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UNIFORM DENSITY THEOREM FOR THE HUBBARD MODEL

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Abstract: A general class of hopping models on a bipartite lattice is considered, including the Hubbard model and the Falicov-Kimball model. For the half-filled band, the single-particle density matrix $\rho(x, y)$ in the ground state and in the canonical and grand canonical ensembles is shown to be constant on the diagonal $x = y$, and to vanish if $x \neq y$ and if x and y are on the same sublattice. Physical implications of this result are discussed.

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The one-particle reduced density matrix, $\rho(x,y)$, of a many-electron quantum system can reveal a good deal about the presence or absence of spatial uniformity. We have uncovered a curious — and, to us, surprising — fact about ρ in the case of a half-filled band in certain tight binding models, including the Hubbard model and the Falicov-Kimball model. Our result, which is applicable to a bipartite lattice, is that $\rho(x,x)$ is always exactly equal to one for all x on a finite lattice, even though the hopping matrix elements and interaction are nonuniform, random and uncorrelated. Furthermore $\rho(x,y) = 0$ when $x \neq y$ but x and y are in the same sublattice. This result applies not only to ground states but also to positive temperature states. (The infinite volume state will be discussed at the end of this paper.) This striking result — the persistence of uniformity in the face of randomness — presumably has physical consequences. For instance, it hints at the stability of some periodic structures in solids, which is to say that the occurrence of periodic structures in a system might be insensitive to some of the details of the Hamiltonian of the system. It is noteworthy that this interesting result has a simple proof — essentially based on hole-particle symmetry.

To establish some notation, we consider a finite graph (lattice) consisting of sites labeled by x, y, etc. and edges (or bonds) connecting certain pairs of sites. We assume that the graph is bipartite, i.e., the vertices can be divided into two disjoint subsets A and B such that there is no edge connecting x and y if x and y are both in A or both in B. The total number of sites in Λ, A or B is denoted by $|\Lambda|, |A|$ and $|B|$. We assume that $|A| \geq |B|$. We are given a hermitian $|\Lambda| \times |\Lambda|$ hopping matrix T with elements $t_{xy} = t^*_{yx}$. These elements are nonzero only if x and y are connected by an edge; in particular the elements t_{xy} are zero whenever x and y are both in A or both in B. Physically, T is real in the absence of magnetic fields that interact with the electron orbital motion.

It is easy to see that the nonzero eigenvalues of T come in opposite pairs, i.e. for every eigenvalue λ there is an eigenvalue $-\lambda$. The two corresponding eigenvectors ϕ^λ and $\phi^{-\lambda}$ are simply related: if $\phi^\lambda = (f^\lambda, g^\lambda)$ with f^λ being the A-part of ϕ^λ and g^λ being the B-part of ϕ^λ then $\phi^{-\lambda} = (f^\lambda, -g^\lambda)$. Alternatively, if $V = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = V^\dagger$ is the diagonal unitary matrix that multiplies ϕ by -1 on the B-sites, then $VTV = -T$. It is possible that T has zero-modes; indeed if $|A| > |B|$ then T will have at least $|A| - |B|$ zero-modes and all these $\lambda = 0$ eigenvectors have the form $\phi = (f, 0)$.

Suppose now that we have a half-filled band, i.e., $N = |\Lambda|$ electrons. By virtue of the two spin states for each electron we have that the ground state energy of $H_0 = \sum_{x,y} t_{xy} c_x^\dagger c_y$ is $E = 2\sum_{\lambda<0} \lambda$. (Note: If $|\Lambda|$ is odd there is at least one zero-mode, and so this formula is correct even in this case.) The ground state of H_0 might be degenerate, however (because of zero-modes). We *define* the density matrix for spin σ in the ground state to be

$$\rho_\sigma(x,y) = \sum_{\lambda<0} \phi^\lambda(x)\phi^\lambda(y)^* + \tfrac{1}{2}\sum_{\lambda=0} \phi^\lambda(x)\phi^\lambda(y)^*. \tag{1}$$

We see that $\mathrm{Tr}\,\rho_\sigma = \sum_x \rho_\sigma(x,x) = |\Lambda|/2$, as it should, and that ρ_σ agrees with the $\beta \to \infty$ limit of the positive temperature density matrix, defined in the *grand canonical* ensemble by

$$\rho_{\beta\sigma}(x,y) = \sum_{\lambda} \phi^\lambda(x)\phi^\lambda(y)^* e^{-\beta\lambda}/(1+e^{-\beta\lambda}). \tag{2}$$

Note that we have used zero chemical potential which, by virtue of the $\lambda, -\lambda$ symmetry, always yields $|\Lambda|$ as the average particle number. If there is more than one zero-mode the ground state, and the ρ_σ in the ground state, is not unique. Eq. (1) serves to fix ρ_σ for our purposes. The Gibbs state is always unique for a finite volume.

Another Gibbs state with which we shall be concerned is the *canonical* ensemble. The density matrix here will be denoted by $\widetilde{\rho}_{\beta\sigma}(x,y)$. Its definition is well known and we shall not write it explicitly for H_0, but we note that the $\beta \to \infty$ limit of $\widetilde{\rho}_{\beta\sigma}$ also equals ρ_σ.

The following simple observation about (1) is the starting point of our further analysis. If $x \in A$ and $y \in A$ then, using the fact that $\phi^{\lambda}(x) = \phi^{-\lambda}(x)$, we have that

$$\rho_\sigma(x,y) = \tfrac{1}{2} \sum_{\text{all }\lambda} \phi^{\lambda}(x)\phi^{\lambda}(y)^* = \tfrac{1}{2}\delta_{x,y}$$

since the ϕ^{λ}'s form an orthonormal basis. A similar remark holds for $x, y \in B$. Thus, $\rho_\sigma(x,x) = \frac{1}{2}$ for all $x \in \Lambda$ and $\rho_\sigma(x,y) = 0$ for $x, y \in A$ or $x, y \in B$. (This result is a slight improvement of an earlier theorem announced in [1] because the zero-mode sum in eq. (1) is explicit here.) As we shall see from the following general theorem (by specializing to zero interaction) the same conclusion applies to $\rho_{\beta\sigma}(x,y)$ and $\widetilde{\rho}_{\beta\sigma}(x,y)$.

The interacting system we shall be concerned with is the *generalized* Hubbard model defined by the Hamiltonian (with spin dependent hopping)

$$H = \sum_{\sigma} \sum_{x,y\in\Lambda} t_{xy\sigma} c^\dagger_{x\sigma} c_{y\sigma} + \sum_{\sigma,\tau} \sum_{x,y\in\Lambda} U_{xy\sigma\tau}(2n_{x\sigma} - 1)(2n_{y\tau} - 1), \tag{3}$$

where $n_{x\sigma} = c^\dagger_{x\sigma} c_{x\sigma}$ and with $U_{xy\sigma\tau}$ real (but not necessarily of one sign). $T_\sigma = \{t_{xy\sigma}\}$ is hermitian and bipartite for each $\sigma =\uparrow$ or $\downarrow$. If we take $T_\uparrow = T_\downarrow$ and $U_{xy\sigma\tau} = U\delta_{xy}$ then H is the usual Hubbard Hamiltonian (apart from a trivial *additive* constant) with interaction $4U \sum n_{x\uparrow} n_{x\downarrow}$. The noninteracting case, H_0, corresponds to $U_{xy\sigma\tau} = 0$. In general, the total spin angular momentum ($SU(2)$ symmetry) will be conserved if we require $t_{xy\sigma}$ and $U_{xy\sigma\tau}$ to be independent of the spin labels σ and τ; for our purposes we do not require this $SU(2)$ invariance.

The positive temperature, grand canonical density matrix $\rho_{\beta\sigma}$ is defined to be

$$\rho_{\beta\sigma}(x,y) = \mathrm{Tr}[c^\dagger_{x\sigma} c_{y\sigma} e^{-\beta H}]/\mathrm{Tr}[e^{-\beta H}]. \tag{4}$$

Formula (4) reduces to (2) for the noninteracting case. The trace is over the full Fock space containing all particle numbers ranging from 0 to $2|\Lambda|$. Again, the zero chemical potential in (4) insures that Tr $\rho_{\beta\sigma} = |\Lambda|/2$.

The canonical density matrix $\widetilde{\rho}_{\beta\sigma}(x,y)$ for this model is also given by (4), but where the trace is only over the N-particle sector (note that both H and $c^\dagger_{x\sigma}c_{y\sigma}$ leave this sector invariant). The half-filled band is defined by $N = |\Lambda|$. Since $(\mathrm{Tr}ABC)^* = \mathrm{Tr}\ C^\dagger B^\dagger A^\dagger = \mathrm{Tr}\ B^\dagger A^\dagger C^\dagger$ we see that $\rho_{\beta\sigma}$ and $\widetilde{\rho}_{\beta\sigma}$ are hermitian matrices for each σ.

THEOREM: *The canonical and the grand canonical density matrices satisfy:*

$$\widetilde{\rho}_{\beta\sigma}(x,x) = \rho_{\beta\sigma}(x,x) = 1/2 \quad \textit{for all } x \in \Lambda \tag{5}$$

$$\widetilde{\rho}_{\beta\sigma}(x,y) = \rho_{\beta\sigma}(x,y) = 0 \qquad \textit{if } x,y \in A \textit{ or } x,y \in B. \tag{6}$$

Proof: The proof for $\widetilde{\rho}_{\beta\sigma}$ will be the same as that for $\rho_{\beta\sigma}$ so we shall only give the proof for the latter.

First, we consider real T. The following version of the hole-particle unitary transformation,

$$c_{x\sigma} \leftrightarrow c^\dagger_{x\sigma} \text{ for } x \in A, \qquad c_{x\sigma} \leftrightarrow -c^\dagger_{x\sigma} \text{ for } x \in B, \tag{7}$$

evidently leaves the Hamiltonian H and the relevant Hilbert spaces invariant. If this unitary transformation is denoted by W we have that $W^2 = 1$, $W = W^\dagger$, $WHW = H$ and hence $\mathrm{Tr}[e^{-\beta H}]\rho_{\beta\sigma}(x,y) = \mathrm{Tr}[Wc^\dagger_{x\sigma}c_{y\sigma}WWe^{-\beta H}W] = \mathrm{Tr}[Wc^\dagger_{x\sigma}W)(Wc_{y\sigma}W)e^{-\beta H}]$. If $x,y \in A$ we can use (7) and the fermion commutation rule to conclude that $\rho_{\beta\sigma}(x,y) = \delta_{x,y} - \rho_{\beta\sigma}(y,x)$. The same is true if $x,y \in B$. If T is real, $\rho_{\beta\sigma}$ is evidently real; since $\rho_{\beta\sigma}$ is also hermitian the theorem is proved in the real case.

The complex case is a bit subtle. The Hamiltonian H is no longer invariant under the hole-particle transformation W, but it is invariant under the *antiunitary* transformation $Y = JW$, in which J is complex conjugation. More precisely, any vector Ψ in our Hilbert space can be written as a linear combination, with complex coefficients, of the basis vectors consisting of monomials in the $c^\dagger_{x\sigma}$'s applied to the vacuum. The antiunitary map J acts on Ψ by replacing each coefficient by its complex conjugate. We note that $JW = WJ$ and therefore $Y^2 = \mathbf{1}$. It is also easy to see that $YHY = H$ and that $Yc_{x\sigma}Y = Wc_{x\sigma}W$, which is given by (7).

Now suppose that K is an arbitrary linear operator, and consider $L \equiv JKJ$. Although J is nonlinear, it is easy to check that L is linear. In fact the matrix elements of L in the above mentioned basis are simply the complex conjugates of the corresponding elements of K. Therefore, even though $J^2 = 1$, it is *not* generally true that $\mathrm{Tr}L = \mathrm{Tr}JKJ = \mathrm{Tr}KJ^2 = \mathrm{Tr}K$. What is true is that $\mathrm{Tr}L = (\mathrm{Tr}K)^*$.

In our case we have, for $x, y \in A$ or $x, y \in B$, $\{\mathrm{Tr}e^{-\beta H}\}\rho_{\beta\sigma}(x,y)^* = \mathrm{Tr}[JWc^\dagger_{x\sigma}c_{y\sigma}e^{-\beta H}WJ]$ $= \mathrm{Tr}[(Yc^\dagger_{x\sigma}Y)(Yc_{y\sigma}Y)(Ye^{-\beta H}Y)] = \mathrm{Tr}[c_{x\sigma}c^\dagger_{y\sigma}e^{-\beta H}] = \{\mathrm{Tr}e^{-\beta H}\}\{\delta_{xy} - \rho_{\beta\sigma}(y,x)\}$. The hermiticity of $\rho_{\beta\sigma}$ now implies the theorem. QED.

It is worth noting that only the invariance of H under Y and the bipartite structure of the lattice have been used. Thus the theorem (with some obvious modifications) applies to the case where the kinetic energy has spin-flip terms and is given by $\sum\limits_{x,y,\sigma,\tau} t_{xy\sigma\tau}c^\dagger_{x\sigma}c_{y\tau}$ with $t_{xy\sigma\tau} = \overline{t_{yx\tau\sigma}}$ and where, for fixed σ and τ, $t_{xy\sigma\tau}$ is a hopping matrix on a bipartite graph. $\rho_{\beta\sigma}(x,y)$ is replaced by $\rho_{\beta\sigma\tau}(x,y) = \rho_{\beta\tau\sigma}(y,x)^*$, and the extended theorem states that it equals $\frac{1}{2}\delta_{xy}\delta_{\sigma\tau}$ when x, y are on the same sublattice. In the interest of simplicity of notation and exposition we have relegated this generalization — relevant to some physical models — to the remark here.

We conclude with some additional remarks about some limiting cases of the Theorem.

I. The Falicov-Kimball model [2]: In this model there is one species of mobile, spinless electrons and one species of arbitrarily fixed particles. It is the same as the Hubbard model with the choice $t_{xy\downarrow} \equiv 0$ and $t_{xy\uparrow} = t_{xy}$. The theorem applies to this model as a special case. Note that it says that *both* the mobile and immobile particles have density 1/2.

II. Ground States: If we define the ground state ρ_σ as the limit $\beta \to \infty$ of the canonical $\widetilde{\rho}_{\beta\sigma}$, then (5) and (6) apply there, too. (Note: We do not have a proof — or even know if it is true — that the $\beta \to \infty$ limit of the canonical ensemble is the same as for the grand canonical ensemble.) In general the ground state is not unique, however, and there are other possibilities for ρ_σ, in which case (5) and (6) apply to states that are invariant under $Y = WJ$. Not every ground state is Y invariant. In the case of the usual Hubbard model on a connected lattice with $U > 0$ and real Y it is known [3] that the ground state has spin angular momentum $S = (|A| - |B|)/2$ and it is unique apart from the $(2S+1)$-fold degeneracy associated with $S^z = \frac{1}{2}(N_\uparrow - N_\downarrow) \in \{-S, -S+1, \ldots, +S\}$. Ground states that are Y invariant are mixtures of states with S^z and $-S^z$, i.e., $\frac{1}{2}|S^z\rangle\langle S^z| + \frac{1}{2}|-S^z\rangle\langle -S^z|$ in Dirac's notation. The reason we can be sure that $Y|S^z\rangle = |-S^z\rangle$ is this: $Y|S^z\rangle$ is — in any event — a state with $\frac{1}{2}(N_\uparrow - N_\downarrow) = -S^z$. It is also a ground state. By uniqueness, this state must be $|-S^z\rangle$. In the general model (3), we cannot be sure that spin flip = hole-particle transformation.

III. Infinite Volume States: These states can, of course, be different from finite volume states. One way to define them is as limits of finite volume states with specified boundary conditions that need not respect Y symmetry. One example concerns the Falicov-Kimball model with $U > 0$ on a hypercubic lattice in D dimensions: For $D \geq 2$ it has long-range order in the ground state and at low temperatures, in which the up spins preferentially occupy the A-sites and the down spins the B-sites (or vice versa) [4,5]. Similarly, the usual Hubbard model is expected to show the same behavior when $D \geq 3$ if $U > 0$, at least if $U > 0$ is large enough. This has not been proved, however. These examples violate (5), but they do suggest that the charge density satisfies $\rho_{\beta\uparrow}(x,x) + \rho_{\beta\downarrow}(x,x) = 1$ in these models. If we now introduce nearest neighbor repulsion (which is allowed in our general model) then even this constancy of the charge density might be violated, however.

What is significant about our finite volume theorem (5), (6) — and which does remain true in the infinite volume limit — is that for every state with non-constant (spin or charge) density there is another equally good state with the complementary density. In other words, one cannot invent a non-translationally invariant Hamiltonian (either by altering the hopping matrix or the potential energy) with the property that it *forces* the density to increase in some specified regions and to decrease in others — even though one might have thought *a-priori* that the density can be controlled by the hopping or potential energy. Any attempt to cause a non-constant density will always result in the certainty that *exactly* the reverse of the desired non-constancy will occur with the hole-particle reversed boundary condition.

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