UNIFORM DENSITY THEOREM FOR THE HUBBARD MODEL

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Elliott H. Lieb*
Departments of Physics and Mathematics, Princeton University, P.O. Box 708, Princeton, NJ 08544-0708

Michael Loss†
School of Mathematics, Georgia Institute of Technology, Atlanta, GA 30332-0160

Robert J. McCann‡
Department of Mathematics, Princeton University, Princeton, NJ 08544-1000

Abstract: A general class of hopping models on a finite 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. For free electron hopping models, it is shown in addition that there are no correlations between sites of the same sublattice in any higher order density matrix. Physical implications 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. For a general class of tight binding models, including the Hubbard model and the Falicov-Kimball model, $\rho(x, y)$ turns out to have a particularly simple form in the case of the half-filled band. The 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 fact has been long appreciated in the chemistry literature, in the context of certain models describing π electrons in

* E-mail: lieb@math.princeton.edu
† E-mail: loss@math.gatech.edu
‡ E-mail: mccann@math.princeton.edu

conjugated carbon systems[1]. It was first observed for the Hückel (free electron) model[2] by Coulson and Rushbrooke[3], who used it to justify the assumption that the effective potential should be the same at each carbon site in a self-consistent molecular orbital treatment. MacLachlan[4,5] extended the result via a hole-particle symmetry argument to the Pariser-Parr-Pople (interacting electron) model[6,7], of which the Hubbard model is formally a special case. For so-called *alternant* molecules, i.e., those in which the carbon atoms form a bipartite lattice, MacLachlan showed that to each N electron eigenstate corresponds a $2|\Lambda| - N$ electron eigenstate with the complementary density. (Here $|\Lambda|$ is the number of carbon sites, and there are 2 allowed spins at each site). These states have the same energy, up to a shift which is proportional to $|\Lambda| - N$. He used this *pairing theorem* to explain the identical spectra which had been observed for positive and negative ions of the same alternant molecule. Despite its usefulness, the result has remained unknown in the statistical mechanics and solid state physics literature, where the same models are used to investigate phase transitions and the existence of long range order. In this context, the persistence of uniformity in the face of randomness is striking. 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. We therefore present the theorem in the context of statistical mechanical ensembles at positive and zero temperature, together with an extremely simple proof. Along the way, we extend the applicability of the theorem to include Hamiltonians with spin dependent hopping and spin-flip interactions. Thus consequences are extracted for some additional models of current physical interest, such as the Falicov-Kimball model. Finally, the infinite volume limit is discussed; if the infinite volume Gibbs state has non-constant density then it is not unique, and the theorem guarantees the existence of another Gibbs state having the complementary density.

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 $|\Lambda|, |A|$ or $|B|$. 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; thus the elements t_{xy} are zero whenever x and y are both in A or both in B. (In particular, $t_{xx} = 0$ for all x.) Physically, T originates in overlap integrals and 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: for every eigenvalue λ there is an eigenvalue $-\lambda$. The two corresponding eigenvectors ϕ^λ and $\phi^{-\lambda}$ are conjugates in the following sense: 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 are zero-modes the ground state, and the ρ_σ in the ground state, will not be 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.

Coulson and Rushbrooke's[3] observation regarding (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

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

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 $x, y \in B$. 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 GENERALIZED HUBBARD MODEL

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

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

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 $8U \sum n_{x\uparrow} n_{x\downarrow}$. 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

$$\rho_{\beta\sigma}(x, y) = Z^{-1} \mathrm{Tr}[c^\dagger_{x\sigma} c_{y\sigma} e^{-\beta H}], \tag{4}$$

where $Z = \mathrm{Tr}\left[e^{-\beta H}\right]$. 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: (Uniform Density in the Generalized Hubbard Model).

The canonical and the grand canonical density matrices satisfy:

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

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

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. MacLachlan's version[5] 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 $Z\rho_{\beta\sigma}(x, y) = \mathrm{Tr}[Wc^\dagger_{x\sigma} c_{y\sigma} WWe^{-\beta H} W] = \mathrm{Tr}[(Wc^\dagger_{x\sigma} W)(Wc_{y\sigma} W)e^{-\beta H}]$. If $x, y \in A$ we can use (7) and the fermion commutation rule to conclude that $\rho_{\beta\sigma}(x, y) = \delta_{xy} - \rho_{\beta\sigma}(y, x)$. 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 $x, y \in B$, $Z\rho_{\beta\sigma}(x,y)^* = \mathrm{Tr}[JWc^\dagger_{x\sigma}c_{y\sigma}e^{-\beta H}WJ]$ $= \mathrm{Tr}[(Yc^\dagger_{x\sigma}Y)(Yc_{y\sigma}Y)(Ye^{-\beta H}Y)] = \mathrm{Tr}[c_{x\sigma}c^\dagger_{y\sigma}e^{-\beta H}] = Z\,(\delta_{xy} - \rho_{\beta\sigma}(y,x))$. 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

$$\sum_{x,y,\sigma,\tau} t_{xy\sigma\tau}c^\dagger_{x\sigma}c_{y\tau}. \tag{8}$$

Hermiticity requires $t_{xy\sigma\tau} = t^*_{yx\tau\sigma}$; to be a hopping model on a bipartite lattice imposes another condition on T which will be made clear in a moment. To apply the previous theorem, we observe that this model is equivalent to a system of spinless fermions living on a lattice twice as large as Λ, with new co-ordinates (x,σ), where $x \in \Lambda$ and $\sigma \in \{\uparrow,\downarrow\}$. The new lattice should be bipartite, which is to say that it can be divided into two sublattices such that $t_{xy\sigma\tau} = 0$ when both (x,σ) and (y,τ) are in the same sublattice. $\rho_{\beta\sigma}(x,y)$ is replaced by $\rho_\beta(x,\sigma;y,\tau) = \rho_\beta(y,\tau;x,\sigma)^*$, and the extended theorem states that it equals $\frac{1}{2}\delta_{xy}\delta_{\sigma\tau}$ when (x,σ) and (y,τ) are both on the same sublattice. In practice, the only subtlety is the identification of the sublattices. For example, let Λ be decomposed into A and B. Then the theorem applies if $t_{xy\sigma\tau} = 0$ whenever $x, y \in A$ or $x, y \in B$. In this case one of the sublattices would consist of those sites (a,σ) for which $a \in A$ and $\sigma \in \{\uparrow,\downarrow\}$. Alternatively, we could have taken the condition to be $t_{xy\sigma\sigma} = 0$ when $x, y \in A$ or $x, y \in B$, and $t_{xy\uparrow\downarrow} = 0$ whenever one of x, y is in A and the other in B. This model also satisfies the hypothesis, but in this case one of the sublattices consists of $\{\ (a,\uparrow) \mid a \in A\ \} \bigcup \{\ (b,\downarrow) \mid b \in B\ \}$. The latter scenario would be realized if we had only on-site spin-flip terms: $t_{xy\uparrow\downarrow} = t_x\delta_{xy}$, a physically appealing possibility. In the interest of simplicity of notation and exposition we have relegated this generalization — relevant to some physical models — to the remark here.

The theorem also extends to include spin-spin interactions of a more general nature than those manifested in (3). This is particularly welcome, since many physical models — the t-J model for example — require SU(2) invariant spin couplings. Let $x \in \Lambda$ and consider the operators $S^3_x = (n_{x\uparrow} - n_{x\downarrow})/2$ and $S^+_x = c^\dagger_{x\uparrow} c_{x\downarrow}$. They generate the usual SU(2) algebra at site x:

$$\vec{S_x} = \big((S^+_x + S^-_x)/2,\, (S^+_x - S^-_x)/2i,\, S^3_x\big)$$

where $S^-_x = (S^+_x)^\dagger$ and the total spin at x is $\vec{S_x} \cdot \vec{S_x}$. In terms of these operators, the spin-spin interaction realized in (3) is of the form $S^3_x S^3_y$ where $x, y \in \Lambda$; it occurs with a coupling constant proportional to $(U_{xy\uparrow\uparrow} + U_{xy\downarrow\downarrow}) - (U_{xy\uparrow\downarrow} + U_{xy\downarrow\uparrow})$. Since $S^3_x \leftrightarrow -S^3_x$ under the hole-particle inversion Y, the invariance of this interaction is manifest, but it clearly destroys the SU(2) symmetry of the Hamiltonian. However, the antiunitary transformation Y does not single out the 3-direction; indeed it follows that $\vec{S_x} \leftrightarrow -\vec{S_x}$ under Y. As a result, the conclusions of the uniform density theorem, (5) and (6), are valid for any system described by a Hamiltonian

$$H' = \sum_\sigma \sum_{x,y\in\Lambda} t_{xy\sigma} c^\dagger_{x\sigma} c_{y\sigma} + \sum_{x,y\in\Lambda} U_{xy}(n_x - 1)(n_y - 1) + \sum_{x\neq y} \sum_{i,j=1}^{3} J^{ij}_{xy} S^i_x S^j_y .$$

Here $n_x = n_{x\uparrow} + n_{y\downarrow}$ and $(S^1_x, S^2_x, S^3_x) = \vec{S_x}$, $t_{xy\sigma}$ is as in (3) and the U_{xy} and J^{ij}_{xy} $(i, j = 1, 2, 3)$ are completely arbitrary real constants. The case $J^{ij}_{xy} = J_{xy}\delta_{ij}$ corresponds to the SU(2) invariant interaction $\vec{S_x} \cdot \vec{S_y}$. We have omitted the spin-charge couplings $(n_x - 1)S^i_y$, which would appear in the most general form of H', in order to maintain its physical simplicity.

We conclude by discussing some consequences and extensions of the Theorem in certain limiting cases.

I. No Correlations within a Sublattice for the Free Electron Model:

For the free electron model, the interaction terms $U_{xy\sigma\tau}$ are zero, leaving a purely kinetic Hamiltonian of the form (3) — or (8), although we continue to suppress this generalization for notational convenience. This Hamiltonian is quadratic in the creation and annihilation operators, i.e., it is a one-body operator. Wick's theorem[8] therefore applies to the grand canonical ensemble[9], for which it states that all operator product expectations are expressible in terms of pair expectations. We use this observation together with the vanishing of $\rho_{\beta\sigma}(x, y)$ for x, y in the same sublattice to show that there can be no correlations between the electron densities on sites in this sublattice. This striking result does not seem to appear previously in the literature, although it generalizes a comment made on p. 86 of Salem's book[1] about two particle correlations in the ground state.

Electron correlations are manifested in the n-particle reduced density matrices $\rho^{(n)}_{\beta\sigma}$ which, for the grand canonical ensemble at inverse temperature β, are defined by

$$\rho^{(n)}_{\beta\sigma}(x_1, \ldots, x_n; y_1, \ldots y_n) = Z^{-1}\mathrm{Tr}\left[c^\dagger_{x_1\sigma} c^\dagger_{x_2\sigma} \ldots c^\dagger_{x_n\sigma} c_{y_n\sigma} \ldots c_{y_2\sigma} c_{y_1\sigma} e^{-\beta H}\right].$$

The trace is over the full Fock space containing all particle numbers 0 to $2|\Lambda|$, and the normalization corresponds to $\mathrm{Tr}\,\rho_{\beta\sigma}^{(n)} = \mathrm{Tr}[N_\sigma(N_\sigma-1)\cdots(N_\sigma-n+1)e^{-\beta H}]/Z$, where N_σ counts the number of spin σ particles.

Diagonalizing the hopping matrix through a change of basis, the Hamiltonian becomes $H=\sum_\lambda \lambda b_\lambda^\dagger b_\lambda$. Here λ runs over $2|\Lambda|$ values. $b_\lambda^\dagger$ and b_λ are quasi-particle creation and annihilation operators, and are related to $c_{x\sigma}^\dagger$ and $c_{x\sigma}$ through a unitary matrix ϕ:

$$c_{x\sigma}^\dagger = \sum_\lambda \phi^\lambda(x,\sigma)^* b_\lambda^\dagger \qquad c_{x\sigma} = \sum_\lambda \phi^\lambda(x,\sigma) b_\lambda. \tag{9}$$

Consequently, $b_\lambda^\dagger$ and b_λ obey the fermion anticommutation relations

$$\left\{b_\lambda^\dagger, b_\mu\right\} = \delta_{\lambda,\mu} \qquad \left\{b_\lambda^\dagger, b_\mu^\dagger\right\} = \left\{b_\lambda, b_\mu\right\} = 0.$$

Of course, $\rho_{\beta\sigma}^{(n)}$ can be expressed in terms of $b_\lambda^\dagger$ and b_λ via (9), and it is in this form that it will be most easily evaluated.

Letting $n_\lambda = b_\lambda^\dagger b_\lambda$, the anticommutation relations imply

$$\mathrm{Tr}\left[b_{\lambda_1}^\dagger \cdots b_{\lambda_n}^\dagger b_{\mu_n} \cdots b_{\mu_1} e^{-\beta H}\right] = \det\left[\delta_{\lambda_i \mu_j}\right]_{i,j=1}^n \mathrm{Tr}\left[n_{\lambda_1}\cdots n_{\lambda_n} e^{-\beta H}\right] \tag{10}$$

since the left hand side vanishes unless the λ_i are distinct and $\mu_i = \lambda_{\pi(i)}$ for some permutation $\pi \in S_n$ on n labels. The antisymmetry is manifested in the determinant. For the grand canonical ensemble, the trace is over the full Fock space, which is an (antisymmetrized) tensor product of the one particle Hilbert space. Taking the trace in the $b_\lambda^\dagger$ basis, H is diagonal so

$$Z^{-1}\mathrm{Tr}\left[n_{\lambda_1}\cdots n_{\lambda_n} e^{-\beta H}\right] = \prod_{i=1}^n (1+e^{\beta\lambda_i})^{-1}.$$

Because this is a product, it can be absorbed into the determinant in (10). The right hand side of (10) then becomes $Z\det\left[\delta_{\lambda_i\mu_j}(1+e^{\beta\lambda_i})^{-1}\right]_{i,j=1}^n$. As a particular instance, $Z^{-1}\mathrm{Tr}\left[b_\lambda^\dagger b_\mu e^{-\beta H}\right] = \delta_{\lambda\mu}(1+e^{\beta\lambda})^{-1}$, thus,

$$Z^{-1}\mathrm{Tr}\left[b_{\lambda_1}^\dagger \cdots b_{\lambda_n}^\dagger b_{\mu_n}\cdots b_{\mu_1} e^{-\beta H}\right] = \det\left[Z^{-1}\mathrm{Tr}\left[b_{\lambda_i}^\dagger b_{\mu_j} e^{-\beta H}\right]\right]_{i,j=1}^n.$$

Multiplying both sides by $\phi^{\lambda_1}(x_1,\sigma)^*\cdots\phi^{\lambda_n}(x_n,\sigma)^*\phi^{\mu_1}(y_1,\sigma)\cdots\phi^{\mu_n}(y_n,\sigma)$ and summing over all λ's and μ's brings us back to the position basis through (9). Since the determinant is termwise multilinear in the $b_{\lambda_i}^\dagger$ and b_{μ_j}, we obtain Wick's Theorem:

$$\rho_{\beta\sigma}^{(n)}(\{x_i;y_i\}_i) = \det\left[\rho_{\beta\sigma}^{(1)}(x_i,y_j)\right]_{i,j=1}^n.$$

Now take all $x_1, \ldots, x_n, y_1, \ldots, y_n$ in the same sublattice, either A or B. By the Uniform Density Theorem,

$$\rho^{(n)}_{\beta\sigma}(\{x_i; y_i\}_i) = 2^{-n} \det \left[\delta_{x_i y_j}\right]^n_{i,j=1} .$$

Explicitly, $\rho^{(n)}_{\beta\sigma}(x_1, \ldots, x_n; y_1, \ldots y_n) = \pm 2^{-n}$ when the x_i are distinct and $x_i = y_{\pi(i)}$ for some fixed permutation $\pi \in S_n$. The sign of $\rho^{(n)}_{\beta\sigma}$ is selected by the parity of π. Otherwise, $\rho^{(n)}_{\beta\sigma} = 0$.

This is to say that there can be no spatial correlations in the electron density between sites of the same sublattice, save only that the probability of finding more than one electron in the same site and spin state vanishes. As an example, if $x, y \in A$ (or B) the σ-electron pair density is $\rho^{(2)}_{\beta\sigma}(x, y; x, y) = (1 - \delta_{xy})/4$, the product of the one-particle densities at $x \neq y$. Thus the Pauli pressure is not felt between the electrons at these sites. This is surprising since one generally expects, and indeed will find, correlations between arbitrary sites $x \in A$ and $y \in B$.

The extension to Hamiltonians of the form (8) is immediate. The n-particle reduced density matrices now depend on spin as well as spatial co-ordinates, and are defined in the obvious way. Taking all the (x_i, σ_i) and (y_i, τ_i) to be in the same sublattice, the conclusion is that

$$\rho^{(n)}_{\beta}(x_1, \sigma_1, \ldots, x_n, \sigma_n; y_1, \tau_1, \ldots, y_n, \tau_n) = 2^{-n} \det \left[\delta_{x_i y_j} \delta_{\sigma_i \tau_j}\right]^n_{i,j=1} .$$

Unfortunately, these results extend neither to the canonical ensemble nor to the interacting Hamiltonian. For the canonical ensemble, correlations result from the fixed number of available particles. To see this, consider a six site lattice in which four of the sites are totally isolated, and the remaining two are joined by a a non-zero hopping matrix element t. The hopping matrix eigenvalues are 0 with multiplicity four, and $\pm|t|$. If this lattice is populated with spinless fermions, then each of the 16 ground states will involve one particle hopping between the connected sites, and zero to four particles distributed over the isolated sites. However, only 6 of these states, those having a total of three particles, will be represented in the canonical Gibbs state. Select any two of the isolated sites, and consider the probability of finding them both occupied. In the grand canonical ensemble, we have seen that this must be 1/4 at any temperature. However, in the zero temperature canonical ensemble, the likelihood of this event is $\binom{4}{2}^{-1} = 1/6$. Of course, this is a finite size effect. On the other hand, it is easy to create transparent counterexamples for the interacting case by taking $T = 0$. In particular, the Ising model Hamiltonian $H = \sum_{i,j \in L} J_{ij} s_i s_j$ can be embedded in the interaction term of (3). The identifications are $L = \Lambda \times \{\uparrow, \downarrow\}$, $s_i = 2n_{x\sigma} - 1$ where $i = (x, \sigma)$, and $J_{ij} = U_{xy\sigma\tau}$ so that an occupied spin-site state corresponds to an up Ising spin. This model is well known to have correlations between all sites for a connected lattice.

Actually, we have just discussed two trivial limits for the standard Hubbard model in which $U_{xy\sigma\tau} = U\delta_{xy}$. The $U \to 0$ limit is the free electron model, while $U \to \infty$ (or equivalently $T \to 0$) corresponds to a (spatially) disconnected Ising model. In both of these limits all spatial correlations which are detectable on a sublattice must vanish — at least for finite lattices and $\beta < \infty$, where the observables are continuous functions of U. In particular, the antiferromagnetic correlations (which can be computed to be present on a small lattice, and are conjectured to be long range for $D \geq 3$ dimensional square lattices) are clearly seen to be a result of interference between the kinetic and potential terms in the Hamiltonian.

II. The Falicov-Kimball model[10]: 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 Uniform Density Theorem applies to this model as a special case. Note that it says that *both* the mobile and immobile particles have density 1/2.

III. 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: For the interacting Hamiltonian, it is not clear that $\rho_\beta = \widetilde{\rho}_\beta$ in the $\beta \to \infty$ limit. Certainly the canonical ensemble and the grand canonical ensemble do not coincide in this limit, even for the free electron model. In Remark I. above, we gave a contrived example involving a six site lattice for which $\rho_\beta^{(2)} \neq \widetilde{\rho}_\beta^{\,(2)}$ at $\beta \to \infty$, in the process of showing that certain correlations did not vanish in the canonical Gibbs state.) Of course, the ground state is not generally unique, 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[11] 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.

IV. Infinite Volume Gibbs States: These states can, of course, have different properties 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)[12,13]. 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 Gibbs state corresponding to the same temperature which has the complementary density. In other words, *one cannot invent a non-translationally invariant Hamiltonian* (either by altering the hopping matrix or the pair potentials) 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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