Principle of Maximum Entanglement Entropy and Local Physics of Correlated many-body Electron-Systems

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We argue that, because of the quantum-entanglement, the local physics of the strongly-correlated materials at zero temperature is described in very good approximation by a simple generalized Gibbs distribution, which depends on a relatively small number local quantum thermodynamical potentials. We demonstrate that our statement is exact in certain limits, and we perform numerical calculations of the iron compounds FeSe and FeTe and of the elemental cerium by employing the Gutzwiller Approximation (GA) that strongly support our theory in general.

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The strongly-correlated electron-systems display an extremely rich variety of phenomena, such as the Mott localization and the high-Tc superconductivity, which do not exist in conventional materials. The key element at the basis of the unconventional physical effects exhibited by the strongly-correlated materials is that the Coulomb interaction “localizes” part of the electrons, which retain part of their atomic character making it impossible to describe the system within a single-particle picture, and opening up the possibility of an entirely different class of phenomena.

A fundamental object in order to understand the physics of the strongly-correlated materials is the so-called “reduced density-matrix” of the correlated electrons, which is obtained from the exact density matrix of the solid by tracing over all degrees of freedom except for those of the correlated local orbitals of interest, e.g., the d-electrons of a transition-metal compound. In fact, this object encodes the whole local physics of the corresponding electronic degrees of freedom. For instance, it enables us to study the average-populations, the mixed-valence character [1, 2] and the entanglement-entropy [3, 4] of the correlated orbitals, which are fundamental concepts in modern condensed matter theory.

The scope of this work is to understand how the reduced density matrix of the correlated electrons is affected by the quantum environment in a solid at zero temperature. Note that while this is a fundamental problem of great interest, the answer is definitively non-trivial, as the size of the reduced density matrix grows exponentially with the number of correlated orbitals, and the interaction between the local correlated orbitals and their environment is generally very strong, and depends both on the chemical composition and on the arrangement of the atoms within the solid.

Let us reformulate the problem from a general perspective, without confining explicitly the discussion to the correlated electron-systems. We consider a generic “large” isolated system $U$ (the lattice), and represent its Hamiltonian as

$$\hat{H}_U = \hat{H}_S + \hat{H}_B + \hat{H}_{SB},$$

where $\hat{H}_S$ is the Hamiltonian of a subsystem $S$ (a subset of local atomic orbitals), $\hat{H}_B$ represents the Hamiltonian of its environment $B$, and $\hat{H}_{SB}$ represents the interaction between $S$ and $B$. Finally, we assume that $U$ is in the ground-state $|\Psi_{E_S}^U\rangle$ of $\hat{H}_U$ and we consider the corresponding reduced density-matrix

$$\hat{\rho}_S = \text{Tr}_B |\Psi_{E_S}^U\rangle \langle \Psi_{E_S}^U|.$$ (2)

How does $\hat{\rho}_S$ depend on the coupling between $S$ and its environment?

In this work we argue that, because of the quantum-entanglement, $\hat{\rho}_S$ exhibits thermodynamical properties pertinent to statistical averages. More precisely we argue that, due to the property of $|\Psi_{E_S}^U\rangle$ to be quantum-entangled, $\hat{\rho}_S$ has, approximately, a simple generalized Gibbs form, which depends only on few local thermodynamical parameters.

Before to expose our theory it is useful to discuss briefly an important recent related result: the canonical-typicality theorem [3, 4]. This theorem states that, given a system represented as in Eq. (1) — with a very small hybridization $\hat{H}_{SB}$ — the reduced density matrix $\rho_S$ of any “typical” $|\Psi_{E_S}^U\rangle \in U_{\langle E,E+dE\rangle}$, where $U_{\langle E,E+dE\rangle}$ is the Hilbert subspace generated by the eigenstates of $\hat{H}_U$ with energy in $[E, E + dE]$, is

$$\hat{\rho}_S = e^{-\hat{H}_S/T_S} / \text{Tr}[e^{-\hat{H}_S}/T_S],$$ (3)

where the temperature $T_S$ is determined by the average energy $E_S \equiv \text{Tr}[\hat{\rho}_S \hat{H}_S]$. Note that the Gibbs form of $\hat{\rho}_S$ arises as an individual property of the typical $|\Psi_{E_S}^U\rangle$ — a
pure state, — without calling in cause the construction of an ensemble. The key concept underlying this important theorem is the quantum-entanglement. A simple way to make this interpretation clear is that Eq. (3) is characterized by the condition

\[ S[\hat{\rho}_S] = \max \{ S[\hat{\rho}] \mid \text{Tr}[\hat{\rho} \hat{H}_S] = E_S \}, \tag{4} \]

where \( S[\hat{\rho}] = -\text{Tr}[\hat{\rho} \log \hat{\rho}] \) is the EE of \( S \), and \( \Omega_S \) is the set of all of the local (that is, in \( S \)) density-matrices. Since the entanglement-entropy is a measure of the quantum-entanglement between \( S \) and \( B \), this characterization of \( \hat{\rho}_S \) shall be regarded as a consequence of the individual property of the typical \( |\Psi_E^n \rangle \in \mathcal{U}_{[E,E+dE]} \) to be highly-entangled \( \hat{\rho} \).

Let us now drop the assumption that the interaction between \( S \) and \( B \) is negligible (which is certainly not the case in materials), and focus on our questions concerning the reduced density matrix \( \hat{\rho}_S \) of the ground-state \( |\Psi_E^n \rangle \) of \( \mathcal{U} \), see Eq. (2) and text below. The key message of this work is that, even in this case, a proper generalization of Eq. (3) holds — albeit only approximately.

In order to demonstrate our statement, let us consider the density-matrix \( \hat{\rho}(a_1, ..., a_n) \) characterized by the condition

\[ S[\hat{\rho}(a_1, ..., a_n)] = \max \{ S[\hat{\rho}] \mid \text{Tr}[\hat{\rho} \hat{A}_i] = a_i \forall i \}. \tag{5} \]

It is known that the solution \( \hat{\rho}(a_1, ..., a_n) \) of Eq. (5) has, if it is nondegenerate, the following “generalized canonical” form [11]

\[ \hat{\rho}(\lambda_1, ..., \lambda_n) = e^{-\sum_{i=1}^n \lambda_i \hat{A}_i} / \text{Tr}[e^{-\sum_{i=1}^n \lambda_i \hat{A}_i}]. \tag{6} \]

From now on we refer to Eq. (6) as the principle of maximum entanglement entropy (PMEE) relative to the set of observables \( \{ \hat{A}_1, ..., \hat{A}_n \} \), and to the constraints in Eq. (5) as the corresponding “testable information”.

A possible way to quantify the goodness of a given PMEE is the following quantity:

\[ \Delta[\hat{A}_1, ..., \hat{A}_n] = \min_{\lambda_1, ..., \lambda_n} D[\hat{\rho}(\lambda_1, ..., \lambda_n), \hat{\rho}_S], \tag{7} \]

where \( \hat{\rho}_S \) is the actual reduced density matrix of the system, and

\[ D[\hat{\rho}_1, \hat{\rho}_2] = \text{Tr}((\hat{\rho}_1 - \hat{\rho}_2)^2) / 2 \in [0,1] \tag{8} \]

is a standard trace-distance [11], that represents the maximal difference between \( \hat{\rho}_1 \) and \( \hat{\rho}_2 \) in the probability of obtaining any measurement outcome.

In summary, we have proposed a systematic method to construct and verify the goodness of a generalized Gibbs ansatz for the reduced density-matrix \( \hat{\rho}_S \) of a generic system. The key step is the identification of a subset of local observables \( \hat{A}_i \equiv \{ \hat{A}_1, ..., \hat{A}_n \} \), whose expectation-values are expected — e.g., on the basis of physical considerations — to be directly “controlled” by the system-environment interaction. Note that \( \Delta[\hat{A}] \equiv 0 \) in the limit in which \( \hat{A} \) coincides with the set of all of the local observables. In fact, any density-matrix is uniquely defined by all of the expectation-values of the observables within its Hilbert space.

As we are going to show, the PMEE is a very useful theoretical tool, as a subset \( \hat{A} \) containing only “few” observables is often sufficient to have \( \Delta[\hat{A}] \approx 0 \). In other words, it is generally possible to define a series of observables \( \hat{A}_i \) such that the corresponding series of trace-distances

\[ \Delta_n \equiv \Delta[\hat{A}_1, ..., \hat{A}_n] \tag{9} \]

converges “rapidly” to zero as a function of \( n \), regardless the details of the environment \( B \) and its coupling with \( S \).

We point out that the PMEE [Eq. (6)] has a twofold interpretation: (1) the only “relevant” testable information of \( \hat{\rho}_S \) consists in the expectation-values \( a_i \) of the observables \( \hat{A}_i \in \hat{A} \); (2) the \( S \) degrees of freedom are essentially in an interaction encoded in a “renormalized” local Hamiltonian

\[ \hat{F}_S = \sum_{i=1}^n \lambda_i \hat{A}_i \quad (\hat{A}_i \in \hat{A}), \tag{10} \]

that is generally different from to the original \( \hat{H}_S \). This twofold interpretation reflects the Legendre-duality between the expectation-values \( a_i \) and the corresponding generalized chemical potentials \( \lambda_i \).

Strongly-correlated electron-systems.— From now on we restrict the attention to the many-body correlated electron-systems in their ground state. More precisely, we consider a generic multi-band Hubbard model (HM)

\[ \hat{H}_\text{HM} = \sum_{i \neq j} \sum_{a,b=1}^{\nu} c_{i,a}^\dagger c_{j,b} + \sum_{i} \hat{H}_i^{\text{loc}}[\{c_{i,a}^\dagger\}, \{c_{i,a}\}]; \tag{11} \]

where \( i, j \) are “site” labels and \( a, b, c = 1, ..., \nu \) label both the spin \( \sigma \) and the orbital \( m \). The Hamiltonian \( \hat{H}_\text{HM} \) can be separated as in Eq. (11), with \( \hat{H}_S \) corresponding to the \( i \)-local operator \( \hat{H}_i^{\text{loc}} \) — which, in general, can include both a quadratic term \( \hat{H}_i^{\text{quadratic}} \) and a quartic term \( \hat{H}_i^{\text{quartic}} \) (representing the on-site Coulomb interaction).

In order to define a PMEE for the \( S \) reduced density-matrix we need to understand which local observables have to be included in \( \hat{A} \), see Eq. (10), to describe approximately the local physics of the system.

Due to the coupling between the environment and the local space, the expectation-value of \( \hat{H}_S \) with respect to \( \hat{\rho}_S \) is controlled by their reciprocal interaction. In other words, \( S \) and \( B \) exchange energy (as in the canonical case), which implies that the expectation-value of \( \hat{H}_S \) has to be included in \( \hat{A} \). On the other hand, since \( \hat{H}_{SB} \) is not generally small, there are at least two additional key physical mechanisms that our PMEE shall take into account. (1) Due to the hybridization effect, also the individual local orbital populations are controlled by the
coupling with the environment. (II) We expect that the effective local interaction $\hat{F}_S$ experienced by the local degrees of freedom is renormalized. Furthermore, we expect that $\hat{F}_S$ is not isotropic, but is invariant only under the point-group of the system.

From the above heuristic arguments, we conclude that $\mathcal{A}$ should include at least all of the quadratic and quartic operators compatible with the symmetry of the system. According to our scheme, the corresponding PMEE is

$$\hat{F}_S^\mu = e^{-\hat{F}_S}/\text{Tr}[e^{-\hat{F}_S}], \quad (12)$$

where the operator $\hat{F}_S$ is a generic linear combination of quadratic and quartic operators. Note that Eq. (12) represents an extremely “special” density-matrix, since the number of parameters that determine it grows only quadratically with $\nu$, see Eq. (11), rather than exponentially.

We point out that Eq. (12) is exact not only in the so called “atomic limit” $\hat{H}_{\text{SS}} \rightarrow 0$, but also for any quadratic $\hat{H}_{\text{loc}}$. This is a simple consequence of the Wick’s theorem, which ensures that the expectation-value of any local observable depends only on the “Wick’s contractions” $\langle \hat{S}_{\nu}^E | \hat{c}_{\nu}^E \hat{c}_{\nu}^\dagger | \hat{S}_{\nu}^E \rangle$, that can be readily reproduced by Eq. (12) within a proper quadratic $\hat{F}_S$.

For later convenience, we define the following series of PMEE for the local reduced density matrix $\hat{\rho}_S$ of a generic HM. (i) $\Delta_1$, corresponding to $\mathcal{A}_1 \equiv \{ \hat{H}_{\text{loc}}, \hat{N} \}$, where $\hat{H}_{\text{loc}}$ is the on-site Hamiltonian and $\hat{N}$ is number operator of $\mathcal{S}$-electrons; (ii) $\Delta_2$, corresponding to $\mathcal{A}_2$ containing $\hat{H}_{\text{loc}}$ and all of the quadratic operators commuting with the point group of the system; (iii) and $\Delta_3$, corresponding to $\mathcal{A}_3$ containing all of the quadratic and the quartic operators that commute with the point group of the system. As a reference, it is also useful to define the trace-distance $\Delta_0$ between $\hat{\rho}_S$ and the maximally-entangled state, which is the local density-matrix proportional to the identity — that corresponds to the PMEE for an empty set of observables, $\mathcal{A}_0 \equiv \{ \}$. The iron chalcogenides. In order to benchmark our theoretical arguments and demonstrate their utility to the study of materials, here we consider, as a first example, the reduced local density matrix $\hat{\rho}_d$ of a realistic HM representing the iron compound FeSe.

We construct the HM of FeSe adopting the same bands-structure $\epsilon$, see Eq. (11), used in Ref. [12], which was generated using Density Functional Theory with the Generalized Gradient Approximation for the exchange-correlation potential, according to the Perdew-Burke-Ernzerhof recipe implemented in Quantum Espresso [26], and applying Wannier90 [27] to compute the maximally localized Wannier orbitals. Finally, we make use of the Slater parametrization of the on-site interaction $\hat{H}_{\text{int}}$. Since the HM can not be solved exactly, we solve it approximately within the GA [14], which is a very reliable approximation for the ground-state of the correlated metals. In particular, we employ the numerical implementation developed in Refs. [18, 19].

In the first panel of Fig. 1 the quasi-particle renormalization weights of FeSe. The normal-metal phase (small $U$) and the Janus phase (large $U$) are indicatively separated by a vertical shaded line, Lower panel: PMEE trace-distances $\Delta_n$ for the reduced density matrix $\hat{\rho}_d$ of FeSe. The series shown in the insets correspond to the three values of $U$ indicated by vertical lines in the main panel. The calculations are performed at fixed $J/U = 0.224$ as a function of $U$. In the second panel of Fig. 1 is shown the evolution of the PMEE trace-distances $\Delta_0, \Delta_1, \Delta_2, \Delta_3$. The corresponding series $\Delta_n$, see Eq. (19), is shown explicitly in the inset for three values of $U$ as a function of the respective number of fitting parameters required. Remarkably, $\Delta_n$ converges very rapidly to 0 for all $U$’s, see Eq. (19). In fact, although the number of independent parameters of $\hat{\rho}_d$ is 2516, the $\Delta_n$ PMEE, which is defined by only 53 free parameters, is sufficient to obtain a very accurate fit for every $U$ considered — as indicated by the trace-distance $\Delta_3 \ll 1$.

In order to get an even better idea of how accurate our PMEE fits are, we show also the histogram of the local configuration probabilities of the eigenstates of $\hat{H}_{\text{loc}}$,

$$P_E \equiv \text{Tr} \left[ \hat{\rho}_d \hat{P}_E \right] /d_E, \quad (13)$$

FIG. 1: (Color online) Upper panel: quasi-particle renormalization weights of FeSe. The normal-metal phase (small $U$) and the Janus phase (large $U$) are indicatively separated by a vertical shaded line. Lower panel: PMEE trace-distances $\Delta_n$ for the reduced density matrix $\hat{\rho}_d$ of FeSe. The series shown in the insets correspond to the three values of $U$ indicated by vertical lines in the main panel. The calculations are performed at fixed $J/U = 0.224$ as a function of $U$. In the second panel of Fig. 1 is shown the evolution of the PMEE trace-distances $\Delta_0, \Delta_1, \Delta_2, \Delta_3$. The corresponding series $\Delta_n$, see Eq. (19), is shown explicitly in the inset for three values of $U$ as a function of the respective number of fitting parameters required. Remarkably, $\Delta_n$ converges very rapidly to 0 for all $U$’s, see Eq. (19). In fact, although the number of independent parameters of $\hat{\rho}_d$ is 2516, the $\Delta_n$ PMEE, which is defined by only 53 free parameters, is sufficient to obtain a very accurate fit for every $U$ considered — as indicated by the trace-distance $\Delta_3 \ll 1$. In order to get an even better idea of how accurate our PMEE fits are, we show also the histogram of the local configuration probabilities of the eigenstates of $\hat{H}_{\text{loc}}$, $P_E \equiv \text{Tr} \left[ \hat{\rho}_d \hat{P}_E \right] /d_E, \quad (13)$.
by the $\Delta$abilities, which is extremely complex, is captured in detail the structure of the computed local configuration probabilities, which is understood by observing the rapid variation of the EE of the $f$ electrons, in correspondence of the signature of the $\gamma$-transition — i.e., concomitantly to the minimum of the bulk-modulus $K = -V dP/dV$.

Let us consider the $\Delta_2$ PMEE for the $f$ local reduced density matrix $\hat{\rho}_f$,

$$\hat{\rho}_f^{\text{fit}} \propto e^{-\frac{[\hat{H}^{\text{loc}} + (\delta\mu_{5/2} n_{5/2} + \delta\mu_{7/2} n_{7/2})]^{2}}{\tau}}. \quad (14)$$

Equation (14) corresponds to maximize the $f$-EE at given average number of $5/2$ and $7/2$ $f$-electrons and given expectation-value of $\hat{H}^{\text{loc}} \equiv \hat{H}^{\text{int}} + \hat{H}^{\text{soc}}$; where $\hat{H}^{\text{int}}$ is the Slater interaction with $U = 6 \text{eV}$ and $J = 0.7 \text{eV}$, and $\hat{H}^{\text{soc}}$ is the spin-orbit-coupling (SOC) operator

$$\hat{H}^{\text{soc}} \equiv \mu_{5/2} \hat{n}_{5/2} + \mu_{7/2} \hat{n}_{7/2}, \quad (15)$$

where the coefficients $\mu_{5/2}$ and $\mu_{7/2}$ are obtained from the LDA Kohn-Sham Hamiltonian.

Note that the parameter $\tau$ of Eq. (14) is not the physical temperature — which is zero by definition in our calculations. In fact, the expectation-value of $\hat{H}^{\text{loc}}$, that is the Legendre-conjugate variable of $\beta$ — is necessarily always higher than its ground-state energy, as the cerium atoms are not isolated, but they are embedded in the fcc lattice-structure. The parameters $\delta\mu_{5/2}$ and $\delta\mu_{7/2}$ renormalize the bare spin-orbit splitting “experienced” by the $f$ electrons, which is

$$\delta_{\text{soc}} \equiv (\mu_{7/2} + \delta\mu_{7/2}) - (\mu_{5/2} + \delta\mu_{5/2}). \quad (16)$$

In the upper panel of Fig. 3 is shown the behavior as a function of the volume of $\Delta_2$ and of the fitting parameters $\tau$, $\delta\mu_{5/2}$ and $\delta\mu_{7/2}$. In the lower panel also the evolution

![FIG. 2: (Color online) Histogram of local configuration probabilities $P_E$ of the eigenstates of $\hat{H}^{\text{loc}}$ of FeSe, in the sectors $N = 5, 6, 7$, for $U = 0.5 \text{eV}$, $U = 2 \text{eV}$ and $U = 4 \text{eV}$ at fixed $J/U = 0.224$. The GA configuration probabilities (red line) are shown in comparison with the local configuration probabilities evaluated using the PMEE density matrices corresponding to the distances $\Delta_2$ and $\Delta_3$. Within each N-sector, the configuration probabilities $P_E$ are sorted in ascending order of energy $E \equiv \langle \psi_E | \hat{H}^{\text{loc}} | \psi_E \rangle$, where $| \psi_E \rangle$ are the eigenstates of $\hat{H}^{\text{loc}}$.]

![FIG. 3: (Color online) Evolution of the PMEE fitting parameters as a function of the volume (upper panels) and corresponding trace-distances (insets). In the lower panel also the evolution of the EE of the computed and fitted reduced $f$ density matrices are also shown. Our results are shown both with (left panels) and without (right panels) taking into account the spin-orbit coupling.]

where $\hat{P}_E$ is the orthonormal projector over the $E$-eigenspace of $\hat{H}^{\text{loc}}$ and $d_E$ is its degeneracy. In Fig. 2 the computed GA configuration probabilities are shown for three values of $U$ in comparison with the local configuration probabilities evaluated using the PMEE density matrices corresponding to the trace-distances $\Delta_2$ and $\Delta_3$. These data confirm the goodness of our PMEE. In fact, the structure of the computed local configuration probabilities, which is extremely complex, is captured in detail by the $\Delta_3$ PMEE, and this agreement is verified for all $U$’s, even though the system undergoes a clear crossover between two electronically distinct phases at $U \simeq 2$.

The same calculations shown above for FeSe are also reported for FeTe in the supplementary material. The results are essentially identical, which further supports our theory.

**The $\gamma$-$\alpha$ transition of cerium.**— As a second example, we consider the elemental cerium at zero temperature, which has been recently studied theoretically within the charge self-consistent Local Density Approximation in combination with the GA, see Ref. [4]. In Ref. [4], the important role of the spin-orbit coupling for the $\gamma$-$\alpha$ iso-structure transition has been understood by observing the rapid variation of the EE of the $f$ electrons, in correspondence of the signature of the $\gamma$-$\alpha$ transition — i.e., concomitantly to the minimum of the bulk-modulus $K = -V dP/dV$.
of $S[\hat{\rho}]$ and $S[\hat{\rho}^\text{fit}]$ is illustrated. As in Ref. [4], our results are shown both by taking into account the SOC and by neglecting it.

We point out that the PMEE $\hat{\rho}^\text{fit}$, see Eq. (14), approximates very well the computed reduced density matrix $\hat{\rho}$, as indicated by the trace-distance $\Delta^2 \ll 1$. The effective temperature $\tau$ decreases by increasing the volume. This is to be expected, as $\tau$ reduces to the actual physical temperature $T = 0$ in the infinite-volume limit. On the contrary, at large volumes the renormalized spin-orbit splitting $\delta_{\text{soc}}$ becomes considerably larger than $\mu_{5/2} - \mu_{7/2}$, which is of the order of $0.3\,eV$ for all volumes considered (not shown).

Remarkably, although the PMEE fitting parameters vary smoothly for all volumes, the entanglement entropy $S[\hat{\rho}]$ changes rapidly at $V \approx 33\,\text{Å}/\text{atom}$ — i.e., around the minimum of the bulk-modulus $K$ [4], — indicating that $\hat{\rho}$ undergoes a rapid crossover. This observation enables us to ascribe the $\gamma$-transition of cerium to the (approximate) generalized Gibbs form [Eq. (14)] of $\hat{\rho}$, and to describe the role of the spin-orbit coupling very neatly as follows. Analogously to a two-level system with a single particle in thermal equilibrium — in which the equilibrium state undergoes a crossover when the temperature becomes comparable with the energy-gap between the two levels, — the crossover of the reduced density matrix $\hat{\rho}$ relates with the discrete structure of the spectrum of $\hat{\rho}_{\text{loc}} \equiv \hat{\rho}_{\text{loc}} + (\delta \mu_{7/2} \hat{n}_{5/2} + \delta \mu_{5/2} \hat{n}_{7/2})$ in relation with the fictitious temperature $\tau$.

The physical picture outlined above might be applicable to describe the volume-collapse transitions in $4f$ and $5f$ systems in general, which is a major subject of investigation in condensed matter physics.

Conclusions.— We have shown that the local physics of the strongly-correlated materials at zero temperature is described by a simple universal generalized Gibbs distribution. This statement is deeply significant, as the interaction between the subsystem (a given atom) and its environment (all of the other atoms) is definitively non-negligible in real materials. Our finding provides a very powerful theoretical viewpoint on the strongly-correlated electron-systems. In fact, as shown explicitly by our calculations, the simple exponential form of the reduced density matrix enables us to understand in terms of few local thermodynamical parameters the behavior of many important physical quantities, such as all of the many-body local configuration probabilities of the correlated electrons — whose number is extremely large in general, as it grows exponentially with the number of correlated orbitals. In the future, our finding might open up the possibility to engineer new compounds with desired physical local properties by directly controlling the local thermodynamical parameters, e.g., through proper structure modifications. Finally, our general interpretation of this results, that is based on the quantum entanglement, suggests that our theory might be applicable not only to materials, but also to other quantum systems.

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PMEE results for FeTe

FIG. 4: (Color online) First panel: quasi-particle renormalization weights of FeTe. The normal-metal phase (small $U$) and the Janus phase (large $U$) are indicatively separated by a vertical shaded line. Second panel: PMEE trace-distances $\Delta_n$ for the reduced density matrix $\rho_d$ of FeSe. The series shown in the insets correspond to the three values of $U$ indicated by vertical lines in the main panel. The calculations are performed at fixed $J/U = 0.224$ as a function of $U$.

Lower panels: Histogram of local configuration probabilities $P_E$ of the eigenstates of $\hat{H}^{\text{loc}}$ of FeTe, in the sectors $N = 5, 6, 7$, for $U = 0.5 \text{ eV}$, $U = 2 \text{ eV}$ and $U = 4 \text{ eV}$ at fixed $J/U = 0.224$. The GA configuration probabilities (red line) are shown in comparison with the local configuration probabilities evaluated using the PMEE density matrices corresponding to the distances $\Delta_2$ and $\Delta_3$. Within each $N$-sector, the configuration probabilities $P_E$ are sorted in ascending order of energy $E \equiv \langle \psi_E | \hat{H}^{\text{loc}} | \psi_E \rangle$, where $|\psi_E\rangle$ are the eigenstates of $\hat{H}^{\text{loc}}$. 