Classical equivalents of one-dimensional quantum-mechanical systems

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Trotter's formula is used to construct two-dimensional classical systems equivalent to some one-dimensional quantum-mechanical systems of interest. The finite-temperature properties of the completely anisotropic Heisenberg chain are expressed in terms of an eight-vertex model in which the vertex weights depend on the size of the lattice. Knowledge of only the largest eigenvalue of the transfer matrix of the eight-vertex model is not sufficient to find the free energy of the chain except in the limit of zero temperature, when Baxter's result for the ground-state energy is recovered. We also examine two models with two species of variables each, and point out that by constructing the equivalent classical problem the trace over one set of variables can be performed.

I. INTRODUCTION

Studies of magnetic systems in one-dimension (1D) are of great interest from both theoretical and experimental points of view. Theoretically, the interest stems from their tractability relative to their two-dimensional (2D) and three-dimensional (3D) counterparts. Experimental interest has increased in recent years, with the recognition that 1D systems can be realized experimentally,[1] and experiments done to check theoretical predictions.[2] One system which has received quite some attention is the spin-$\frac{1}{2}$ fully anisotropic Heisenberg chain [the XYZ model, see Eq. (2)] and its many special cases such as the Ising, XY, XXZ, and XXX (isotropic) models. The ground-state energy E_G and the free energy of both the Ising[3] and XY (Ref. 4) models are known. E_G is known for the XXX and XXZ models,[5] and Baxter recently found E_G for the XYZ model.[6] However, the calculation of the free energy of these models (XXX, XXZ, and XYZ) remains an unsolved problem. In this paper we reformulate this problem as a classical 2D problem.

The existence of a connection between 2D classical problems and ground-state properties of 1D quantum-mechanical systems is known. For instance, Baxter found E_G for the XYZ model[6] by first finding the partition function of the eight-vertex model,[7,8] which is a 2D classical problem. Here we show that the finite-temperature properties of the XYZ model also map onto an eight-vertex model, but one in which coupling constants (i.e., vertex weights) depend on the length of the 2D system. The mapping is based on the use of the Trotter formula[9,10]

$$\exp\sum_{r=1}^{n} A_r = \lim_{m\to\infty}\left(\prod_{r=1}^{n} e^{A_r/m}\right)^m . \tag{1}$$

The application of this formula to the conversion of d-dimensional quantum-mechanical problems to $(d+1)$-dimensional classical ones was pioneered by Suzuki,[11] and has been applied to both spin and fermion systems.[11–13] The method used in this paper is similar, but we have examined the equivalent classical problem somewhat more carefully, though we have not aimed at mathematical rigor. The approach runs in a direction which is opposite to the transfer matrix method, which reduces the effective dimensionaltiy of a classical problem by one at the expense of introducing off-diagonal matrix elements.

The plan of the paper is as follows. In Sec. II we consider the XYZ model and reformulate it as a classical problem. This problem is then interpreted as an arrow-vertex model by prescribing rules for drawing arrows. It is shown that the free energy of the XYZ model can be obtained from that of the eight-vertex model with certain weights. In Sec. III we consider the zero-temperature limit, and recover Baxter's result for E_G. In Sec. IV we examine two other 1D systems, viz., (i) a coupled electronic-spin–nuclear-spin model and (ii) the Falicov-Kimball model, and obtain their classical equivalents. The motivation for doing this is that one can do the trace over half the degrees of freedom in the equivalent classical problems. We conclude with a discussion of our results in Sec. V.

II. *XYZ* MODEL AS THE EIGHT-VERTEX MODEL

A. Application of Trotter's formula

The Hamiltonian of the spin-$\frac{1}{2}$ XYZ linear chain is

$$\mathcal{H} = -\sum_{i-1}^{N}(J_x S_i^x S_{i+1}^x + J_y S_i^y S_{i+1}^y + J_z S_i^z S_{i+1}^z) \quad , \tag{2}$$

where N is the number of spins. Various special cases of interest are (i) Ising ($J_x = J_y = 0$); (ii) XY ($J_z = 0$); (iii) isotropic Heisenberg, XXX ($J_x = J_y = J_z$); and (iv) XXZ ($J_x = J_y$). Let us define

$$\mathcal{H}^0 = -\sum_{i=1}^{N} J_z S_i^z S_{i+1}^z \quad , \tag{3}$$

$$V_i = -(J_x S_i^x S_{i+1}^x + J_y S_i^y S_{i+1}^y) \quad , \tag{4}$$

$$V_A = \sum_{i\in A} V_i, \quad V_B = \sum_{i\in B} V_i \quad , \tag{5}$$

where A (B) is the set of odd (even) integers. Each of V_A and V_B is the sum of commuting terms in this decomposition. We can write Eq. (2) as

$$\mathcal{H} = \mathcal{H}^0 + V_A + V_B \quad . \tag{6}$$

The partition function is

$$Z = \mathrm{tr} e^{-\beta(\mathcal{H}^0 + V_A + V_B)} \quad , \tag{7}$$

where β is the inverse temperature. On applying Trotter's formula [Eq. (1)] to Eq. (7) we get

$$Z = \lim_{m\to\infty} Z^{(m)} \tag{8}$$

where

$$Z^{(m)} = \mathrm{tr}\left(e^{-\beta\mathcal{H}^0/2m} e^{-\beta V_A/m} \times e^{-\beta\mathcal{H}^0/2m} e^{-\beta V_B/m}\right)^m \quad . \tag{9}$$

We have interchanged the limit $m \to \infty$ and the trace. We now introduce $2m$ complete sets of eigenstates of $\mathcal{H}^0$ (the Ising part) in Eq. (9) and get

$$Z^{(m)} = \sum_{\alpha_1\alpha_2\cdots\alpha_{2m}} \left(\exp\frac{-\beta}{2m}\sum_{r=1}^{2m}\mathcal{H}_r^0\right)\langle\alpha_1|e^{-\beta V_A/m}|\alpha_2\rangle\,\langle\alpha_2|e^{-\beta V_B/m}|\alpha_3\rangle\cdots\langle\alpha_{2m}|e^{-\beta V_B/m}|\alpha_1\rangle \quad , \tag{10}$$

where the states $|\alpha_r\rangle$ are obtained by prescribing the eigenvalues of S_i^z for all i. Thus

$$S_i^z|\alpha_r\rangle = S_{ir}|\alpha_r\rangle \quad , \tag{11}$$

$$\mathcal{H}^0|\alpha_r\rangle = \mathcal{H}_r^0|\alpha_r\rangle \quad . \tag{12}$$

r is a dummy integer which keeps track of which term one is considering in Eq. (10), and each α_r runs over 2^N states. We can now use Eq. (5) to rewrite Eq. (10) in the form

$$Z^{(m)} = \sum_{\alpha_1\alpha_2\cdots\alpha_{2m}} \exp\left(\frac{-\beta}{2m}\sum_{r=1}^{2m}\mathcal{H}_r^0 - \beta\sum_{i\in A}\sum_{r=1}^{2m}h(i,r) - \beta\sum_{i\in B}\sum_{r=1}^{2m}h(i,r)\right) \quad , \tag{13}$$

where

$$e^{-\beta h(i,r)} = \langle S_{ir}S_{i+1r}|e^{-\beta V_i/m}|S_{ir+1}S_{i+1r+1}\rangle \quad . \tag{14}$$

The matrix element of Eq. (14) can be found using the identity

$$\hat{O} \equiv e^{-\beta V_i/m} = (\tfrac{1}{2} + 2S_i^zS_{i+1}^z)\cosh K_- + (\tfrac{1}{2} - 2S_i^zS_{i+1}^z)\cosh K_+ + (S_i^+S_{i+1}^- + S_{i+1}^+S_i^-)\sinh K_+ + (S_i^+S_{i+1}^+ + S_i^-S_{i+1}^-)\sinh K_- \quad , \tag{15}$$

where

$$K_\pm = (\beta/4m)(J_x \pm J_y) \quad . \tag{16}$$

We see that only 8 of the 16 matrix elements in Eq. (14) are nonzero, and these are, in self-evident notation,

$$\begin{aligned}
&\langle\uparrow\uparrow|\hat{O}|\uparrow\uparrow\rangle = \langle\downarrow\downarrow|\hat{O}|\downarrow\downarrow\rangle = \cosh K_- \quad ,\\
&\langle\uparrow\downarrow|\hat{O}|\uparrow\downarrow\rangle = \langle\downarrow\uparrow|\hat{O}|\downarrow\uparrow\rangle = \cosh K_+ \quad ,\\
&\langle\uparrow\downarrow|\hat{O}|\downarrow\uparrow\rangle = \langle\downarrow\uparrow|\hat{O}|\uparrow\downarrow\rangle = \sinh K_+ \quad ,\\
&\langle\uparrow\uparrow|\hat{O}|\downarrow\downarrow\rangle = \langle\downarrow\downarrow|\hat{O}|\uparrow\uparrow\rangle = \sinh K_- \quad .
\end{aligned} \tag{17}$$

Essentially the same matrix element as in Eq. (14) was also calculated by Suzuki.[11] We now interpret Eq. (13) as the partition function of a 2D classical model. Imagine a 2D square lattice (Fig. 1) in which rows are labeled by r ($1 \leq r \leq 2m$) and columns by i ($1 \leq i \leq N$). To each site, assign an Ising spin $S_{ir} = \pm\frac{1}{2}$. $Z^{(m)}$ is now equivalent to a 2D Ising model with four-spin interactions. The effective Hamiltonian can be written explicitly, from Eqs. (13)–(17). Since 8 of the 16 matrix elements vanish, the four-spin interactions corresponding to them must have zero Boltzmann weights, or equivalently, infinite energies.

These constraints can be incorporated in a compact fashion in an arrow-vertex description[7,8,14] (below), so we will not explicitly write the classical Hamiltonian here, and only note that it has (a) two-spin interactions, contained in $\mathcal{H}_r^0$ in Eq. (13). This contribution to the energy is

$$-\frac{J_z}{2m}\sum_{i=1}^{N}\sum_{r=1}^{2m} S_{ir}S_{i+1r} \ ,$$

and corresponds to an interaction energy $\pm J_z/8m$ for every horizontal bond in Fig. 1. (b) Four-spin interactions corresponding to the terms $h(i,r)$ in Eq. (13). These interactions couple spins on the edges of every square whose diagonals have been drawn in Fig. 1.

B. Arrow-vertex representation

In Fig. 1 consider the superlattice formed by the double lines which are the diagonals of every alternate square on the original lattice. This superlattice contains Nm points, which is half the number on the original lattice. Each superlattice point is connected to four spins through bonds. We now place arrows on these bonds, and prescribe the rules which determine their directions in terms of the spin configuration. The rules are if the spin at a corner is pointing up (down), the arrow on the bond through that corner runs north (south) -east or north (south) -west.

These rules lead to continuous arrows on superlattice bonds. The specification of a particular spin configuration on the original lattice uniquely determines the arrow configuration on the superlattice, and vice versa. We illustrate the application of the rules in Fig. 2, where a typical spin configuration and the corresponding arrow configuration are shown.

As only 8 of the 16 matrix elements in Eq. (14) are nonzero, only 8 of the 16 possible configurations of arrows are allowed at a given superlattice vertex. These allowed configurations are shown in Fig. 3. The Boltzmann weight associated with a given lattice configuration is the product of weights associated with each vertex. The allowed vertices (Fig. 3) have weights

$$\begin{aligned}
&\omega_1=\omega_2\equiv a=e^{K_0}\cosh K_- \ ,\\
&\omega_3=\omega_4\equiv b=e^{-K_0}\sinh K_+ \ ,\\
&\omega_5=\omega_6\equiv c=e^{-K_0}\cosh K_+ \ ,\\
&\omega_7=\omega_8\equiv d=e^{K_0}\sinh K_- \ ,
\end{aligned} \tag{18}$$

where

$$K_0=\beta J_z/4m \tag{19}$$

and K_+ and K_- were defined in Eq. (16). Vertices not shown in Fig. 3 have zero weight. The partition function is

$$Z^{(m)}=\sum_{\substack{\text{arrow}\\ \text{configurations}}}\ \prod_{\substack{\text{vertices}\\ \nu}}\omega_\nu \ . \tag{20}$$

This is the partition function of the eight-vertex model defined on the superlattice (Fig. 1), with weights given by Eq. (18).

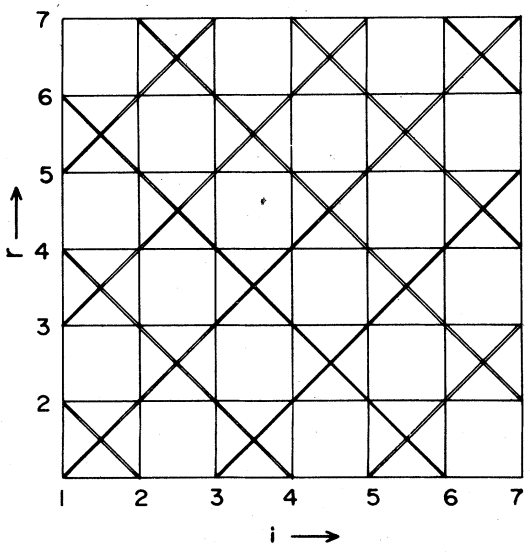

FIG. 1. 2D lattice on which the equivalent classical problem is defined is shown. i labels sites on the original 1D lattice and r is a label along the Trotter direction. Arrows are drawn on the diagonals.

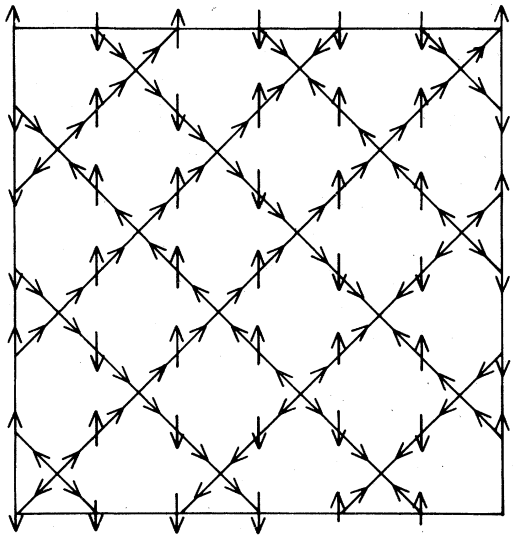

FIG. 2. Typical spin configuration and the corresponding arrow configuration are shown.

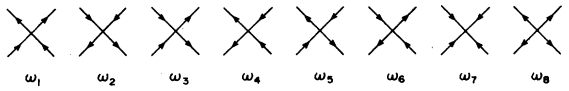

FIG. 3. The eight allowed vertices are shown with their weights.

Denoting the free energy per spin of the XYZ system by f, we have

$$f=-\beta^{-1}\lim_{\substack{m\to\infty\\N\to\infty}}(1/N)\ln Z^{(m)} \quad . \tag{21}$$

The free energy per vertex of the eight-vertex model is

$$f_8^{(N,m)}=-\beta^{-1}(1/Nm)\ln Z^{(m)} \tag{22}$$

and so

$$f=\lim_{\substack{m\to\infty\\N\to\infty}} m f_8^{(N,m)} \quad . \tag{23}$$

This establishes the equivalence between the finite temperature properties of the XYZ system and the properties of an eight-vertex model. The latter has two unfamiliar features on which we comment briefly.

(a) The vertex weights depend on m, which is proportional to the length of one of the sides of the 2D lattice. This dependence has the consequence that some familiar simplifications which usually occur in the thermodynamic limit may not go through, e.g., dropping all eigenvalues of the transfer matrix other than the largest is no longer justified. This is illustrated by means of a simple example in Appendix A.

(b) The superlattice of Fig. 1 has $\frac{1}{2}N+m$ rows and as many columns, but only Nm lattice points, as most rows and columns are truncated. However, when N and m are large, we expect the thermodynamic properties of this system to be the same as that of a rectangular eight-vertex model with m rows and N columns.

In Sec. III we turn to the limit $T\to 0$ °K, and recover Baxter's result for E_G.

III. ZERO-TEMPERATURE LIMIT FOR THE XYZ MODEL

Let us define

$$t=e^{-\beta f_8^{(N,m)}} \tag{24}$$

and

$$u=-\tfrac{1}{4}\beta J_z \quad , \tag{25}$$

where we have chosen $J_z<0$. Then the zero-temperature limit is obtained by letting $u\to\infty$. The ground-state energy per spin is

$$E_G=\tfrac{1}{4}J_z\lim_{\epsilon\to 0}\lim_{u\to\infty}\lim_{N\to\infty}\lim_{m\to\infty}(\ln t/\epsilon) \tag{26}$$

where

$$\epsilon=u/m \quad . \tag{27}$$

As discussed in Appendix B, we must take the limit $m\to\infty$ before $u\to\infty$, thereby implying $\epsilon\to 0$. Otherwise, we get a lower bound on E_G rather than E_G. In the limit $\epsilon\to 0$, t behaves like $1+O(\epsilon)$, and so Eq. (26) can be rewritten as

$$E_G=\tfrac{1}{4}J_z\lim_{u\to\infty}\frac{d}{d\epsilon}\lim_{\substack{m\to\infty\\N\to\infty}}\ln t \quad . \tag{28}$$

We now need to substitute for t, the eight-vertex model partition function. As discussed towards the end of Sec. II, it is not valid at all temperatures to use only the largest eigenvalue of the transfer matrix to find t. However, as illustrated by the example of Appendix A, in the limit of zero temperature the largest eigenvalue may suffice to give the ground-state energy correctly. Thus in order to find E_G we will use Baxter's solution[7] (Baxter I) for t, (which was derived from the largest eigenvalue of the transfer matrix).

We will use Baxter's notation in much of what follows. Expanding the vertex weights in Eq. (18) to lowest order in ϵ, we have

$$a=1-\epsilon,\quad b=-\epsilon\left(\frac{J_x+J_y}{J_z}\right)$$

and (29)

$$c=1+\epsilon,\quad d=\epsilon\left(\frac{J_y-J_x}{J_z}\right) \quad .$$

Using Eqs. (2.5), (7.3), (7.4) and (7.5) of Baxter I, we find to $O(\epsilon)$:

$$l^2=\frac{J_z^2-J_y^2}{J_z^2-J_x^2}+O(\epsilon) \quad , \tag{30}$$

$$\mathrm{sn}^2\zeta=\frac{J_z-J_x}{J_z+J_y}\left[1+\epsilon\left(\frac{J_y+J_x}{J_z}\right)\right] \quad , \tag{31}$$

$$\mathrm{sn}^2 V=\frac{J_z-J_x}{J_z+J_y}\left[1-3\epsilon\left(\frac{J_y+J_x}{J_z}\right)\right] \quad . \tag{32}$$

The three parameters l, ζ, and V characterize the three independent ratios that can be formed from the weights in Eq. (29). In the limit $\epsilon=0$ we can use the doubling formulas for Jacobian elliptic functions and get

$$\mathrm{cn}2\zeta:\mathrm{dn}2\zeta:1=J_x:J_y:J_z \quad . \tag{33}$$

Thus, in the limit $\epsilon=0$, Eqs. (30) and (33) are the same as Eqs. (4.2) and (3.10) of Baxter's second paper[6] (Baxter II), so we have the same parametrization.

Now Baxter's solution[7] [Eqs. (7.7) and (7.8) of Baxter I] is

$$\ln t = \ln c + 2\sum_{n=1}^{\infty} \frac{\sinh^2(\tau-\lambda)n}{n\sinh(2n\tau)\cosh(n\lambda)} \times [\cosh(n\lambda)-\cosh(n\alpha)] \ , \quad (34)$$

where

$$\tau = \pi K_l/K_{l'}, \quad \lambda = \pi\zeta/K_{l'}, \quad \alpha = \pi V/K_{l'} \ . \quad (35)$$

Here $l' = (1-l^2)^{1/2}$ and K_l is a complete elliptic integral of modulus l. As $\epsilon \to 0$, ζ approaches V [Eqs. (31) and (32)], so we need differentiate only the term in braces in the sum in Eq. (34). Using

$$\frac{d}{d\epsilon}[\cosh(n\lambda)-\cosh(n\alpha)]|_{\epsilon=0} = \frac{n\pi\sinh n\lambda}{2K_{l'}\mathrm{sn}\zeta\,\mathrm{cn}\zeta\,\mathrm{dn}\zeta}\frac{d}{d\epsilon}[\mathrm{sn}^2\zeta-\mathrm{sn}^2 V] \ , \quad (36)$$

we find

$$E_G = \frac{J_z}{4} + \frac{J_z\pi\,\mathrm{sn}2\zeta}{K_{l'}} \times \sum_{n=1}^{\infty}\frac{\sinh^2(\tau-\lambda)n}{\sinh 2n\tau}\tanh n\lambda \ . \quad (37)$$

We have recovered Baxter's result for E_G, as Eq. (37) agrees with Eq. (4.6) of Baxter II.

The behavior of E_G has been discussed in Baxter II, where it has been shown that E_G reduces to the previously known ground-state energy in various special cases. In Appendix C here, we discuss the derivation of E_G for the XY chain without going through this route; in the XY case, the vertex weights obey the free-fermion condition of Fan and Wu,[8] and we are able to use their solution to find E_G.

IV. SYSTEMS WITH TWO SPECIES OF VARIABLES

In this section we consider the classical problems equivalent to two 1D quantum models, each of which involves more than one type of variable. We then find that we can trace over half the variables in the equivalent classical problems though this could not have been done directly in the quantum problems.

A. Coupled electronic-spin–nuclear-spin Hamiltonian

The hyperfine coupling of nuclear spins to exchange-coupled electronic spins is known to have interesting consequences, e.g., indirect coupling between nuclear spins.[15] The partition function of such a system involves a trace over both electronic and nuclear spins. The latter trace can be carried out explicitly if (a) both electronic and nuclear spins involve only Ising interactions[16] and (b) the electronic spins are classical, though not necessarily the nuclear spins.[17] Here we consider a model in which the nuclear trace cannot be carried out so straightforwardly. We take

$$\mathcal{H}_{SI} = \mathcal{H}_S - A\sum_i I_i^z S_i^z \ , \quad (38)$$

where the I_i are nuclear spins, the S_i are electronic spins and $\mathcal{H}_S$, which involves only S_i's, does not commute with the second term. To fix ideas, suppose that $\mathcal{H}_S$ is the XYZ Hamiltonian of Eq. (2). Then the equivalent classical problem can be constructed following the method used in Sec. II. We have

$$Z^{(m)} = \sum_{\substack{\alpha_1\alpha_2\cdots\alpha_{2m}\\ \gamma_1\gamma_2\cdots\gamma_{2m}}} \langle\alpha_1\gamma_1|e^{-\beta\mathcal{H}_0'/2m}e^{-\beta V_A/m}|\alpha_2\gamma_2\rangle\langle\alpha_2\gamma_2|e^{-\beta\mathcal{H}_0'/2m}e^{-\beta V_B/m}|\alpha_3\gamma_3\rangle\cdots\langle\alpha_{2m}\gamma_{2m}|e^{-\beta\mathcal{H}_0'/2m}e^{-\beta V_B/m}|\alpha_1\gamma_1\rangle \ , \quad (39)$$

where

$$\mathcal{H}_0' = \mathcal{H}_0 - A\sum_i I_i^z S_i^z \quad (40)$$

and $\mathcal{H}_0$, V_A, and V_B were defined in Eqs. (3)–(5). Here $|\alpha_r\gamma_r\rangle$ stands for an electron-spin–nuclear-spin direct product state in the Ising basis. As the hyperfine coupling is diagonal in this basis and $\mathcal{H}_S$ does not involve any I_i's, the states $|\gamma_r\rangle$ must be the same for all r. Thus we have

$$Z = \sum_{\alpha_1\alpha_2\cdots\alpha_{2m}}\sum_{\gamma}\left(\exp\frac{\beta A}{2m}\sum_i I_i^z\sum_r S_{ir}\right)e^{-\beta\mathcal{H}_S^{eq}} \ . \quad (41)$$

Here $\mathcal{H}_S^{eq}$ is the classical Hamiltonain equivalent to $\mathcal{H}_S$ alone. The nuclear trace in Eq. (41) can now be done. Assuming that $I_i^z = \pm\frac{1}{2}$, we find

$$Z = \sum_{\alpha_1\alpha_2\cdots\alpha_{2m}}\left[\prod_{i-1}^{N}2\cosh\left(\frac{\beta A}{4m}\sum_{r=1}^{2m}S_{ir}\right)\right]e^{-\beta\mathcal{H}_S^{eq}} \ . \quad (42)$$

The term in square brackets can be exponentiated to give the total effective Hamiltonian

$$\mathcal{H}_{SI}^{eq}=\mathcal{H}_{S}^{eq}-\frac{1}{\beta}\sum_{i}\ln\left[2\cosh\left(\frac{\beta A}{4m}\sum_{r=1}^{2m}S_{ir}\right)\right] . \quad (43)$$

Note that $\mathcal{H}_{SI}^{eq}$ involves only electronic spins, with a coupling between all spins in the Trotter direction.

B. Falicov-Kimball model

The Falicov-Kimball model[18] involves interactions between electrons in two bands. In 1D the Hamiltonian is

$$\mathcal{H}_{\rm FK}=\mathcal{H}_{d}+\mathcal{H}_{fd} , \quad (44)$$

where

$$\mathcal{H}_{d}=t\sum_{i,\sigma}(d_{i\sigma}^{\dagger}d_{i+1\sigma}+\text{H.c.})-\mu\sum_{i\sigma}n_{di\sigma}+U_{dd}\sum_{i}n_{di\uparrow}n_{di\downarrow} \quad (45)$$

and

$$\mathcal{H}_{fd}=U_{ff}\sum_{i}n_{fi\uparrow}n_{fi\downarrow}+U_{fd}\sum_{i\sigma\sigma'}n_{fi\sigma}n_{di\sigma'}-\mu\sum_{i\sigma}n_{fi\sigma} \quad (46)$$

Here f and d label the two bands, i refers to sites on a lattice and σ is a spin label. The n's are electron occupation numbers, and $d_{i\sigma}^{\dagger}$ creates a d electron of spin σ at site i. t is the d-electron hopping matrix element, U_{dd}, U_{ff}, and U_{fd} are intrasite Coulomb interaction energies, and μ is the chemical potential. $\mathcal{H}_{d}$ is just the 1D Hubbard model, and we have shown in detail how the classical problem equivalent to it can be constructed.[12] $\mathcal{H}_{\rm FK}$ is thought to show diverse interesting behavior (e.g., metal-insulator transitions, exciton formulation[18,19]). Here we show that by going to the equivalent 2D system we can completely trace over the f degrees of freedom. Following the procedure used in Sec. IV A, we arrive at the analog of Eq. (41):

$$Z^{(m)}=\sum_{\alpha_1\alpha_2\cdots\alpha_{2m}}\sum_{\gamma}\exp\left(-\beta U_{ff}\sum_{i}n_{fi\uparrow}n_{fi\downarrow}+\beta\mu\sum_{i\sigma}n_{fi\sigma}-\frac{\beta U_{fd}}{2m}\sum_{i\sigma\sigma'}n_{fi\sigma}\sum_{r}n_{dir\sigma'}\right)e^{-\beta\mathcal{H}_{d}^{eq}} . \quad (47)$$

Here α_r is specified by giving all d-electron occupation numbers, and γ by giving the f-electron occupations. The sum over γ can be done, with the result

$$Z^{(m)}=\sum_{\alpha_1\alpha_2\cdots\alpha_{2m}}\left[\prod_{i=1}^{N}(1+2e^{\beta\mu-\beta U_{fd}\mathfrak{N}_{di}}+e^{-\beta(U_{ff}-2\mu)-2\beta U_{fd}\mathfrak{N}_{di}})\right]e^{-\beta\mathcal{H}_{d}^{eq}} , \quad (48)$$

where

$$\mathfrak{N}_{di}=\frac{1}{2m}\sum_{\sigma,r=1}^{2m}n_{dir\sigma} \quad (49)$$

and $\mathcal{H}_{d}^{eq}$ is the classical Hamiltonian equivalent to $\mathcal{H}_{d}$. The partition function now involves only the d electron degrees of freedom, and can be written as a trace over an effective Hamiltonian involving only the d electrons, as was done for the electronic spins in Sec. IV A.

V. DISCUSSION

A. Results

One of the main aims of this work was to cast the problem of obtaining the free energy of the XYZ linear chain into a classical 2D problem. This was fulfilled in Sec. II where we saw that the classical problem was the eight-vertex model. Baxter's solution of the eight-vertex model[7] (obtained by finding the largest eigenvalue of the transfer matrix) suffices to find the ground-state energy, but not the free energy of the XYZ system. The reason for this (as indicated by the simple example in Appendix A) is the fact that the coupling constants in the classical problem depend on m, the extent of the lattice in the Trotter direction. Our derivation of the ground-state energy provides a useful alternative to Baxter's[6] and does not need to make an assumption regarding the symmetry of the eigenvector. In order to get the free energy of the XYZ Hamiltonian, one needs a "complete solution" for the eight-vertex problem—in terms of the transfer matrix, one needs *all* eigenvalues.

In Sec. IV we saw how the general method of constructing classical equivalences could be used when there was more than one species of variable in the 1D problem. In the two examples considered, we saw that one set of variables could be completely traced over in the equivalent classical problem, leaving an effective Hamiltonian involving only electronic spins (in the coupled electronic-spin—nuclear-spin case) and only d electrons (in the 1D Falicov-Kimball model). The result of doing the nuclear-spin or f-electron trace was to introduce many-site interactions in the Trotter direction.

B. Other decompositions and generalization to higher dimensions

The classical problem one obtains depends not only on the quantum problem one starts with, but also on

the method of decomposing the Hamiltonian before applying Trotter's formula. The decomposition should be such that the appropriate matrix elements can be evaluated, preferably with the insertion of as few complete sets of states as possible. (This number was $2m$ in our decomposition.) Other decompositions exist, but often require the insertion of many more complete sets of states. For instance, in the decomposition used in Eq. (5.10) in Ref. 11 for the XYZ Hamiltonian

$$\begin{aligned} &\mathcal{H} = \mathcal{H}_x + \mathcal{H}_y + \mathcal{H}_z, \\ &\mathcal{H}_x = -\sum_{i=1}^{N} J_x S_i^x S_{i+1}^x \ , \end{aligned} \tag{50}$$

etc., one needs to introduce Nm states [otherwise matrix elements like Eq. (5.13) in Ref. 11, viz.,

$$\langle \alpha | \exp\left[\frac{-\beta}{m} \sum_{i=1}^{N} S_i^x S_{i+1}^x\right] | \alpha' \rangle$$

cannot be readily evaluated].

We now discuss the generalizability of our method to higher dimensions than one and to more than nearest-neighbor interactions in 1D. The generalization is straightforward in the case of spin systems, for which operators associated with different sites commute. In the case of fermion systems, operators at different sites anticommute, and a state of the system is specified by the action of certain fermion creation operators on the vacuum, *in a prescribed order*. This ordering becomes important in higher dimensions than one (or in 1D with more than nearest-neighbor coupling). A two-site fermion-hopping matrix element depends not only on the occupation numbers of the two sites in question, but also on the occupation of sites that are in between, in the prescribed ordering of sites. For instance, on a 2-d lattice, suppose all points points are labeled $\{l; l = 1, \ldots N\}$. Then, for the Hubbard model, in the generalization of Eq. (7) of Ref. 12 to 2D, the term $\Delta + \ln \sinh(t/m)$ would be replaced by $\Delta + \ln \sinh(t/m) + i\pi N_{jk\sigma}$, where $N_{jk\sigma} = \sum_{j<l<k} n_{l\sigma}$. Here j,k are nearest neighbors on the actual lattice, and $i\pi N_{jk\sigma}$ accounts for fermion anticommutations. It should be accounted for, but should not lead to additional difficulties in numerical studies of the classical problem (see below).

C. Uses of classical equivalents

Besides providing an alternative means of formulating an important problem (Sec. II) or doing partial traces (Sec. IV), the construction of equivalent classical problems can also provide new ways of looking at old results. For instance, the known equivalence[4] between the XY chain and a Hamiltonian describing free fermions follows since both quantum problems lead to the same classical problem. Another instance is the example of the equivalence of free-fermion and conjugate models[8] discussed in Appendix C and obtained from the equivalence of the XY and YZ models.

A practical use of the classical problem transcription is that one can now use numerical techniques such as Monte Carlo,[11,20] which one could not have used on the original quantum Hamiltonian. Such a procedure obviates the need for diagonalizing the Hamiltonian in order to obtain the thermodynamics.

Numerical studies would perforce be done on lattices with a finite value of m. In this connection we would like to draw attention to an important observation about finite m approximations using the Trotter formula. Any such approximation gives a lower bound on the true free energy, as follows from a theorem due to Golden.[21]

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APPENDIX A

In this appendix we consider the simple example of a single spin in a transverse magnetic field, and construct the classical problem equivalent to it. The Hamiltonian is

$$\mathcal{H} = -hS^x \tag{A1}$$

and it is trivially checked that the ground-state energy and the free energy for the problem are, respectively,

$$E_G = -\tfrac{1}{2}h \tag{A2}$$

and

$$f = -(h/2u)\ln(2\cosh u) \ , \tag{A3}$$

where we have set $u = \frac{1}{2}\beta h$. Since there is one spin, the effective dimensionality of the problem is zero, and one can construct a 1D classical problem equivalent to it. Let us write

$$Z = \lim_{m\to\infty} Z^{(m)} \ , \tag{A4}$$

with

$$Z^{(m)} = \mathrm{tr}(e^{2\epsilon S_x})^m \ , \tag{A5}$$

where $\epsilon = u/m$ and m plays the role of the Trotter integer. Since there are no noncommuting operators, Eq. (A4) would hold even without taking the limit $m \to \infty$. Introducing m complete sets of S^z eigenstates we get

$$Z^{(m)}=\sum_{S_1\cdots S_m}\langle S_1|e^{2\epsilon S^x}|S_2\rangle\,\langle S_2|e^{2\epsilon S^x}|S_3\rangle\cdots\langle S_m|e^{2\epsilon S^x}|S_1\rangle\ , \tag{A6}$$

where

$$S^z|S_r\rangle=S_r|S_r\rangle,\quad S_r=\pm\tfrac{1}{2}\ . \tag{A7}$$

Now

$$\langle S_1|e^{2\epsilon S^x}|S_2\rangle=(\sinh\epsilon\cosh\epsilon)^{1/2}e^{KS_1S_2}\ , \tag{A8}$$

where

$$K=2\ln\coth\epsilon\ . \tag{A9}$$

Thus

$$Z^{(m)}=(\sinh\epsilon\cosh\epsilon)^{m/2}\times\sum_{\{S_r\}}\exp K\sum_{r=1}^{m}S_rS_{r+1}\ . \tag{A10}$$

This is clearly the partition function of a 1D Ising model with periodic boundary conditions. One way to solve this problem is to use a transfer-matrix method.

Let us define the transfer matrix T by

$$\langle S_1|T|S_2\rangle=(\sinh\epsilon\cosh\epsilon)^{1/2}e^{KS_1S_2}\ . \tag{A11}$$

Then

$$T=\begin{pmatrix}\cosh\epsilon & \sinh\epsilon\\ \sinh\epsilon & \cosh\epsilon\end{pmatrix}\ . \tag{A12}$$

Now

$$Z^{(m)}=\mathrm{tr}\,T^m=\lambda_+^m+\lambda_-^m\ , \tag{A13}$$

where

$$\lambda_\pm=e^{\pm\epsilon} \tag{A14}$$

are the eigenvalues of T. Thus the free energy is

$$f^{(m)}=-(h/u)\ln(\lambda_+^m+\lambda_-^m)\ . \tag{A15}$$

This clearly agrees with Eq. (A3). However if we had replaced $\mathrm{tr}\,T^m$ by λ_+^m (as is ordinarily valid in the thermodynamic limit, $m\to\infty$) we would have obtained the wrong answer. The reason that only the largest eigenvalue is not sufficient here is that the coupling constant in the Ising model depends on m, the size of the system. If however, we want only the ground-state energy, the largest eigenvalue suffices, as the omitted term is $O(\lambda_-/\lambda_+)^m$, which vanishes as $T\to 0$.

APPENDIX B

In this appendix we discuss the consequence of taking the $\beta\to\infty$ and $m\to\infty$ limits in the wrong order. For a Hamiltonian $\mathcal{H}$ which is the sum of two parts

$$\mathcal{H}=\mathcal{H}_1+\mathcal{H}_2 \tag{B1}$$

the free energy can be written

$$f=\frac{-\bar{E}}{u}\lim_{m\to\infty}\ln\mathrm{tr}(e^{-u\mathcal{H}_1/m\bar{E}}e^{-u\mathcal{H}_2/m\bar{E}})^m\ . \tag{B2}$$

We have used Trotter's formula [Eq. (1)] and set $\beta=u/\bar{E}$, where $\bar{E}$ is some characteristic energy of the problem. Since the ground-state energy E_G is $\lim_{u\to\infty}f$, it is clear that the limit $u\to\infty$ must be taken after the limit $m\to\infty$ has been taken.

Below we show that if the reverse (incorrect) order is followed, we get a lower bound on E_G rather than its true value. We have

$$e^{-\epsilon\mathcal{H}_i/\bar{E}}\xrightarrow[\epsilon\to\infty]{}|\Phi_i\rangle e^{-\epsilon E_i^0/\bar{E}}\langle\Phi_i|\ , \tag{B3}$$

where $i=1,2$ and $|\Phi_i\rangle$ and E_i^0 are, respectively, the ground state and ground-state energy of $\mathcal{H}_i$ and $\epsilon=u/m$. Substituting Eq. (B3) into the right-hand side of Eq. (B2), we obtain

$$-\lim_{\epsilon\to\infty}\frac{1}{\epsilon m}\ln[|\langle\Phi_1|\Phi_2\rangle|^{2m}e^{-\epsilon m(E_1^0+E_2^0)/\bar{E}}] \tag{B4}$$

$$=(E_1^0+E_2^0)/\bar{E}\ . \tag{B5}$$

This is clearly a lower bound on $E_G/\bar{E}$.

APPENDIX C

Here we obtain the ground-state energy of the XY model. The Hamiltonian is obtained by setting $J_z=0$ in Eq. (2) and we put $J_x=J$, $J_y=\gamma J$, and $\beta=u/J$. Then the eight-vertex model weights are [from Eq. (20)]

$$a=\cosh\tfrac{1}{4}\epsilon(1-\gamma),\quad b=\sinh\tfrac{1}{4}\epsilon(1+\gamma)\ ,$$
$$c=\cosh\tfrac{1}{4}\epsilon(1+\gamma),\quad d=\sinh\tfrac{1}{4}\epsilon(1-\gamma)\ , \tag{C1}$$

where $\epsilon=u/m$. These weights obey the "free fermion" condition of Fan and Wu,[8] viz., $a^2+b^2=c^2+d^2$. The ground-state energy is

$$E_G/J=-\lim_{u\to\infty;N\to\infty;m\to\infty}\left(\frac{d}{d\epsilon}\ln t\right)_{\epsilon=0} \tag{C2}$$

and we can use the free-fermion solution of Fan and Wu to write

$$\ln t=\frac{1}{2}\int_0^{2\pi}\int_0^{2\pi}\frac{d\theta}{2\pi}\frac{d\phi}{2\pi}\ln(2a'+2d_+\cos\theta\cos\phi+2d_-\sin\theta\sin\phi)\ , \tag{C3}$$

where

$$a' = a^2 + b^2 \ ,$$
$$d_+ = \sinh^2 \tfrac{1}{4}\epsilon(1+\gamma) - \cosh^2 \tfrac{1}{4}\epsilon(1-\gamma) \qquad \text{(C4)}$$
$$d_- = \cosh^2 \tfrac{1}{4}\epsilon(1+\gamma) - \sinh^2 \tfrac{1}{4}\epsilon(1-\gamma)$$

Doing the θ integral in Eq. (C3) we get

$$\frac{E_G}{J} = -\frac{1}{2}\frac{d}{d\epsilon} \times \int_0^{2\pi} \frac{d\phi}{2\pi} \ln[1 + 2\epsilon(1+\gamma^2+2\gamma\cos 2\phi)^{1/2}] \ , \qquad \text{(C5)}$$

where we have retained terms to $O(\epsilon)$ in (C5). Carrying out the differentiation we find

$$\frac{E_G}{J} = -\frac{(1+\gamma)}{2\pi} E\left(\frac{2\sqrt{\gamma}}{1+\gamma}\right) \ , \qquad \text{(C6)}$$

where

$$E(k) = \int_0^{\pi/2} d\phi (1 - k^2 \sin^2\phi)^{1/2} \ . \qquad \text{(C7)}$$

It is interesting to note that if we consider the YZ model in place of the XY model, we obtain a "conjugate model" rather than the free-fermion model. Thus the invariance properties of the Hamiltonian (2) leads to the (known) equivalence[8] of the free-fermion and conjugate models, in this way of looking at these models.

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