eigenvalue of $M$, then $0 \leq \lambda \leq \langle \chi | \chi \rangle$ (we do not assume that $|\chi\rangle$ is normalized) (43). For a short proof of this result, see the SM.

We now review some facts about operator norms of Hermitian matrices. The operator norm $||A||$ of a Hermitian matrix $A$ is equal to the maximum of the absolute values of the eigenvalues of $A$. For the fermion density matrix $M$ from the last paragraph, we then find that $||M|| \leq \langle \chi | \chi \rangle$. Next, if $A_{ij}$ is any matrix element of $A$, we have $|A_{ij}| \leq ||A||$ (this follows from the Cauchy-Schwarz inequality). Finally, the operator norm is submultiplicative, which means that $||AB|| \leq ||A|| ||B||$ for any two matrices $A$ and $B$.

**Finishing the proof of Lemma 1:** We now use this information to bound the sum involving $M_{kq}^{(\alpha)}$. First, let $M^{(\alpha)}$ be the Hermitian matrix with matrix elements $M_{kq}^{(\alpha)}$, and let $N^{(\alpha)}$ be the square of this matrix, $N^{(\alpha)} = M^{(\alpha)} M^{(\alpha)*}$. Then

$$\sum_{q} |M_{kq}^{(\alpha)}|^2 = N_{kk}^{(\alpha)} = |N_{kk}^{(\alpha)}| ,$$

and we have

$$\sum_{q} |M_{kq}^{(\alpha)}|^2 \leq ||N^{(\alpha)}|| \leq ||M^{(\alpha)}||^2 \leq \langle \chi_\alpha | \chi_\alpha \rangle^2 .$$

(27)

Combining all of our results leads to

$$|\langle \phi | c_{k \uparrow}^\dagger U, c_{k \uparrow} | \phi \rangle| \leq \frac{1}{|\Lambda|} \sum_{\alpha} \sqrt{u(A\Lambda)^2 \langle \chi_\alpha | \chi_\alpha \rangle^2} ,$$

(28)

and then the bound $|\langle \phi | c_{k \uparrow}^\dagger U, c_{k \uparrow} | \phi \rangle| \leq |u|$ follows from the normalization condition (21) for the states $|\chi_\alpha\rangle$. 
Conclusion: For the Hubbard and Kondo models, in the ground state and at non-zero temperature, we have derived rigorous bounds on the deviation of the average momentum occupation numbers $\langle n_{k\sigma} \rangle$ from their non-interacting values. In the future it would be interesting to derive similar results for models with more general interactions, for example spinless fermions with a density-density interaction of the form $\sum_{\mathbf{x},\mathbf{r}} v_{\mathbf{r}} n_{\mathbf{x}} n_{\mathbf{x}+\mathbf{r}}$ and where the interaction potential $v_{\mathbf{r}}$ satisfies a summability condition such as $\sum_{\mathbf{r}} |v_{\mathbf{r}}| \leq O(1)$ (or any similar condition). It would also be interesting to try and derive similar bounds for time-dependent quantities such as Green’s functions.

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I. RESULTS FOR GENERALIZED HUBBARD MODELS

A. The models

In this section we study generalized Hubbard models with Hamiltonians of the form

$$H = \sum_{k, \sigma} \epsilon_k n_{k\sigma} - \sum_{x, \sigma} \mu_x n_{x\sigma} + \sum_{x} u_x n_{x\uparrow} n_{x\downarrow}. \quad (1.1)$$

The main differences between this Hamiltonian and the one from the main text is that we now have a spatially-varying single-particle potential $\mu_x$ and a spatially-varying Hubbard interaction $u_x$.

We now introduce some notation that will help us express our results for this generalized model. First, we define $\bar{\mu}$ and $s_\mu$ to be the mean and standard deviation, respectively, of the coefficients $\mu_x$, $\bar{\mu} = \frac{1}{|\Lambda|} \sum_x \mu_x$ and $s^2_\mu = \frac{1}{|\Lambda|} \sum_x (\mu_x - \bar{\mu})^2$. If $\mu_x = \mu$ for all $x$ then $\bar{\mu} = \mu$, $s_\mu = 0$, and the single-particle potential term in $H$ reduces to the ordinary chemical potential term $-\mu N$. However, when the $\mu_x$ are not uniform the standard deviation $s_\mu$ serves as a natural measure of the disorder in the single-particle potential. [We always consider a single Hamiltonian with fixed values of the $\mu_x$ and $\mu$, i.e., we do not do any disorder averaging.] Next, we define $\bar{\pi}$ and $s_\pi$ to be the mean and standard deviation of the interaction coefficients $u_x$. Finally, we also define $u_{\text{rms}}$ to be the root mean square of the Hubbard interaction strength, $u^2_{\text{rms}} = \sum_x u^2_x / |\Lambda|$. Note that $u^2_{\text{rms}} = \bar{u}^2 + s^2_u$ and so $u_{\text{rms}} \leq \bar{u} + s_u$ by subadditivity of the square root.

In what follows we write $H$ in the form

$$H = H_0 + V \quad (1.2)$$

where now

$$H_0 = \sum_{k, \sigma} (\epsilon_k - \bar{\mu}) n_{k\sigma} \quad (1.3)$$

and

$$V = \sum_{x, \sigma} (\bar{\mu} - \mu_x) n_{x\sigma} + \sum_{x} u_x n_{x\uparrow} n_{x\downarrow}. \quad (1.4)$$

Note that the chemical potential in $H_0$ is now the average $\bar{\mu}$ of the coefficients $\mu_x$ for the single-particle potential. Then $H_0$ is again the Hamiltonian for a translation invariant free fermion system, and we can think of $V$ as a perturbation to $H_0$ that introduces both interactions and disorder.

B. Non-zero temperature result

For our generalized Hubbard models at non-zero temperature, we now wish to compare $\langle n_{k\sigma} \rangle$ with the Fermi-Dirac distribution $f_k$ with the average chemical potential $\bar{\mu}$. In this case our result reads as follows.

**Theorem 1 (generalized Hubbard, non-zero temperature):** Let $f_k$ denote the Fermi-Dirac distribution with chemical potential $\bar{\mu}$, $f_k = (e^{\beta (\epsilon_k - \bar{\mu})} + 1)^{-1}$. For any $\beta < \infty$, the momentum occupation numbers $\langle n_{k\sigma} \rangle$ for the Hamiltonian (1.1) obey the bounds

$$-\delta f_k \leq \langle n_{k\sigma} \rangle - f_k \leq \delta (1 - f_k), \quad (1.5)$$

where the constant $\delta$ is given by

$$\delta = \beta (s_\mu + u_{\text{rms}}). \quad (1.6)$$

We see that in this more general case the deviation of $\langle n_{k\sigma} \rangle$ from $f_k$ is controlled by $s_\mu$, which is a natural measure of the disorder in the single-particle potential, and by $u_{\text{rms}}$, which is a natural measure of the non-uniform Hubbard interaction strength.
In this case we again find that \( \langle n_{k\sigma} \rangle \) is close to the result for a low temperature free fermion system if \( s_\mu + u_{\text{rms}} \ll k_B T \ll \epsilon_F \) (recall that \( \epsilon_F := |e_0 - \overline{\mu}| \) is the Fermi energy for \( H_0 \)). In other words, the presence of disorder has no qualitative effect on our conclusions.

The proof of this theorem follows the same steps as the proof of Theorem 1 in the main text except that now \( H_0 \) contains the average potential \( \overline{\mu} \), and we also need to replace the translation invariant Hubbard interaction \( U = u \sum_{x,\sigma} n_{x\uparrow} n_{x\downarrow} \) with the more general perturbation \( V \) from Eq. (1.4). We also need a new version of Lemma 1 for this general case.

**Lemma 1 (generalized Hubbard model):** Let \( |\phi\rangle \) be any normalized state in the Fock space of the spin-up and spin-down fermions, and let \( V \) be the perturbation term from (1.4). Then for any \( k \) and \( \sigma \) the expectation value \( \langle \phi | c_{k\sigma}^\dagger [V, c_{k\sigma}] | \phi \rangle \) obeys

\[
|\langle \phi | c_{k\sigma}^\dagger [V, c_{k\sigma}] | \phi \rangle | \leq s_\mu + u_{\text{rms}} ,
\]

and an identical bound holds for \( |\langle \phi | c_{k\sigma}^\dagger [V, c_{k\sigma}] | \phi \rangle| \).

To prove this version of Lemma 1, we first write \( V = V_1 + V_2 \) where \( V_1 = \sum_{x,\alpha} (\overline{\mu} - \mu_x) n_{x\alpha} \) contains the single-particle potential terms and \( V_2 = \sum_{x} u_x n_{x\uparrow} n_{x\downarrow} \) contains the Hubbard interaction. By the triangle inequality we have

\[
|\langle \phi | c_{k\sigma}^\dagger [V, c_{k\sigma}] | \phi \rangle| \leq |\langle \phi | c_{k\sigma}^\dagger [V_1, c_{k\sigma}] | \phi \rangle| + |\langle \phi | c_{k\sigma}^\dagger [V_2, c_{k\sigma}] | \phi \rangle| .
\]

(1.8)

We will now show that that \( |\langle \phi | c_{k\sigma}^\dagger [V_1, c_{k\sigma}] | \phi \rangle| \leq s_\mu \) and that \( |\langle \phi | c_{k\sigma}^\dagger [V_2, c_{k\sigma}] | \phi \rangle| \leq u_{\text{rms}} \).

To bound the term involving \( V_2 \) we follow almost the exact same steps as in the proof of Lemma 1 in the main text. The only difference is that we now define \( A_{kq}^{(\alpha)} \) by

\[
A_{kq}^{(\alpha)} := \sum_{x} u_x (\alpha |\tilde{n}_{x\downarrow}\rangle |\alpha\rangle e^{-i(k-q)\cdot x} ,
\]

(1.9)

and we then find that

\[
\sum_{q} |A_{kq}^{(\alpha)}|^2 = |\Lambda| \sum_{x} u_x^2 (\alpha |\tilde{n}_{x\downarrow}\rangle |\alpha\rangle)^2 \leq (u_{\text{rms}} |\Lambda|)^2 ,
\]

(1.10)

where the first equality again follows from the Plancherel theorem. We can now follow the same steps as in the main text to conclude that \( |\langle \phi | c_{k\sigma}^\dagger [V_2, c_{k\sigma}] | \phi \rangle| \leq u_{\text{rms}} \).

Next, we prove the bound involving \( V_1 \). The proof in this case is much simpler and we do not need to use a decomposition of the state \( |\phi\rangle \) like we had in Eq. 18 of the main text (that decomposition was only needed to handle the Hubbard interaction term). In this case we simply have

\[
c_{k\sigma}^\dagger [V_1, c_{k\sigma}] = \frac{1}{|\Lambda|} \sum_{x,q} (\mu_x - \overline{\mu}) c_{k\sigma}^\dagger c_{q\sigma} e^{-i(k-q)\cdot x} ,
\]

(1.11)

and we can write

\[
\langle \phi | c_{k\sigma}^\dagger [V_1, c_{k\sigma}] | \phi \rangle = \frac{1}{|\Lambda|} \sum_{q} A_{kq} M_{kq}
\]

(1.12)

where now

\[
A_{kq} := \sum_{x} (\mu_x - \overline{\mu}) e^{-i(k-q)\cdot x}
\]

(1.13a)

\[
M_{kq} := \langle \phi | c_{k\sigma}^\dagger c_{q\sigma} | \phi \rangle .
\]

(1.13b)

Since \( |\phi\rangle \) is a normalized state, the same manipulations from the main text (Cauchy-Schwarz, Plancherel theorem, Fermi statistics) immediately lead to the desired bound \( |\langle \phi | c_{k\sigma}^\dagger [V_1, c_{k\sigma}] | \phi \rangle| \leq s_\mu \).

This completes the proof of Theorem 1 and Lemma 1 for the family of generalized Hubbard models defined in Eq. (1.1).

**C. Ground state result**

We now prove our results for the momentum occupation numbers in the ground state of the generalized Hubbard model (1.1). In particular, Theorem 2 from the main text will follow from a special case of the more general results that we state and prove here.
We start by stating our ground state result. For this result recall that, even if the ground state of this model is degenerate, we can always choose a basis for the space of ground states such that each state is a simultaneous eigenstate of $\mathbb{N}_\uparrow$ and $\mathbb{N}_\downarrow$. In the statement of our result we assume that the ground state $|\psi\rangle$ is chosen from such a basis in the case where the model has a ground state degeneracy. As in the main text, we denote the eigenvalue of $\mathbb{N}_\sigma$ for $|\psi\rangle$ by $N_\sigma, N_\sigma|\psi\rangle = N_\sigma|\psi\rangle$, and then $\rho_\sigma = N_\sigma/|\Lambda|$ is the filling fraction for spin $\sigma$.

**Theorem 2 (generalized Hubbard, ground state):** In any ground state of the Hamiltonian (1.1) the momentum occupation numbers $\langle n_{k\sigma}\rangle$ obey

$$
\langle n_{k\sigma}\rangle \leq \frac{s_{\mu} + |\pi\sqrt{\beta_\sigma} + s_u}{\epsilon_k - \pi + \pi\rho_\sigma} , \text{ if } \epsilon_k - \pi + \pi\rho_\sigma > 0 \\
1 - \langle n_{k\sigma}\rangle \leq \frac{s_{\mu} + |\pi\sqrt{\beta_\sigma} + s_u}{|\epsilon_k - \pi + \pi\rho_\sigma|} , \text{ if } \epsilon_k - \pi + \pi\rho_\sigma < 0 ,
$$

where $\sigma$ is the opposite of $\sigma$ (e.g., $\uparrow = \downarrow$).

The proof of this ground state result differs from the proof of our non-zero temperature results in a few important ways, and we highlight the differences below. We only discuss the proof of the first inequality in Theorem 2 for the case of spin-up, as the proofs of the remaining cases are very similar.

The proof again starts with a local version of the variational principle, but in this case we only need to use the familiar variational principle for the ground state. In particular, we use the fact that, for any operator $O$, the variational principle implies that $\langle O^\dagger[H,O]\rangle \geq 0$, where the expectation is taken in the ground state $|\psi\rangle$. If we choose $O = c_{k\uparrow}$, then we find that

$$
- (\epsilon_k - \pi)\langle n_{k\uparrow}\rangle + \langle c_{k\uparrow}^\dagger[V,c_{k\uparrow}]\rangle \geq 0 .
$$

The next step is to analyze the term $\langle c_{k\uparrow}^\dagger[V,c_{k\uparrow}]\rangle$. To do this we use a new decomposition of $V$ as $V = V_1' + V_2' + V_3'$, where $V_1' = \sum_{x} (\pi - \mu_x) n_{x\uparrow}$ like before, but now $V_2' = \pi \sum_{x} n_{x\uparrow} n_{x\downarrow}$ contains the average Hubbard interaction and $V_3' = \sum_{x} (\pi - \mu_x) n_{x\uparrow} n_{x\downarrow}$ contains the deviation of the Hubbard interaction from its average.

We start with the term containing $V_2'$. After some algebra we find that

$$
\langle c_{k\uparrow}^\dagger[V_2',c_{k\uparrow}]\rangle = - \frac{\pi}{|\Lambda|} \sum_{x,q} \hat{c}_{k\uparrow}^\dagger \hat{c}_{q\uparrow} \hat{n}_{x\downarrow} e^{-i(k-q)\cdot x} ,
$$

where the operators $\hat{c}_{k\sigma}$ (fermions with tildes) were defined in the main text. Next, we split the expectation $\langle c_{k\uparrow}^\dagger[V_2',c_{k\uparrow}]\rangle$ into two pieces by separating out the $q = k$ term in the sum. The contribution from the $q = k$ term is

$$
- \frac{\pi}{|\Lambda|} \langle \hat{n}_{k\uparrow} \sum_x \hat{n}_{x\downarrow} \rangle = - \frac{\pi}{|\Lambda|} \langle n_{k\uparrow},N_{\downarrow}\rangle = - \pi\rho_\downarrow \langle n_{k\uparrow}\rangle .
$$

[Recall that any number operator with a tilde is equal to the corresponding operator without the tilde.] If we also define the quantity $\langle c_{k\uparrow}^\dagger[V_2',c_{k\uparrow}]\rangle_{not\; k}$ by

$$
\langle c_{k\uparrow}^\dagger[V_2',c_{k\uparrow}]\rangle_{not\; k} := - \frac{\pi}{|\Lambda|} \sum_{x,q \neq k} \hat{c}_{k\uparrow}^\dagger \hat{c}_{q\uparrow} \hat{n}_{x\downarrow} e^{-i(k-q)\cdot x} ,
$$

then we can now write Eq. (1.15) in the form

$$
(\epsilon_k - \pi + \pi\rho_\downarrow) \langle n_{k\uparrow}\rangle \leq \langle c_{k\uparrow}^\dagger[V_1',c_{k\uparrow}]\rangle + \langle c_{k\uparrow}^\dagger[V_2',c_{k\uparrow}]\rangle_{not\; k} + \langle c_{k\uparrow}^\dagger[V_3',c_{k\uparrow}]\rangle .
$$

This inequality of course implies that

$$
(\epsilon_k - \pi + \pi\rho_\downarrow) \langle n_{k\uparrow}\rangle \leq |\langle c_{k\uparrow}^\dagger[V_1',c_{k\uparrow}]\rangle| + |\langle c_{k\uparrow}^\dagger[V_2',c_{k\uparrow}]\rangle_{not\; k}| + |\langle c_{k\uparrow}^\dagger[V_3',c_{k\uparrow}]\rangle| ,
$$

which will be useful when $\epsilon_k - \pi + \pi\rho_\downarrow > 0$. We can now use the same techniques that we used to prove Lemma 1 to show that $|\langle c_{k\uparrow}^\dagger[V_1',c_{k\uparrow}]\rangle| \leq s_\mu$ and that $|\langle c_{k\uparrow}^\dagger[V_3',c_{k\uparrow}]\rangle| \leq s_u$.

The last step of the proof is to show that $|\langle c_{k\uparrow}^\dagger[V_2',c_{k\uparrow}]\rangle_{not\; k}| \leq |\pi|\sqrt{\beta_\downarrow}$. To prove this bound we follow most of the proof of Lemma 1 from the main text, but we then follow a different procedure at the end. Specifically, we start by decomposing the ground state $|\psi\rangle$ as

$$
|\psi\rangle = \sum_{a,\alpha} W_{a\alpha} |\alpha\rangle \otimes |\alpha\rangle ,
$$

(1.21)
where now the states $|\alpha\rangle$ are a real space occupation number basis for the $N_\uparrow$-particle sector of $\tilde{F}_\uparrow$, and the states $|\alpha\rangle$ are a real space occupation number basis for the $N_\downarrow$-particle sector of $\tilde{F}_\downarrow$ (the main difference from the main text is that we are now working in a sector with a fixed number of particles of each spin). If we now follow the same steps as in the main text, then we will arrive at the inequality

$$
|\langle c_{k\uparrow}^\dagger [V_2, c_{k\uparrow}] \rangle|_{\text{not } k} \leq \frac{1}{|\mathcal{A}|} \sum_{\alpha} \sqrt{\left( \sum_{q \neq k} |A_{kq}^{(\alpha)}|^2 \right) \left( \sum_{q \neq k} |M_{kq}^{(\alpha)}|^2 \right)},
$$

where now

$$
A_{kq}^{(\alpha)} := \prod_x (\langle \alpha | \tilde{n}_{x\uparrow} | \alpha \rangle e^{-i(k-q)\cdot x}),
$$

$$
M_{kq}^{(\alpha)} := \langle \chi_\alpha | e^{\dagger}_{k\uparrow} \tilde{c}_{q\uparrow} | \chi_\alpha \rangle,
$$

and we again have $|\chi_\alpha\rangle := \sum_\alpha W_{\alpha\alpha} |\alpha\rangle$ and $\sum_\alpha \langle \alpha | \tilde{n}_{x\uparrow} | \alpha \rangle = 1$.

Next, we again need to bound the sums involving $A_{kq}^{(\alpha)}$ and $M_{kq}^{(\alpha)}$. To do this we first note that $\sum_{q \neq k} |A_{kq}^{(\alpha)}|^2 \leq \sum_q |A_{kq}^{(\alpha)}|^2$ (i.e., we add back in the $q = k$ term), and likewise for the sum involving $M_{kq}^{(\alpha)}$. Next, we bound $\sum_q |M_{kq}^{(\alpha)}|^2$ using Fermi statistics exactly as in the main text. Finally, for the sum over $A_{kq}^{(\alpha)}$ we first have

$$
\sum_q |A_{kq}^{(\alpha)}|^2 = \pi^2 |\mathcal{A}| \sum_x \langle \alpha | \tilde{n}_{x\uparrow} | \alpha \rangle^2.
$$

Then, since $\langle \alpha | \tilde{n}_{x\uparrow} | \alpha \rangle^2 = \langle \alpha | \tilde{n}_{x\uparrow} | \alpha \rangle$ (because $\langle \alpha | \tilde{n}_{x\uparrow} | \alpha \rangle$ equals 0 or 1), we have

$$
\sum_q |A_{kq}^{(\alpha)}|^2 = \pi^2 |\mathcal{A}| \sum_x \langle \alpha | \tilde{n}_{x\uparrow} | \alpha \rangle = \pi^2 |\mathcal{A}| N_\downarrow.
$$

Putting these results together then yields the bound $|\langle c_{k\uparrow}^\dagger [V_2, c_{k\uparrow}] \rangle|_{\text{not } k} \leq |\pi| \sqrt{N_\downarrow}$.

After all of this work, we end up with the inequality

$$
(\epsilon_k - \pi + \pi \rho_\downarrow)(\tilde{n}_{\downarrow}) \leq s_\mu + |\pi| \sqrt{\rho_\downarrow} + s_u,
$$

and then the first inequality in Theorem 2 follows for any $k$ that satisfies $\epsilon_k - \pi + \pi \rho_\downarrow > 0$.

Finally, to derive the second inequality in Theorem 2 one should repeat this proof but choose $\mathcal{O} = c_{k\uparrow}^\dagger$ instead of $\mathcal{O} = c_{k\uparrow}$ in the first step where we used the variational principle.

**II. RESULTS FOR GENERALIZED KONDO MODELS**

In this section we present the proofs of our results for the Kondo model, namely the proofs of Theorem 1 (the Kondo part) and Theorem 3 from the main text. We will actually prove these results for a more general Kondo model that includes more than one impurity spin.

We now consider generalized Kondo models that feature a finite number $M$ of impurity spins $\tilde{S}_1, \ldots, \tilde{S}_M$ at arbitrary locations and with arbitrary values of their spin and Kondo coupling. The $i$th impurity spin, for $i \in \{1, \ldots, M\}$, has spin $s_i \in \{1/2, 1, 3/2, \ldots\}$. These spins couple to the fermions on $M$ distinct lattice sites $x_1, \ldots, x_M$. Finally, the spin $\tilde{S}_i$ couples to the fermion at site $x_i$ with a Kondo coupling $J_i$. The Hamiltonian for this generalized Kondo model takes the form $H_{\text{Kondo}} = H_0 + V$, where $H_0 = \sum_{k, \sigma} (\epsilon_k - \mu) n_{k\sigma}$ and

$$
V = \sum_{i=1}^M V_i
$$

$$
V_i = J_i \tilde{S}_i \cdot \left( \sum_{\tau, \tau'} c_{x_i, \tau}^\dagger \frac{\sigma_{\tau, \tau'}}{2} c_{x_i, \tau'} \right).
$$

Our main results for this generalized Kondo model are as follows.
Theorem 1 (generalized Kondo, non-zero temperature): Let \( f_k \) denote the Fermi-Dirac distribution with chemical potential \( \mu \), \( f_k = (e^{\beta(\epsilon_k - \mu)} + 1)^{-1} \). For any \( \beta < \infty \), the momentum occupation numbers \( \langle n_{k\sigma} \rangle \) for \( H_{\text{Kondo}} \) obey

\[
- \delta f_k \leq \langle n_{k\sigma} \rangle - f_k \leq \delta (1 - f_k),
\]

where the constant \( \delta \) is given by

\[
\delta = \frac{3}{2 \sqrt{|A|}} \sum_i |J_i| s_i. \tag{2.2}
\]

Theorem 3 (generalized Kondo, ground state): In any ground state of \( H_{\text{Kondo}} \) the momentum occupation numbers \( \langle n_{k\sigma} \rangle \) obey

\[
\langle n_{k\sigma} \rangle \leq \frac{3}{2 \sqrt{|A|}} \sum_i |J_i| \epsilon_k - \mu, \quad \text{if } \epsilon_k - \mu > 0,
\]

\[
1 - \langle n_{k\sigma} \rangle \leq \frac{3}{2 \sqrt{|A|}} |\epsilon_k - \mu|, \quad \text{if } \epsilon_k - \mu < 0. \tag{2.4a, 2.4b}
\]

The main structure of the proofs of these results is identical to the Hubbard model case. The only difference is in the specific bound on the terms involving the interaction, and so in this section we will only derive that specific bound. In particular, we will prove the following result.

Lemma 1 (generalized Kondo model): Let \( |\phi\rangle \) be any normalized state, and let \( V \) be the Kondo interaction term from Eq. (2.1). Then for any \( k \) and \( \sigma \) the expectation value \( \langle \phi | c_{k\sigma}^\dagger [V,c_{k\sigma}] |\phi\rangle \) obeys the bound

\[
|\langle \phi | c_{k\sigma}^\dagger [V,c_{k\sigma}] |\phi\rangle| \leq \frac{3}{2 \sqrt{|A|}} \sum_i |J_i| s_i, \tag{2.5}
\]

and an identical bound holds for \(|\langle \phi | c_{k\sigma} [V,c_{k\sigma}^\dagger] |\phi\rangle|\).

We now prove this result for the case of spin-up. We start by writing out the Kondo interaction in more detail. For any index \( i \) we have

\[
V_i = \frac{J_i}{2} \left( S_{i\uparrow}^x c_{i\uparrow}^\dagger c_{i\downarrow} + S_{i\downarrow}^x c_{i\downarrow}^\dagger c_{i\uparrow} + \text{H.c.} \right) + \frac{J_i}{2} S_{i\downarrow}^z (n_{i\downarrow} - n_{i\uparrow}), \tag{2.6}
\]

where H.c. = Hermitian conjugate. By the triangle inequality we have \(|\langle \phi | c_{k\sigma}^\dagger [V,c_{k\sigma}] |\phi\rangle| \leq \sum_i |\langle \phi | c_{k\sigma}^\dagger [V_i,c_{k\sigma}] |\phi\rangle|\), and the individual terms \( c_{k\uparrow}^\dagger [V_i,c_{k\uparrow}] \) take the form

\[
c_{k\uparrow}^\dagger [V_i,c_{k\uparrow}] = \frac{J_i}{2 \sqrt{|A|}} e^{-ik \cdot x_i} \left( -S_{i\uparrow}^x c_{k\uparrow}^\dagger c_{i\downarrow} + i S_{i\downarrow}^y c_{k\uparrow}^\dagger c_{i\uparrow} + S_{i\downarrow}^z c_{k\uparrow}^\dagger c_{i\uparrow} \right). \tag{2.7}
\]

The triangle inequality then gives

\[
|\langle \phi | c_{k\uparrow}^\dagger [V_i,c_{k\uparrow}] |\phi\rangle| \leq \frac{|J_i|}{2 \sqrt{|A|}} \left( |\langle \phi | S_{i\uparrow}^x c_{k\uparrow}^\dagger c_{i\downarrow} |\phi\rangle| + |\langle \phi | S_{i\downarrow}^y c_{k\uparrow}^\dagger c_{i\uparrow} |\phi\rangle| + |\langle \phi | S_{i\downarrow}^z c_{k\uparrow}^\dagger c_{i\uparrow} |\phi\rangle| \right). \tag{2.8}
\]

To proceed further we now derive a bound on the absolute value of a general expectation value of the form \( \langle \phi | S_{i}^{\alpha} c_{k\sigma} c_{x_i \tau} |\phi\rangle \) where \( \alpha \in \{x,y,z\} \) and \( \sigma, \tau \in \{\uparrow, \downarrow\} \). To start, the Cauchy-Schwarz inequality gives

\[
|\langle \phi | S_{i}^{\alpha} c_{k\sigma} c_{x_i \tau} |\phi\rangle| \leq \sqrt{\langle \phi | (S_{i}^{\alpha})^2 |\phi\rangle} \sqrt{\langle \phi | c_{k\sigma} c_{k\sigma}^{\dagger} c_{x_i \tau} c_{x_i \tau} |\phi\rangle}. \tag{2.9}
\]

Since we are working with an impurity of spin \( s_i \), we have \( \langle \phi | (S_{i}^{\alpha})^2 |\phi\rangle \leq s_i^2 \). For the other term we have

\[
\langle \phi | c_{k\sigma} c_{k\sigma}^{\dagger} c_{x_i \tau} c_{x_i \tau} |\phi\rangle = \langle \phi | c_{k\sigma}^{\dagger} (1 - n_{k\sigma}) c_{x_i \tau} |\phi\rangle \\
\leq \langle \phi | c_{k\sigma}^{\dagger} c_{x_i \tau} |\phi\rangle \\
\leq 1, \tag{2.10}
\]

where we used the fact that the operators \( 1 - n_{k\sigma} \) and \( c_{k\sigma}^{\dagger} c_{x_i \tau} = n_{x_i \tau} \) both have a maximum eigenvalue equal to 1 (this is where the Fermi statistics of the particles is used to derive our result for the Kondo model). Putting these results together yields the bound

\[
|\langle \phi | S_{i}^{\alpha} c_{k\sigma} c_{x_i \tau} |\phi\rangle| \leq s_i, \tag{2.11}
\]

which is enough to complete the proof of the stated bound on \(|\langle \phi | c_{k\sigma}^\dagger [V,c_{k\sigma}] |\phi\rangle|\).
III. EIGENVALUES OF FERMION DENSITY MATRICES

In this last section we present a short proof of the fact about fermion density matrices that we stated in the main text and used in the proof of Lemma 1.

We first recall the setup that we had in the main text. We considered a set of fermion creation and annihilation operators $c_i, c_i^\dagger$ obeying $\{c_i, c_j\} = 0$ and $\{c_i, c_j^\dagger\} = \delta_{ij}$, where the indices $i$ and $j$ take values in some finite index set $I$. We then picked a particular state $|\chi\rangle$ in the Fock space of these fermions, and we used it to define a Hermitian matrix $M$ whose matrix elements are given by $M_{ij} := \langle \chi | c_i^\dagger c_j | \chi \rangle$. In the main text we claimed that, if $\lambda$ is any eigenvalue of $M$, then $0 \leq \lambda \leq \langle \chi | \chi \rangle$ (we do not assume that $|\chi\rangle$ is normalized). We now present a short proof of this result.

Let $v_i$ be the components of a normalized eigenvector of $M$ with eigenvalue $\lambda$, so $\sum_j M_{ij} v_j = \lambda v_i$ for all $i$ and $\sum_i |v_i|^2 = 1$. If we define a new fermion operator $C_v$ by $C_v := \sum_i v_i c_i$, then we have $\lambda = \sum_{i,j} v_i^* v_j M_{ij} v_j = \langle \chi | C_v^\dagger C_v | \chi \rangle$ (the star denotes complex conjugation). One can check that $C_v$ obeys the standard anticommutation relations $\{C_v, C_v\} = 0$ and $\{C_v, C_v^\dagger\} = 1$. Then the number operator $C_v^\dagger C_v$ has eigenvalues 0 and 1, which implies that $0 \leq \lambda \leq \langle \chi | \chi \rangle$. 