

d -DIMENSIONAL HUBBARD MODEL AS A ($d + 1$)-DIMENSIONAL CLASSICAL PROBLEM

Mustansir BARMA and B. SRIRAM SHASTRY

Tata Institute of Fundamental Research, Homi Bhabha Road, Bombay 400005, India

Received 14 February 1977

We show an exact equivalence between the partition function of a d -dimensional model of electrons with short range interactions and a ($d + 1$)-dimensional classical problem. For $d = 1$ the latter is the combinatorial problem of two coupled arrow-vertex models.

Recently Suzuki [1] has proved interesting theorems using Trotter's formula [2] to demonstrate that the partition function of a d -dimensional quantum-mechanical spin system is equivalent to that of a ($d + 1$)-dimensional problem involving only classical (Ising) variables. In this letter we use Trotter's formula to study an interacting Fermi system in d dimensions, and establish a similar correspondence with a ($d + 1$)-dimensional system whose only variables are commuting operators^{†1}. Besides its intrinsic interest, this result is important from the point of view of numerical studies, as it becomes possible to perform Monte Carlo calculations for the equivalent classical system [1].

The model we study is that of a single band of electrons with short-range interactions [4–6] – commonly referred to as the Hubbard model. It is of considerable interest both in the study of itinerant magnetism [7] and as a candidate for a metal-insulator transition [8]. The Hamiltonian (appropriate to a grand canonical ensemble) is

$$\mathcal{H} = U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} - \mu \sum_{i,\sigma} \hat{n}_{i\sigma} - t \sum_{\langle ij \rangle} (c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma}). \quad (1)$$

Here $c_{i\sigma}^\dagger$ creates an electron of spin σ in a Wannier state centred at site i and $\hat{n}_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$. U is the short ranged repulsion, μ is the chemical potential and t is a hopping matrix element which we take to be non zero only between nearest neighbor sites.

Few exact results exist on the system described by \mathcal{H} for finite t and U . For example the ground state energy [9] and spectrum of low-lying excitations [10, 11] are known in one-dimension. Also in 1-D, \mathcal{H} can be mapped onto a (quantum) spin Hamiltonian with two spins per site [12]. Also, there are numerical studies of rings and chains with a finite number of sites [13, 14].

The equivalence of H to a classical Hamiltonian \mathcal{H}_{eff} that we get is valid in any dimension d . \mathcal{H}_{eff} , which involves only commuting operators, includes 4-site interactions on a ($d + 1$)-dimensional lattice. For clarity, we present the case $d = 1$ in detail, and indicate the generalization to higher dimensions. For $d = 1$, we further show the combinatorial problem is equivalent to that of the partition function of two interpenetrating vertex models [15, 16].

Define $\tilde{\mathcal{H}} = -\beta\mathcal{H}$ where β is the inverse temperature, and partition $\tilde{\mathcal{H}}$ thus:

$$\tilde{\mathcal{H}} = \mathcal{H}_0 + T_1 + T_2, \quad \text{where} \quad \mathcal{H}_0 = -\tilde{U} \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} + \tilde{\mu} \sum_{i,\sigma} \hat{n}_{i\sigma},$$

$$T_1 = \tilde{t} \left\{ \sum_{i \in A} (c_{i\uparrow}^\dagger c_{i+1\uparrow} + c_{i+1\uparrow}^\dagger c_{i\uparrow}) + \sum_{i \in B} (c_{i\downarrow}^\dagger c_{i+1\downarrow} + c_{i+1\downarrow}^\dagger c_{i\downarrow}) \right\},$$

^{†1} An entirely different approach to establishing quantum-classical equivalences for such problems has been discussed in ref. [3].

$$T_2 = \tilde{t} \left\{ \sum_{i \in A} (c_{i\downarrow}^\dagger c_{i+1\downarrow} + c_{i+1\downarrow}^\dagger c_{i\downarrow}) + \sum_{i \in B} (c_{i\uparrow}^\dagger c_{i+1\uparrow} + c_{i+1\uparrow}^\dagger c_{i\uparrow}) \right\}.$$

Here $\tilde{U} = -\beta U$, $\tilde{\mu} = -\beta\mu$ and $\tilde{t} = -\beta t$. A is the set of all odd sites in the chain, and B the set of all even sites. Notice that each of \mathcal{H}_0 , T_1 and T_2 is the sum of commuting terms. Trotter's formula gives⁺²

$$e^{\tilde{\mathcal{H}}} = \lim_{m \rightarrow \infty} [e^{\tilde{\mathcal{H}}_0/2m} e^{T_1/m} e^{\tilde{\mathcal{H}}_0/2m} e^{T_2/m}]^m, \quad (3)$$

so that the grand partition function $Z = \lim_{m \rightarrow \infty} Z^{(m)}$ where

$$Z^{(m)} = \sum_{\alpha_1 \dots \alpha_{2m}} \langle \rho_{\alpha_1} | e^{\tilde{\mathcal{H}}_0/2m} e^{T_1/m} | \rho_{\alpha_2} \rangle \langle \rho_{\alpha_2} | e^{\tilde{\mathcal{H}}_0/2m} e^{T_2/m} | \rho_{\alpha_3} \rangle \dots \langle \rho_{\alpha_{2m}} | e^{\tilde{\mathcal{H}}_0/2m} e^{T_2/m} | \rho_{\alpha_1} \rangle. \quad (4)$$

Here $|\rho_{\alpha_r}\rangle$ stands for a member of the complete set of eigenstates of \mathcal{H}_0 and is obtained by prescribing the eigenvalues of the operators $\hat{n}_{i\sigma} \forall i, \sigma$ for a given r as follows

$$\hat{n}_{i\sigma} |\rho_{\alpha_r}\rangle = n_{ir\sigma} |\rho_{\alpha_r}\rangle, \quad (5)$$

where $n_{ir\sigma}$ denotes the eigenvalue of the operator $\hat{n}_{i\sigma}$, and finally finds an interpretation as the value of the number operator in a $(d+1)$ -dimensional classical system.

Since $|\rho_{\alpha_r}\rangle$ is an eigenfunction of \mathcal{H}_0 , the evaluation of a typical matrix element in eq. (4) involves only terms like

$$M^\sigma(i, r) = \langle n_{ir\sigma} n_{i+1r\sigma} | e^{\tilde{t}/m} (c_{i\sigma}^\dagger c_{i+1\sigma} + c_{i+1\sigma}^\dagger c_{i\sigma}) | n_{ir+1\sigma} n_{i+1r+1\sigma} \rangle$$

$M^\sigma(i, r)$ is a function of the four occupation numbers and can be calculated straightforwardly. We find

$$M^\sigma(i, r) = \lim_{\Delta \rightarrow \infty} e^{h_\sigma(i, r)} \quad (6)$$

with

$$\begin{aligned} h_\sigma(i, r) = & -\Delta + \Delta(n_{ir\sigma} n_{i+1r\sigma} n_{ir+1\sigma} n_{i+1r+1\sigma} + \bar{n}_{ir\sigma} \bar{n}_{i+1r\sigma} \bar{n}_{ir+1\sigma} \bar{n}_{i+1r+1\sigma}) \\ & + [\Delta + \ln \cosh(\tilde{t}/m)] (n_{ir\sigma} \bar{n}_{i+1r\sigma} n_{ir+1\sigma} \bar{n}_{i+1r+1\sigma} + \bar{n}_{ir\sigma} n_{i+1r\sigma} \bar{n}_{ir+1\sigma} n_{i+1r+1\sigma}) \\ & + [\Delta + \ln \sinh(\tilde{t}/m)] (n_{ir\sigma} \bar{n}_{i+1r\sigma} \bar{n}_{ir+1\sigma} n_{i+1r+1\sigma} + \bar{n}_{ir\sigma} n_{i+1r\sigma} n_{ir+1\sigma} \bar{n}_{i+1r+1\sigma}). \end{aligned} \quad (7)$$

Here $\bar{n}_{ir\sigma} = (1 - n_{ir\sigma})$. The limit $\Delta \rightarrow \infty$ guarantees that $M^\sigma(i, r)$ is non zero only if $n_{ir\sigma} + n_{i+1r\sigma} = n_{ir+1\sigma} + n_{i+1r+1\sigma}$ as the kinetic energy conserves the number of particles with a given spin.

Let us regard r as a coordinate in a direction perpendicular to the original 1-D lattice. Then (i, r) labels points on a 2-D lattice and we have

$$Z^{(m)} = \text{Tr} \lim_{\Delta \rightarrow \infty} e^{\mathcal{H}_{\text{eff}}(m, \Delta)} \quad (8)$$

where

$$\mathcal{H}_{\text{eff}}(m, \Delta) = \frac{1}{2m} \sum_{r=1}^{2m} \mathcal{H}_{0r} + \sum_{\substack{i \in A \\ r \in A'}} h_\uparrow(i, r) + \sum_{\substack{i \in B \\ r \in B'}} h_\uparrow(i, r) + \sum_{\substack{i \in A \\ r \in B'}} h_\downarrow(i, r) + \sum_{\substack{i \in B \\ r \in A'}} h_\downarrow(i, r), \quad (9)$$

with $A'(B')$ labelling the set of all odd (even) r . For a given r , \mathcal{H}_{0r} has the same form as \mathcal{H}_0 except that the vari-

⁺² We thank Dr. S. Dattagupta for bringing to our notice misprints in eqs. (3) and (4) in the original manuscript.

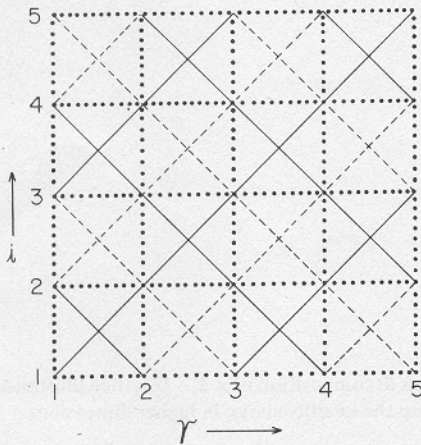


Fig. 1. \mathcal{H}_{eff} is defined on the dotted lattice. Arrows are drawn on the interpenetrating dashed and solid lattices according to the rules of fig. 2.

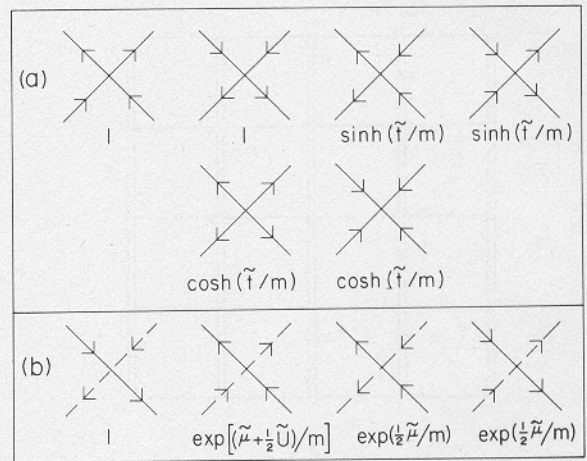


Fig. 2. Allowed vertices are shown with their weights. (a) These vertices result from up-spin hopping. Down spin hopping gives the corresponding dashed vertices with corresponding weights. (b) These vertices are associated with the localized interaction. For each one, the interchange of a solid and dashed line gives an allowed vertex of equal weight.

ables $\hat{n}_{i\sigma}$ in \mathcal{H}_0 are replaced by $n_{i\sigma}$. The h_σ terms involve 4-site interactions. We now show how the partition function $Z^{(m)}$ for the classical Hamiltonian \mathcal{H}_{eff} can be associated with a certain arrow-vertex model [15–16].

In fig. 1, the dotted lines indicate the lattice on which \mathcal{H}_{eff} is defined. The solid and dashed lines form interpenetrating lattices on which arrows will be drawn. The intersection of a pair of solid lines is associated with the 4-spin terms in the $(A - A')$ and $(B - B')$ summations, whereas intersections of dashed lines correspond to terms in the $(A - B')$ and $(A' - B)$ sums. The rule for drawing an arrow on a solid (dashed) bond is that an arrow pointing northeast or northwest represents the presence of an up-spin (down-spin) particle at the site at the centre of the bond, whereas an arrow pointing southeast or southwest represents its absence. With these rules it is easy to verify that the partition function has contributions from the vertex configurations shown in fig. 2a, with the corresponding weight factors. Identical weight factors hold for arrow configurations on the dashed lattice. Vertices at the intersection of a solid and a dashed bond give weight factors corresponding to \mathcal{H}_{0r} . There are eight such vertices, and four are shown in fig. 2(b). The other four are obtained on interchanging the role of solid and dashed bonds and have identical weight factors.

Thus the problem of evaluating Z is reduced to summing over all allowed vertex configurations, and weighting with the appropriate factors. The chemical potential μ is now determined from the constraint $\sum_{r,\sigma} (n_{i\sigma}/2m) = N$, the total number of electrons.

Turning to higher dimensions, we can demonstrate a similar equivalence with a classical system. The problem is one of partitioning the kinetic energy into parts, each of which is the sum of commuting terms. One possibility for a $2 - D$ lattice is illustrated with the help of fig. 3. Decompose the sum of the hopping over all nearest neighbor bonds into $T_1 + T_2 + T_3 + T_4$ where for instance T_1 includes the hopping on all the single dashed bonds (for up spins) and single solid bonds (for down spins). Trotter's formula can be used again, and on inserting $4m$ complete sets of states, we can convert the problem into a $3 - D$ classical problem. It should be noted that relations like

$$\langle n_{i\sigma} n_{j\sigma'} \rangle_{\mathcal{H}} = \frac{1}{2m} \sum_r \langle n_{ir\sigma} n_{jr\sigma'} \rangle_{\mathcal{H}_{\text{eff}}},$$

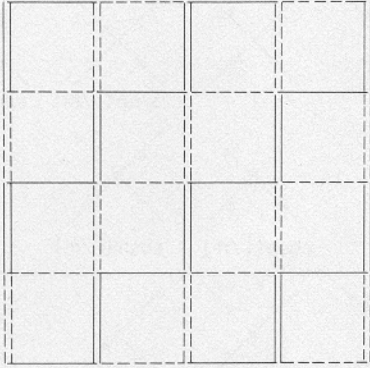


Fig. 3. This decomposition of a $2 - D$ lattice illustrates how to break up the kinetic energy in higher dimensions.

enable correlation functions for the quantum system to be calculated using the effective classical Hamiltonian.

In conclusion, it is worth pointing out that in our treatment, the $(d + 1)$ th dimension enters the classical problem on the same footing as the original d dimensions, unlike in other treatments of the problem [3].

B.S.S. thanks Professor M. Suzuki for a stimulating discussion which led to our interest in this problem.

References

- [1] M. Suzuki, Prog. of Theor. Phys. 56, No. 5 (1976).
- [2] H.F. Trotter, Proc. Am. Math. Soc. 10 (1959) 545.
- [3] J. Hertz, Phys. Rev. B14 (1976) 1165;
- [4] J. Hubbard, Proc. Roy. Soc. A276 (1963) 238.
- [5] J. Kanamori, Prog. Theor. Phys. 30 (1963) 275.
- [6] M.C. Gutzwiller, Phys. Rev. Lett. 10 (1963) 159.
- [7] C. Herring, in: Magnetism, vol. 4, eds. G.T. Rado and H. Suhl (Academic Press, New York, 1966) Ch. X.
- [8] D. Adler, in: Solid State Physics, vol. 21, eds. F. Seitz, D. Turnbull and H. Ehrenreich, (Academic Press, New York, 1968).
- [9] E.H. Lieb and F.Y. Wu, Phys. Rev. Lett. 20 (1968) 1445.
- [10] A.A. Ovchinnikov, JETP 30 (1970) 1160.
- [11] C.F. Coll, Phys. Rev. B9 (1974) 2150.
- [12] H. Shiba, Prog. Theor. Phys. 48 (1972) 2171.
- [13] H. Shiba and P. Pincus, Phys. Rev. B5 (1972) 1966.
- [14] D. Cabib and T.A. Kaplan, Phys. Rev. B7 (1973) 2199.
- [15] R.J. Baxter, Ann. Phys. (N.Y.) 70 (1972) 193.
- [16] E.H. Lieb and F.Y. Wu, in: Phase transitions and critical phenomena vol. 1, eds. C. Domb and M.S. Green (Academic Press, New York, 1972).