Orbital-driven melting of a bosonic Mott insulator

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(Dated: August 5, 2014)

In order to study the interplay between localized and dispersive orbital states in a system of ultracold atoms in an optical lattice, we investigate the possibility to coherently couple the lowest two Bloch bands by means of resonant periodic forcing. Considering bosons in one dimension, it is shown that a strongly interacting Floquet system can be realized, where at every lattice site two (and only two) near-degenerate orbital states are relevant. By smoothly tuning both states into resonance we find that the system can undergo an orbital-driven Mott-insulator-to-superfluid transition. As an intriguing consequence of the kinetic frustration in the system, this transition can be either continuous or first-order, depending on parameters such as lattice depth and filling.

PACS numbers: 37.10.Jk, 03.75.Lm, 67.85.-d, 75.30.Mb

Orbital degrees of freedom play an important role in solid-state systems. A prominent example is the intriguing physics of heavy-fermion compounds emerging from the interplay between dispersive conduction-band orbitals and strongly localized orbitals with a large effective mass and strong Coulomb interactions. In systems of ultracold atoms in optical-lattice in the interesting deep-lattice tight-binding regime where interactions are strong, on-site orbital degrees of freedom spanning Bloch bands above a large energy gap, are typically frozen out.

In first experiments, atoms were transferred to excited bands of optical lattices in a non-adiabatic fashion in different ways. Moreover, coherent band coupling via lattice shaking has recently been employed in the weakly interacting regime, where condensation into two possible momentum states led to domain formation. Such band-coupling via periodic driving has been studied theoretically for single or weakly interacting particles. Also band coupling via magnetic resonances has been proposed. Furthermore, there has been a lot of theoretical interest in the physics of excited orbitals not involving lower-lying states. Finally, the perturbative admixture of excited orbitals has been investigated in theory and experiment.

Here, we investigate the possibility to coherently open on-site orbital degrees of freedom also in a strongly interacting optical-lattice system by means of near-resonant lattice shaking. Already for the simple case of spinless bosons in one dimension (1D), an intriguing “dressed-lattice” system can thus be realized, where effectively at every lattice site the strongly localized (heavy) ground-band orbital is nearly degenerate and coupled to the much more dispersive (light) first-excited-band orbital. The tunneling matrix elements of the two orbitals differ strongly in magnitude and also in sign, with the latter leading to kinetic frustration. We predict an orbital-driven phase transition between a Mott insulator (MI) and a superfluid (SF) state when the population of the light orbitals is adiabatically increased by lowering the interorbital detuning. As a consequence of frustration and strong interorbital interactions, this transition is found to be either continuous or discontinuous (first-order), depending on parameters such as filling or lattice depth.

Realizing the two-orbital model Consider spinless bosonic atoms in a 1D bichromatic optical lattice \( V(x) = V_0 \sin^2(k_L x) - V_1 \sin^2(2k_L x) \) [Fig. 1(a)]. The transversal directions shall be frozen out by a deep lattice \( V_{\perp} \sin^2(k_{Ly}) + \sin^2(k_L z) \), we take \( V_{\perp}/E_R = 30 \). The recoil energy \( E_R = \hbar^2 k_L^2 / 2m \) with mass \( m \) is needed to localize a particle on a lattice constant \( \pi / k_L \) and will serve as energy unit. Throughout this work we will assume parameters of Rb 87, where a typical wave length of \( 2\pi / k_L = 852 \text{ nm} \) gives \( E_R = 2\pi \hbar \cdot 3.16 \text{ kHz} \). The system is described by the 1D multi-band Bose-Hubbard Hamiltonian \( \hat{H}_0 = \hat{H}_\text{kin} + \hat{H}_\text{os} \), with

\[
\hat{H}_\text{kin} = - \sum_\ell \sum_\alpha \langle \ell | \hat{a}^\dagger \hat{b}_\alpha \rangle \langle \ell+1 | \hat{b}_\alpha \hat{a}^\dagger + \text{h.c.}, \tag{1}
\]

\[
\hat{H}_\text{os} = - \sum_\ell \left[ \sum_\alpha \epsilon_{\alpha} \hat{n}_\alpha + \sum_\{\alpha\} \frac{U(\alpha)}{2} \hat{b}_\alpha^\dagger \hat{b}_\alpha \hat{b}_\alpha^\dagger \hat{b}_\alpha \right]. \tag{2}
\]

Here \( \hat{b}_\alpha^\dagger \) and \( \hat{n}_\alpha \) are the creation and number operator for a boson in the real Wannier orbital \( w_\alpha(x - x_\ell) \) of Bloch band \( \alpha = 0, 1, 2 \ldots \) localized at \( x_\ell = \ell \pi / k_L \). Further, one has band-center energies \( 0 = \epsilon_0 < \epsilon_1 < \ldots \) and tunneling matrix elements \( 0 < J_0 < J_1 < \ldots \). The interaction strengths \( U(\alpha) \equiv U_{\alpha_1 \alpha_2 \alpha_3 \alpha_4} = (2\hbar^2 a_\alpha^2 / m) \int dx w_{\alpha_1}(x) w_{\alpha_2}(x) w_{\alpha_3}(x) w_{\alpha_4}(x) \) vanishing for odd \( \sum \alpha_1 \), since \( \epsilon_{\alpha}(x) = (-)^\alpha \epsilon_{\alpha}(-x) \), and contain the transverse localization length \( a_{\perp} \equiv (V_{\perp} / E_R)^{1/4} / k_L \) and the scattering length \( a_s \) (\( \approx 5.6 \text{ nm} \) for Rb 87).

In the deep-lattice regime of strong interactions \( \epsilon_1 \) is typically much larger than the temperature and the chemical potential so that the orbital degree of freedom \( \alpha \) is frozen out. We wish to coherently open this freedom by means of time periodic forcing with near-resonant frequency \( \omega_0 \approx \epsilon_1 \). In particular, the lowest band \( \alpha = 0 \) shall be coupled to the more dispersive first excited band \( \alpha = 1 \), without creating coupling to...
even higher-lying bands \((\alpha \geq 2)\). In order to achieve such a controlled situation—also in the regime where interactions are strong compared to tunneling—we combine two strategies: On the one hand we choose a driving scheme, namely lattice shaking, that for weak forcing does not lead to multi-“photon” interband transitions at resonances \(\Delta_{\alpha'\alpha} \equiv \epsilon_{\alpha'} - \epsilon_{\alpha} \approx m\hbar\omega\) with integer \(|m| \geq 2\). On the other hand we engineer the band structure by varying \(V_1/V_0\) such that transitions to band 2 remain off resonant: With increasing \(V_1/V_0\) the bands organize in pairs \((0,1)\), \((2,3)\), \ldots such that \(\Delta_{10}\) and \(\Delta_{22}\) as well as \(J_1/J_0\) and \(J_3/J_2\) decrease, while \(\Delta_{21}\) increases. For an intermediate \(V_1/V_0 = 0.5\) and \(V_0 = 10E_R\), we find \(\Delta_{10} \approx 3.7E_R\) already noticeably smaller than \(\Delta_{21} \approx 5.3E_R\), rendering the \(\Delta_{21}\) transition off-resonant when \(\hbar\omega \approx \Delta_{10}\). At the same time the ratio \(J_1/J_0 \approx 5.7\) is still relatively large, retaining the crucial feature that \(\alpha = 0\) particles are much heavier than \(\alpha = 1\) particles [Fig. 1(b,d)].

Sineoidal lattice shaking with amplitude \(\Delta x = K_{KL}/(\pi m\omega^2)\) gives rise to an inertial force that is captured in the Hamiltonian by

\[
\hat{H}_{\Delta}(t) = K\cos(\omega t) \sum_\ell \left[ \sum_\alpha \ell \hat{n}_{\alpha\ell} + \sum_{\alpha'} \eta_{\alpha'\alpha} \hat{b}_{\alpha'\ell}^\dagger \hat{b}_{\alpha\ell} \right],
\]

where \(\eta_{\alpha'\alpha} = (K_{KL}/\pi) \int dx w_{\alpha'}(x) x w_{\alpha}(x)\) vanishes for even \(\alpha' + \alpha\). We employ a time-periodic unitary transform-

\[
\hat{U}(t) = \exp\left(-i \sum_\ell \hat{n}_{\alpha\ell} \nu_{\alpha\ell} t\right)
\]

with integers \(\nu_{\alpha\ell}\), designed to shift all band energies \(\epsilon_{\alpha} \equiv \epsilon_{\alpha} - \nu_{\alpha} \hbar\omega \in (-\hbar\omega/2, \hbar\omega/2)\) that are as close as possible to \(\epsilon_0 = \epsilon' = 0\). This gives \(|\epsilon'\| = |\epsilon_1 - \hbar\omega| \ll \hbar\omega\) by choice of \(\omega\) and \(|\epsilon_2| = |\epsilon_2 - \hbar\omega| \sim \hbar\omega\) by choice of \(V_1/V_0\); all other \(\epsilon_{\alpha}^\prime\) are scattered somehow between \(-\hbar\omega/2\) and \(\hbar\omega/2\). The periodic time dependence of the transformed Hamiltonian \(\hat{H}(t) = \hat{U}(t)\hat{H}_0 \hat{U}(t)^\dagger\) appears in the interband coupling parameters \(K\eta_{\alpha'\alpha} \cos(\omega t) e^{i(\nu_{\alpha'\ell} - \nu_{\alpha\ell}) t}\) and \(U_{\alpha}(t) e^{i(\nu_{\alpha'\ell} + \nu_{\alpha'\ell} - \nu_{\alpha\ell} - \nu_{\alpha\ell}) t}\). For weak forcing \(K \ll \hbar\omega\) the driving frequency \(\hbar\omega \sim \Delta_{10}\) is large compared to the intraband terms as well as to the band coupling [Fig. 1(d)]. This allows to average the rapidly oscillating terms in the Hamiltonian over one driving period and to approximately describe the system by the effective time-independent Hamiltonian \(\hat{H}_{\text{eff}} = \frac{1}{\tau} \int_0^\tau dt \hat{H}(t)\) reading

\[
\hat{H}_{\text{eff}} = \hat{H}_{\text{kin}} + \sum_\ell \left[ \sum_{\alpha} \epsilon_\alpha \hat{n}_{\alpha\ell} + K \sum_{\alpha'\alpha} \eta_{\alpha'\alpha} \hat{b}_{\alpha'\ell}^\dagger \hat{b}_{\alpha\ell} \right]
\]

\[
+ \sum_{\alpha} \frac{U_{\alpha}(t)}{2} \hat{b}_{\alpha1}^\dagger \hat{b}_{\alpha2} \hat{b}_{\alpha3} \hat{b}_{\alpha4},
\]

with \(\eta_{\alpha'\alpha} = \eta_{\alpha'\alpha}(\delta_{\nu_{\alpha'\ell},\nu_{\alpha\ell}} + \delta_{\nu_{\alpha'\ell},\nu_{\alpha\ell}-1})/2\) and \(U_{\alpha}(t) = U_{\alpha}(\hat{b}_{\alpha1} + \hat{b}_{\alpha2} + \hat{b}_{\alpha3} + \hat{b}_{\alpha4}).\) A more systematic derivation of Eq. (4) relies on Floquet theory. Defining \(\hat{H}_{\text{eff}}\) as the generator of the time evolution over one period \([2,22]\), it can be computed using degenerate perturbation theory in the extended Floquet Hilbert space \([23]\). An example for such a treatment is found in Refs. [13,45]. In leading order one recovers Eq. (4), whereas the leading correction contains tiny second-order coupling to bands \(\alpha \geq 3\) of order \(\epsilon^2/\hbar\omega\). Here \(\epsilon \lesssim 0.1E_R\) is a typical interband coupling matrix element and \(\hbar\omega \gtrsim 3E_R\).

It is a crucial property of lattice shaking \([3]\) that the single-particle interband coupling \(K\eta_{\alpha'\alpha}\) allows for single-photon transitions with \(\nu_{\alpha'} = \nu_{\alpha} \pm 1\) only and that the scattering processes \(\alpha \leftrightarrow \alpha\) allow for zero-photon transitions with \(\nu_{\alpha1} + \nu_{\alpha2} = \nu_{\alpha3} + \nu_{\alpha4}\) only. In contrast, a modulation of the lattice depth would lead also to multi-photon transitions. As a consequence, in the Hamiltonian \((4)\) the bands 0 and 1 are coupled to band 2 only, namely via the processes sketched in Fig. 1(c). These processes are, however, off resonant, since \(\epsilon_2 \sim \hbar\omega\). In the high-frequency limit the bands 0 and 1 are, therefore, decoupled from all other bands and described by

\[
\hat{H}_{\text{eff}} = \hat{H}_{\text{kin}} + \sum_\ell \left[ \delta \hat{n}_{1\ell} - \gamma (\hat{b}_{\ell}^\dagger \hat{b}_{\ell} + \text{h.c.}) + 2U_{00} \hat{n}_{0\ell} \hat{n}_{1\ell} + \frac{U_{00}}{2} \hat{n}_{0\ell} (\hat{n}_{1\ell} - 1) + \frac{U_{11}}{2} \hat{n}_{1\ell} (\hat{n}_{1\ell} - 1) \right],
\]

where \(\gamma = -K\eta_{00}/2\), \(U_{\alpha\alpha} \equiv U_{\alpha\alpha'\alpha'\alpha}\) and \(\delta = \Delta_{10} - \omega\). For \(V_0 = 10E_R\), \(V_1/V_0 = 1/2\), and \(K = 0.5E_R\) we obtain \(J_0 \approx 0.030E_R\), \(J_1 \approx 0.17E_R\), \(\gamma \approx 0.13E_R\), \(U_{00} \approx 0.58E_R\), \(U_{01} \approx 0.36E_R\), and \(U_{11} \approx 0.50E_R\).
incompressible MI phases at different integer filling of \( n = n_0 + n_1 \) particles per site, interrupted by compressible SF phases with fractional \( n \) in \( \mu \) direction. In turn, for large negative \( \delta \) the system is a compressible SF.

In the intermediate regime, where \(|\delta|\) becomes comparable to the band coupling \( \gamma \), an orbital-driven Mott transition occurs: Within the MI state the occupation \( n_1 \) will continuously increase when \( \delta \) is lowered and the larger \( n_1 \) the larger is the reduction of kinetic energy \( \approx 2J_1(n_1+1) \) (or \( \approx 2J_1n_1 \)) that a particle (or a hole) can achieve by delocalizing along leg 1 on the MI background. Roughly, when the kinetic energy reduction of a particle-hole pair exceeds its interaction-energy cost \( \approx (U_{11} + 2U_{01}n_0\delta_{n_1,1}) \), these excitations proliferate and the ground state becomes a SF. This transition can be observed in Fig. 2(c,middle) where we plot both ground-state correlations \( \chi_{\alpha'\alpha} = \langle \hat{b}_{\alpha'}^\dagger \hat{b}_0 \rangle / \sqrt{n_{\alpha'} n_\alpha} \) and imbalance \( n_0 - n_1 \) for fixed filling \( n = 1 \) versus \( \delta \), with \( V_1/V_0 = 0.5 \) and \( V_0/E_R = 15,10,5 \) (from top to bottom). Numerical data in (b) and (c) obtained for \( M = 30 \) runs under periodic boundary conditions using iTEBD [46, 47].

The MI parameter \( \delta \) can be used to tune the relative occupation between both legs. For large positive (negative) \( \delta \) only leg 0 (1) will be occupied and the system effectively reduces to a 1D chain. For integer filling of \( n \) particles per site, the ground state of a simple Bose-Hubbard chain with tunneling \( J \) and on-site repulsion \( U \) is a gapped (i.e. incompressible) MI with localized particles if \( J/U < (J/U)^{(n)}_c \), where \( (J/U)^{(1)}_c \approx 0.26 \) [50]. Otherwise, it is a gapless SF with quasilong-range order. For the parameters assumed, this makes the system a MI for \( \delta \gg |\gamma| \), since \( J_0/U_{00} \approx 0.051 \) and a SF for \( -\delta \gg |\gamma| \), since \( J_1/U_{11} \approx 0.34 \). We introduce the chemical potential \( \mu \) and compute the ground-state compressibility \( \partial_{\mu n} \) in the \( \mu-\delta \) plane [Fig. 2(b)] by imaginary-time-evolving block decimation (iTEBD) [46, 47]. As expected, on the left-hand side (where \( \delta > 0 \)) the system features

**Fig. 2.** (color online) (a) Sketch of the effective model, grey (white) circles correspond to the \( \alpha = 1 \) (0) state at each site \( \ell \), with energy \( \delta (0) \). (b) Ground-state compressibility \( \partial_{\mu n} \) in the \( \mu-\delta \) plane for \( V_0/E_R = 10 \) and \( V_1/V_0 = 1/2 \). (c) Correlations \( \chi_{\alpha'\alpha} = \langle \hat{b}_{\alpha'}^\dagger \hat{b}_0 \rangle / \sqrt{n_{\alpha'} n_\alpha} \) and imbalance \( n_0 - n_1 \) for fixed filling \( n = 1 \) versus \( \delta \), with \( V_1/V_0 = 0.5 \) and \( V_0/E_R = 15,10,5 \) (from top to bottom). Numerical data in (b) and (c) obtained for \( M = 30 \) runs under periodic boundary conditions using iTEBD [46, 47].

**Orbital-driven Mott transition** The effective Hamiltonian [5] describes a highly tunable 1D ladder system [Fig. 2(a)] with interesting properties: The tunneling matrix elements along both legs of the ladder (i.e. in both bands) differ in sign and magnitude. The former leads to localization than leg 1. The hybridization between both legs is controlled by the energy separation \( \delta \) and the coupling \( \gamma \), which can be tuned via the frequency and strength of the driving, respectively. Finally, the system features strong interorbital interactions \( U_{10} \), with two-particle energies \( 2U_{01} > U_{00} > U_{11} \).

The parameter \( \delta \) can be used to tune the relative occupation between both legs. For large positive (negative) \( \delta \) only leg 0 (1) will be occupied and the system effectively reduces to a 1D chain. For integer filling of \( n \) particles per site, the ground state of a simple Bose-Hubbard chain with tunneling \( J \) and on-site repulsion \( U \) is a gapped (i.e. incompressible) MI with localized particles if \( J/U < (J/U)^{(n)}_c \), where \( (J/U)^{(1)}_c \approx 0.26 \) [50]. Otherwise, it is a gapless SF with quasilong-range order. For the parameters assumed, this makes the system a MI for \( \delta \gg |\gamma| \), since \( J_0/U_{00} \approx 0.051 \) and a SF for \( -\delta \gg |\gamma| \), since \( J_1/U_{11} \approx 0.34 \). We introduce the chemical potential \( \mu \) and compute the ground-state compressibility \( \partial_{\mu n} \) in the \( \mu-\delta \) plane [Fig. 2(b)] by imaginary-time-evolving block decimation (iTEBD) [46, 47]. As expected, on the left-hand side (where \( \delta > 0 \)) the system features
transition to occur already when \( n_0 - n_1 \approx 0.94 \), well before the MI_{01}-to-MI_{1} transition can happen near the estimated value of \( n_0 - n_1 \approx 0.23 \). In this case the Mott transition is found to be discontinuous (first order), as can be seen in Fig. 2(c,bottom). The discontinuity results from an abrupt change in the structure of the short-range correlations along leg 0. Namely in the SF phase the correlations along leg 0 are adapted to those of leg 1 (hence the label SF_{1}). This implies that the short-range correlations along leg 0 have to undergo a finite jump at the MI_{01}-to-SF_{1} transition. Hence, when lowering \( V_0/E_R \) the continuous MI_{01}-to-MI_{1} and MI_{1}-to-SF_{1} transitions merge to a single discontinuous MI_{01}-to-SF_{1} transition. A first-order transition is also found for \( V_0/E_R = 10 \) at filling \( n = 2 \). The discontinuous orbital-driven Mott transition results from kinetic frustration, tunneling imbalance \( J_1 \gg J_0 \), and strong interband interactions \( U_{01} \), all stemming from the spatial structure of the Wannier orbitals.

**Preparation dynamics** In order to investigate the physics of the effective model \( 5 \) the following experimental protocol can be pursued. After the system is prepared close to the undriven ground state, populating band 0, the driving strength \( K \) is ramped up smoothly to the desired value. During this step \( \omega \) is chosen such that \( \delta \) is still large enough to suppress any significant occupation of band 1. In a second step, \( \delta \) can then be lowered in order to open the orbital degree of freedom. For a sufficiently slow parameter variation the system is expected to approximately follow the ground state of the effective two-band (2B) model \( 5 \), unless the first-order transition is crossed. This desired dynamics is effectively adiabatic \( 14 \), meaning that it is adiabatic with respect to the approximate effective Hamiltonian \( 3 \), but diabatic with respect to tiny coupling matrix elements appearing in higher-order of the high-frequency approximation.

We have simulated the time evolution of the second step [Fig. 3(a)] using TEBD \( 16, 47 \). For parameters like in Fig. 2(c,middle), \( \delta/E_R \) is ramped from 1 to \( -0.5 \) within a time \( T_r = 500\hbar/E_R \approx 25\mathrm{ms} \). In order to probe the validity of the 2B model \( 5 \), we include the major “loss” processes depicted in Fig. 1(c) by employing Hamiltonian \( 4 \) with three bands (\( \alpha = 0,1,2 \)). In Fig. 3(a), one can clearly see that the \( \alpha = 2 \) occupation \( n_2 \) remains very low and that the overlap with the instantaneous 2B ground state stays close to 1. Both clearly justifies a description of the driven system in terms of the effective 2B model \( 5 \). It, moreover, indicates that an effectively adiabatic time evolution is possible, despite a noticeable dip of the overlap at the Mott transition. Thus, the protocol allows for the preparation of stable low-entropy states in an excited Bloch band.

In Fig. 3(b) we investigate how effective adiabaticity depends on \( T_r \) and \( K \). Too small \( T_r \) and \( \gamma \propto K \) spoil the adiabatic dynamics within the 2B model. In turn, for too large \( K \) the coupling to band 2 becomes relevant. Moreover, for too large \( K \) and \( T_r \) slow second-order loss processes (not included) can occur. Finally, Fig. 3(c) shows that while a minimum dimerization \( V_1/V_0 = 0.5 \) is crucial, values \( V_1/V_0 > 0.5 \) are not detrimental [Fig. 3(b)]. For a simple cosine lattice with \( V_1/V_0 = 0 \) we observe significant population transfer to band 2.

**Conclusion and outlook** We have shown that lattice shaking is a feasible tool to coherently open on-site orbital degrees of freedom in a strongly interacting optical lattice system and that the interplay between Wannier orbits of different structure gives rise to rich physics already for spinless bosons in 1D. Extending the scheme to spinful fermions, the interplay between strongly localized and dispersive orbital states should permit to mimic aspects of the intriguing heavy-fermion physics and to realize periodic-Anderson-like models \( 1, 4 \). The extension to higher dimensional lattices should provide a feasible scheme for the preparation of low-entropy states in excited bands as they have been discussed before \( 21 \), and, moreover, to couple them to strongly localized lowest-band orbits. Finally, by employing sufficiently off resonant forcing, keeping \( \delta \) large enough, one might enhance and control the perturbative admixtures of excited bands \( 28, 11 \), e.g. in order to enhance superexchange processes by engineering density-dependent tunneling.

We thank Miklós Gulácsi for discussions. CS acknowledges support by the Studienstiftung des deutschen Volkes.
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see supplemental material for the perturbative treatment of transitions within the MI phase.
SUPPLEMENTAL MATERIAL

Transition between M10 and M101

For large negative δ, one can treat both γ and the tunneling matrix elements \( J_\alpha \) as a perturbation. For unit filling \( n = 1 \) the unperturbed ground state takes the simple form

\[
|\psi_0\rangle = \prod_\ell \hat{b}_{\ell 0}^\dagger |\text{vac}\rangle
\]

with the vacuum state \(|\text{vac}\rangle\). A finite correlation \( \langle \hat{b}_{10}^\dagger \hat{b}_{11}^\dagger \rangle \) will appear in third order. Namely one has

\[
\langle \psi | \hat{b}_{10}^\dagger \hat{b}_{11}^\dagger |\psi\rangle \simeq \langle \psi_1 | \hat{b}_{10}^\dagger \hat{b}_{11}^\dagger |\psi_1\rangle + \langle \psi_2 | \hat{b}_{10}^\dagger \hat{b}_{11}^\dagger |\psi_1\rangle
\]

\[
= 2 \langle \psi_1 | \hat{b}_{10}^\dagger \hat{b}_{11}^\dagger |\psi_2\rangle
\]

with \(|\psi_k\rangle\) denoting the state correction appearing in \( k \)th order perturbation theory. Here the relevant term of \(|\psi_1\rangle\) reads

\[
\frac{-\gamma \hat{b}_{10}^\dagger \hat{b}_{00}^\dagger |\psi_1\rangle}{-\delta} = \frac{\gamma}{\delta} \hat{b}_{10}^\dagger \prod_{\ell \neq 0} \hat{b}_{\ell 0}^\dagger |\text{vac}\rangle,
\]

and the relevant term of \(|\psi_2\rangle\) takes the form

\[
\left( \frac{\gamma \hat{b}_{11}^\dagger \hat{b}_{11}^\dagger |\psi_1\rangle}{2 U_{01} + \delta} + \frac{J_1 \hat{b}_{10}^\dagger \hat{b}_{10}^\dagger |\psi_0\rangle}{2 U_{01} + \delta} \right) = \left( \frac{2 J_0}{U_{00}} - \frac{J_1}{\delta} \right) \frac{\gamma}{2 U_{12} + \delta} \hat{b}_{11}^\dagger \prod_{\ell \neq 0} \hat{b}_{\ell 0}^\dagger |\text{vac}\rangle.
\]

With that we arrive at

\[
\langle \hat{b}_{10}^\dagger \hat{b}_{11}^\dagger \rangle \simeq \left( \frac{2 J_0}{U_{00}} - \frac{J_1}{\delta} \right) \frac{2 \gamma^2}{2 U_{12} + \delta}
\]

leading to a sign change when both terms in the round bracket cancel each other. The change from positive to negative sign corresponds to the transition from M10 to M101 that is thus expected to occur at

\[
\delta = \frac{U_{00} J_1}{2 J_0}.
\]

Transition between M101 and M11

We assume sharp filling \( n = n_0 + n_1 = 1 \) and treat the tunnel terms as a perturbation. The unperturbed on-site problem is then given by

\[
\hat{H}_0 = \delta \hat{n}_1 - \gamma (\hat{b}_{00}^\dagger \hat{b}_{00} + \hat{b}_{01}^\dagger \hat{b}_{01}) + 2 U_{01} \hat{n}_0 \hat{n}_1
\]

\[
+ \frac{U_{00}}{2} \hat{n}_0 (\hat{n}_0 - 1) + \frac{U_{11}}{2} \hat{n}_1 (\hat{n}_1 - 1)
\]

where we dropped the site index \( \ell \). In the subspace of one particle on a site the unperturbed ground state reads

\[
|\psi^{(0)}\rangle = (a_0 \hat{b}_{00}^\dagger + a_1 \hat{b}_{11}^\dagger)|\text{vac}\rangle,
\]

with energy \( \varepsilon_0 = \frac{\delta}{2} - \frac{1}{2} [\delta^2 + 4 \gamma^2]^{1/2} \) per site and \( a_1 / a_0 = -\varepsilon_0 / \gamma \), with \( a_0^2 + a_1^2 = 1 \), giving in leading order perturbation theory

\[
n_0 \simeq a_0^2 \quad \text{and} \quad n_1 \simeq a_1^2.
\]

In the course of the perturbation calculation we also need defect states with one particle less (a hole) and one extra particle. The hole state is simply given by the vacuum

\[
|\psi^{(h)}\rangle = |\text{vac}\rangle,
\]

with energy \( \varepsilon_h = 0 \). The subspace with two particles on a site contains three states. For simplicity, we neglect the hybridization coupling \( \gamma \) and approximate the eigenstates with an additional particle by states with sharp occupations of the orbitals \( \alpha \),

\[
\langle \psi^{(p_{20})}\rangle = \frac{1}{\sqrt{2}} (\hat{b}_{0}^\dagger)^2 |\text{vac}\rangle,
\]

\[
\langle \psi^{(p_{11})}\rangle = \hat{b}_{0}^\dagger |\text{vac}\rangle,
\]

\[
\langle \psi^{(p_{20})}\rangle = \frac{1}{\sqrt{2}} (\hat{b}_{1}^\dagger)^2 |\text{vac}\rangle,
\]

with unperturbed energies \( \varepsilon_{p_{20}} = U_{00}, \varepsilon_{p_{11}} = 2 U_{01} + \delta, \) and \( \varepsilon_{p_{20}} = 2 U_{11} + 2 \delta \).

Re-introducing the site index \( \ell \) the unperturbed ground state reads

\[
|\psi_0\rangle = \prod_\ell |\psi_0^{(0)}\rangle = \prod_\ell (a_0 \hat{b}_{0\ell}^\dagger + a_1 \hat{b}_{1\ell}^\dagger)|\text{vac}\rangle.
\]

The correlation function between the neighboring sites 0 and 1 obtains a finite value in the first order of the perturbation expansion with respect to tunneling

\[
\langle \psi_1 | \hat{b}_{00}^\dagger \hat{b}_{01}^\dagger |\psi_1\rangle \simeq \langle \psi_1 | \hat{b}_{00}^\dagger \hat{b}_{01}^\dagger |\psi_1\rangle + \langle \psi_1 | \hat{b}_{00}^\dagger \hat{b}_{01}^\dagger |\psi_0\rangle
\]

\[
= 2 \langle \psi_0 | \hat{b}_{00}^\dagger \hat{b}_{01}^\dagger |\psi_1\rangle.
\]

Here the relevant terms of the first-order state correction \( |\psi_1\rangle \) possess an extra particle in one of the three possible states on site 1 and a hole on site 0. These terms are related to the perturbation \( -J_0 \hat{b}_{01}^\dagger \hat{b}_{00} + J_1 \hat{b}_{11}^\dagger \hat{b}_{10} \) and read

\[
\left[ \frac{a_0^2 J_0}{U_{00} - 2 \varepsilon_0} (\hat{b}_{01}^\dagger)^2 - \frac{a_1^2 J_1}{U_{11} + 2 \delta - 2 \varepsilon_0} (\hat{b}_{11}^\dagger)^2 \right] \prod_{\ell \neq 0,1} (a_0 \hat{b}_{0\ell} + a_1 \hat{b}_{1\ell}) |\text{vac}\rangle.
\]

With this expression we obtain from Eqs. (19) and (14) that

\[
\langle \hat{b}_{00}^\dagger \hat{b}_{01}^\dagger \rangle \simeq \frac{2 n_0}{U_{00}(2 U_{01} + \delta - 2 \varepsilon_0)} \left[ 2 n_0 J_0 (2 U_{01} + \delta - 2 \varepsilon_0) + n_1 (J_1 - J_0) (U_{00} - 2 \varepsilon_0) \right]
\]
and

\[ \langle \hat{b}^\dagger_{10} \hat{b}_{11} \rangle \approx -\frac{2n_1}{(U_{11} + 2\delta - 2\varepsilon_0)(2U_{01} + \delta - 2\varepsilon_0)} \times \left[ 2n_1 J_1 (2U_{01} + \delta - 2\varepsilon_0) + n_0 (J_1 - J_0)(U_{11} + 2\delta - 2\varepsilon_0) \right]. \] (23)

The transition from MI$_{01}$ to MI$_1$ is related to \( \langle \hat{b}^\dagger_{00} \hat{b}_{01} \rangle \) becoming negative. Approximating \( 2U_{01} + \delta - 2\varepsilon_0 \approx 2U_{01} \), which is consistent with our previous approximation to neglect \( \gamma \) on doubly occupied sites, the transition is expected to occur when

\[ \frac{n_1}{n_0} \approx \frac{4J_0 U_{01}}{(J_1 - J_0)U_{00}} \] (24)

or, equivalently, when

\[ n_0 - n_1 \approx \frac{(J_1 - J_0)U_{00} - 4J_0 U_{01}}{(J_1 - J_0)U_{00} + 4J_0 U_{01}}. \] (25)