PHYSICAL REVIEW

LETTERS

VOLUME 66 18 MARCH 1991 Number 11

Interacting-Electron Model Exactly Solvable in Any Dimension

Arianna Montorsi and Mario Rasetti

Dipartimento di Fisica and Unitá Istituto Nazíonale di Fisica della Materia, Politecnico di Torino, 10129 Torino, Italy (Received 6 August 1990; revised manuscript received 17 January 1991)

When processes not conserving the double occupation number are inhibited, one obtains a model like the Kivelson-Schrieffer-Su-Heeger extension of the Hubbard model. We solve this model exactly in any number of dimensions. The system free energy is given for any fixed filling. The ground-state energy and double-occupancy order parameter are discussed for d=2.

PACS numbers: 05.30.Fk, 71.10.+x

The extension of the Hubbard model proposed by Kivelson, Schrieffer, Su, and Heeger¹ (KSSH) includes, besides an extra diagonal term designed to account for Coulomb interaction between nearest-neighbor sites (which in the sequel we shall neglect), an off-diagonal part intended to represent bond-charge repulsion interactions.^{2,3} In the present Letter we consider a further generalization of that model, assuming spin-dependent hopping amplitudes, given by

$$H = \sum_{\mathbf{i},\sigma} \varepsilon n_{\mathbf{i},\sigma} + U \sum_{\mathbf{i}} n_{\mathbf{i},\uparrow} n_{\mathbf{i},\downarrow} + \frac{1}{2} \sum_{\langle \mathbf{i},\mathbf{j} \rangle} \sum_{\sigma,\sigma'} t^{(\sigma,\sigma')} (a_{\mathbf{i},\sigma}^{\dagger} a_{\mathbf{j},\sigma'} + a_{\mathbf{j},\sigma'}^{\dagger} a_{\mathbf{i},\sigma}) - \frac{1}{2} \sum_{\langle \mathbf{i},\mathbf{j} \rangle} \sum_{\sigma,\sigma'} \Delta t^{(\sigma,\sigma')} (a_{\mathbf{i},\sigma}^{\dagger} a_{\mathbf{j},\sigma'} + a_{\mathbf{j},\sigma'}^{\dagger} a_{\mathbf{i},\sigma}) (n_{\mathbf{i},-\sigma} + n_{\mathbf{j},-\sigma'}) , \quad (1)$$

where the last factor represents just the bond-charge repulsion term characteristic of the KSSH model. The extra terms in (1) describing spin-flip (spin-nonconserving) hopping processes can be thought of as due to spin-orbit coupling. As customary, $a_{\mathbf{i},\sigma}^{\dagger}, a_{\mathbf{i},\sigma}$ are fermionic creation and annihilation $\{a_{\mathbf{i},\sigma},a_{\mathbf{j},\sigma}\}=0, \{a_{\mathbf{i},\sigma}^{\dagger},a_{\mathbf{j},\sigma}\}=\delta_{\mathbf{i},\mathbf{j}}\delta_{\sigma,\sigma'}\mathbf{1}, n_{\mathbf{i},\sigma}=a_{\mathbf{i},\sigma}^{\dagger}a_{\mathbf{i},\sigma}\}$ over a d-dimensional lattice $\Lambda^{(d)}$ ($\mathbf{i},\mathbf{j}\in\Lambda^{(d)}$, $\sigma\in\{\uparrow,\downarrow\}$), whereas the parameters ε , U, t, and Δt have the usual meaning, and $\langle\mathbf{i},\mathbf{j}\rangle$ stands, as customary, for nearest neighbors (nn) in $\Lambda^{(d)}$. For simplicity we assume initially $\Lambda^{(d)}$ to be simple d cubic.

As we intend to study the statistical mechanical properties of the itinerant-electron model defined by (1), in particular the equilibrium features it exhibits in the thermodynamic limit, we shall consider hereafter, instead of H, the effective Hamiltonian $\mathcal{H} = H - \mu N_e$ —where μ denotes the chemical potential, and $N_e = \sum_i n_{i,\uparrow} + n_{i,\downarrow}$ the total electron number operator—which is required in the grand-canonical ensemble scheme. \mathcal{H} has, of course, the same form as H, with ε replaced by $\omega = \varepsilon - \mu$.

Contrary to the Hubbard Hamiltonian, the Hamiltonian (1) assigns different amplitudes to the hopping processes, depending on the relative site occupation. In particular, one can check from (1) how the closer Δt is to t, the more the hopping processes between two singly occu-

pied sites and a doubly occupied and an empty site are inhibited.

We factorize $\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1$, where \mathcal{H}_1 includes all the hopping nondiagonal terms, whereas \mathcal{H}_0 is diagonal, as it depends only on the occupation numbers $n_{i,\sigma}$. In the particular case when $t^{(\sigma,\sigma')} \equiv \Delta t^{(\sigma,\sigma')}$, $[\mathcal{H}_0,\mathcal{H}_1] = 0$, obviously implying that both the number of electrons N_e and the number of doubly occupied sites $\sum_i n_{i,\uparrow} n_{i,\downarrow}$ are conserved quantities. In this case we shall solve exactly the model defined by (1) in any number of dimensions d, and with $t^{(\sigma,\sigma)} \equiv t^{(\sigma,-\sigma)} = t$. We expect that if the latter condition were replaced by $t^{(\sigma,-\sigma)} = 0$ (i.e., spin conservation, no spin-flip processes allowed) the combinatorial structure of the model, even though much more complicated, should still lend itself to being exactly solved. This case has been studied for d=1 in Ref. 5.

The condition of commutativity of \mathcal{H}_0 and \mathcal{H}_1 implies equal amplitudes (in absolute value) for the hopping processes from singly occupied to empty sites as for those from doubly occupied to singly occupied sites. Such a constraint can be removed by adding in the bond-charge repulsion term in the Hamiltonian (1) a factor $\eta n_{\mathbf{i}, -\sigma} n_{\mathbf{j}, -\sigma'}$ to $n_{\mathbf{i}, -\sigma} + n_{\mathbf{j}, -\sigma'}$. The latter simply changes the relative amplitude of the allowed hoppings by the arbitrary factor $\eta - 1 = \rho$ without introducing any new pro-

cess, yet preserving the commutativity of \mathcal{H}_0 and \mathcal{H}_1 and the solvability of the model.

On the other hand, the condition $t^{(\sigma,\sigma)} \equiv t^{(\sigma,-\sigma)}$ naturally leads to introducing a new set of local operators,

$$A_{i} = \frac{1}{\sqrt{2}} (a_{i,\uparrow} + a_{i,\downarrow}), \quad N_{i} = A_{i}^{\dagger} A_{i},$$

$$D_{i} = \frac{1}{2} (n_{i,\uparrow} + n_{i,\downarrow} + a_{i,\uparrow} a_{i,\downarrow}^{\dagger} + a_{i,\downarrow} a_{i,\uparrow}^{\dagger}),$$
(2)

such that $n_{i,\uparrow} + n_{i,\downarrow} = N_i + D_i$ and $n_{i,\uparrow} n_{i,\downarrow} = D_i N_i \ \forall \ i \in \Lambda$, and in terms of which the Hamiltonian \mathcal{H} can be easily rewritten as

$$\mathcal{H} = \sum_{i} \omega(N_{i} + D_{i}) + t \sum_{\langle i,j \rangle} \kappa_{i,j} (A_{i}^{\dagger} A_{j} + A_{j}^{\dagger} A_{i})$$
$$+ U \sum_{i} N_{i} D_{i}, \qquad (3)$$

where $\kappa_{i,j} \equiv 1 - D_i - D_j + \eta D_i D_j$. With the particular choice $\omega = 0 = U$, a similar model has been dealt with, e.g., in Ref. 6.

The spinless operators A_i , A_i^{\dagger} , N_i satisfy the usual fermionic commutation relations,

$${A_{i,A_{j}}} = 0, {A_{i,A_{j}}} = \delta_{i,j}1, [A_{j},N_{i}] = A_{i}\delta_{i,j}, (4)$$

and generate the $(N+1)^2$ -dimensional (N denoting the

total number of sites in Λ) \mathbb{Z}_2 -graded algebra

$$\mathcal{A} = \langle N_{\mathbf{i}}, A_{\mathbf{i}}, A_{\mathbf{i}}^{\dagger}, A_{\mathbf{i}}^{\dagger} A_{\mathbf{j}}, 1 | \mathbf{i}, \mathbf{j} \in \Lambda, \mathbf{i} \neq \mathbf{j} \rangle \sim u(\mathcal{N}|1).$$

Moreover, the D_i 's are idempotent operators $(D_iD_i = D_i)$, commuting with all the elements of \mathcal{A} . The latter property not only allows us to deal with the operators D_i as with classical *Ising*-like dynamical variables, but leads to recognizing that the model defined by (3) has a dynamical algebra \mathcal{L} which is the direct sum of $2^{\mathcal{N}}$ copies of \mathcal{A} , each copy \mathcal{A}_{α} corresponding to a given distribution α of eigenvalues $s_i \in \{0,1\}$ of the D_i 's.

The statistical mechanical solution of the model is based, of course, on the evaluation of the grand-canonical partition function $Z_N = \text{Tr}_{\mathcal{L}}\{e^{-\beta\mathcal{H}}\}$ = $\text{Tr}_{\mathcal{L}}\{e^{-\beta\mathcal{H}}\}e^{-\beta\mathcal{H}}\}$, where $\beta = 1/k_BT$.

Because of the above algebraic structure, the trace over \mathcal{L} , Tr, reduces to

$$\operatorname{Tr}_{\mathcal{L}} \equiv \sum_{\{a\}} \operatorname{tr}_{\mathcal{A}_a} \left[\sum_{\{a\}} \equiv \sum_{\{s_i\}} \right].$$
 (5)

The central problem is therefore to evaluate $\operatorname{tr}_{\mathcal{A}_a}$, namely, the trace over the α th copy of \mathcal{A} . In order to tackle such a problem, we refer the Hilbert space of states to the Fock basis $|\psi_k\rangle = \bigotimes_i |v_i\rangle$, $k = 1, \ldots, 2^{\mathcal{N}}$, where $|v_i\rangle$ denotes the eigenvector of the operator N_i : $N_i |v_i\rangle = v_i |v_i\rangle$, $v_i \in \{0,1\}$.

In the above basis,

$$\operatorname{tr}_{\mathcal{A}_{a}}\left\{e^{-\beta\mathcal{H}_{a}}\right\} = \sum_{\{v_{i}\}} \exp\left\{\sum_{i} \left[\left(\omega + Us_{i}\right)v_{i} + \omega s_{i}\right]\right\} \left\langle\psi_{k}\left|e^{-\beta\mathcal{H}_{i}^{(a)}}\right|\psi_{k}\right\rangle,\tag{6}$$

where the index α in \mathcal{H} and \mathcal{H}_1 is meant to keep track of the particular set of values of the s_i 's, labeled just by α , they refer to.

The matrix elements entering (6) can be expanded as a power series in the variable $\tau = -2\beta t$,

$$\langle \psi_{k} | e^{-\beta \mathcal{H}_{1}^{(a)}} | \psi_{k} \rangle = \sum_{l=0}^{\infty} \frac{\tau^{2l}}{(2l)!} \langle \psi_{k} | \left\{ \sum_{\langle i,j \rangle} \kappa_{i,j} A_{i}^{\dagger} A_{j} \right\}^{2l} | \psi_{k} \rangle = 1 + \sum_{l=1}^{\infty} \frac{\tau^{2l}}{(2l)!} \sum_{\{\lambda_{i}\}} \Theta_{\lambda_{i}}(\{s_{i}\}) \Xi_{\lambda_{i}}(\{v_{i}\}) . \tag{7}$$

Here $\{\lambda_l\}$ denotes the collection of all loops in $\Lambda^{(d)}$ with 2l edges (the number of edges is even because $\Lambda^{(d)}$ is cubic). Such loops can be multiply connected, and each edge may possibly cover the same bond in $\Lambda^{(d)}$ more than once. The equivalence between the two series in τ is based on the property that the matrix elements of the lth power of $\mathcal{H}_1^{(a)}$ have nonvanishing contributions only from those factors which are associated with bonds $\langle i,j \rangle$ with nondangling ends. Such contributions are each the product of a term Θ_{λ_l} —originating from the $\kappa_{i,j}$'s, and depending only on the $\{s_i|i\in\lambda_l\}$'s —times a term Ξ_{λ_l} —a diagonal matrix element of a sum of products of an equal number of operators A_i and A_i^{\dagger} along the loop, a function only of the $\{v_i|i\in\lambda_l\}$'s.

It is now convenient to decompose the set $\{\lambda_l\}$ into its disconnected components, the *i*th of which is characterized by the number of edges $2l_i$ and the number of sites touched m_i . We denote the corresponding set by $\{\lambda_{l_i}^{(m_i)}|1 \leq l_i \leq l; 2 \leq m_i \leq L_i\}$ $[L_i \equiv \min(2l_i, \mathcal{N})]$. The sum over $\{\lambda_l\}$ in (7) is then decomposed into

$$\sum_{j=1}^{J_l} \sum_{\{l_i\}} (2l)! \prod_{n=1}^{j} \left[\frac{1}{(2l_n)!} \sum_{m_n=2}^{L_n} \sum_{\{\lambda_{l_n}^{(m_n)}\}} \Theta_{\lambda_{l_n}^{(m_n)}}(\{s_i\}) \Xi_{\lambda_{l_n}^{(m_n)}}(\{v_i\}) \right], \tag{8}$$

where $J_l \equiv \min(l, \frac{1}{2} \mathcal{N})$, and where $\sum_{l=1}^{\infty} denotes$

$$\sum_{l_1 \geq 1} \cdots \sum_{l_i \geq 1} \delta \left[l - \sum_{n=1}^{j} l_n \right].$$

Because of the particular form of $\kappa_{i,j}$, one has

$$\Theta_{\lambda_{l_n}^{(m_n)}}(\{s_i\}) \equiv \prod_{\substack{i=1 \text{mod } m}}^m \kappa_{i,i+1} = \prod_{\substack{i \in \lambda_{l_n}^{(m_n)}}} \delta(s_i,0) + \rho^{2l_n} \prod_{\substack{i \in \lambda_{l_n}^{(m_n)}}} \delta(s_i,1) ,$$
(9)

where i labels the sites of $\lambda_{l_n}^{(m_n)}$ numbered along the loop (so that i+1 is the nn of i). We shall see in the sequel that the

explicit expression of $\Xi_{\lambda_i^{(m_n)}}(\{v_i\})$ is not needed.

Equations (6)-(9) allow us to rewrite Z_N as the sum of two contributions, $Z_N = Z_0 + Z_1$, the first of which —originating from the factor 1 in (7)—has the form

$$Z_0 = \sum_{\{s_i\}} \sum_{\{v_i\}} \exp \left\{ \sum_{i \in \Lambda^{(d)}} \left[(\omega + Us_i) v_i + \omega s_i \right] \right\} = \left[1 + 2e^{-\beta \omega} + e^{-\beta (U + 2\omega)} \right]^{\mathcal{N}} \equiv z_0^{\mathcal{N}},$$
(10)

whereas the second, containing the remaining part of the series, upon inserting the explicit expression (9) for $\Theta_{\lambda_{l_n}^{(m_n)}}(\{s_i\})$ and performing the configuration sums over $\{s_i\}$ and $\{v_i|i \notin \lambda_{l_n}^{(m_n)}\}$, turns out to be

$$Z_{1} = Z_{0} \sum_{l=1}^{\infty} \tau^{2l} \sum_{j=1}^{J_{l}} \sum_{\{l_{j}\}}^{J_{l}} \prod_{n=1}^{j} \left[\mathcal{Q}_{l_{n}}^{(n)}(\omega, z_{0}) + \rho^{2l_{n}} \mathcal{Q}_{l_{n}}^{(n)}(\omega + U, e^{\beta \omega} z_{0}) \right], \tag{11}$$

$$Q_{l_n}^{(n)}(\Omega,\xi_0) = \frac{1}{(2l_n)!} \sum_{m_n=2}^{L_n} \xi_0^{-m_n} \sum_{\substack{\{\nu_i\}\\i \in \lambda_l^{(m_n)}\}}} \sum_{\substack{\{\nu_i\}\\i \in \lambda_l^{(m_n)}}} \Xi_{\lambda_{l_n}^{(m_n)}}(\{\nu_i\}) \prod_i e^{-\beta \Omega \nu_i}.$$
(12)

Equation (12) can be evaluated globally, by comparing the solution to an associated pure tight-binding model obtained by the same procedure adopted above with the conventional solution derived by transforming to wave-vector space.⁷

Let us recall that a pure spinless tight-binding model can be characterized by the Hamiltonian
$$H_{TB} = \omega \sum_{i} N_{i} + t \sum_{\langle i,j \rangle} (A_{i}^{\dagger} A_{j} + A_{j}^{\dagger} A_{i}). \tag{13}$$

Repeating the whole derivation which led from (3) to (11), one obtains the partition function

$$Z_{TB} = \tilde{z}_0^{\mathcal{N}} \left\{ 1 + \sum_{l=1}^{\infty} \tau^{2l} \sum_{j=1}^{J_l} \sum_{\{l_j\}}' \prod_{n=1}^{j} \mathcal{Q}_{l_n}^{(n)}(\omega, \tilde{z}_0) \right\}, \tag{14}$$

where $\tilde{z}_0 \equiv 1 + e^{-\beta \omega}$

On the other hand, the model (13) can be exactly solved in a standard way for any number of dimensions d, as H_{TB} is diagonal in the wave-vector space. One finds in this manner for Z_{TB} an expression formally identical with (14), in

$$\prod_{n=1}^{j} \mathcal{Q}_{l_{n}}^{(n)}(\omega, \tilde{z}_{0}) = \frac{1}{j!} \left[\frac{2e^{-\beta\omega}}{\tilde{z}_{0}^{2}} \right]^{j} \sum_{\mathbf{k}^{(1)}, \dots, \mathbf{k}^{(j)}} \prod_{n=1}^{j} \left[\frac{1}{(2l_{n})!} [\varphi(\mathbf{k}^{(n)})]^{2l_{n}} \right].$$
(15)

In (15), $\mathbf{k} = \{k_1, \dots, k_d\}$ is a vector in reciprocal space, ranging over a half of the first *Brillouin zone*, \mathcal{D} , the double prime in $\sum_{k=0}^{n} \mathbf{k}^{(n)}$ is to remind us of the requirement that each term in the sum must have all indices $\mathbf{k}^{(n)}$, $n=1,\ldots,m$, different from each other, and $\varphi(\mathbf{k}) = 2\sum_{r=1}^{\bar{d}} \cos(k_r)$.

Equation (15) must hold for every j, and provides both the functional form

$$Q_{l_n}^{(n)}(\Omega, \xi_0) = 2 \frac{e^{-\beta \Omega}}{\xi_0^2} \frac{Q_{l_n}^{(n)}}{n}$$

and the recursive equations for the $Q_{l_n}^{(n)}$'s.

Insertion of the solutions for the latter in (11) leads then, after some manipulations, to

$$Z_{1} = Z_{0} \sum_{l=1}^{\infty} \tau^{2l} \sum_{j=1}^{J_{l}} \frac{1}{j!} \sum_{\{l_{i}\}} \prod_{n=1}^{j} \frac{1}{(2l_{n})!} (x + \rho^{2l_{n}} y) \sum_{\mathbf{k}^{(1)}, \dots, \mathbf{k}^{(j)}} \prod_{m=1}^{j} \left[\varphi(\mathbf{k}^{(m)}) \right]^{2l_{m}}, \tag{16}$$

where $x = (2/z_0^2)e^{-\beta\omega}$ and $y = xe^{-\beta(2\omega+U)}$.

Resorting to the integral representation for the δ function, whereby one can explicitly perform the sum $\Sigma'_{\{l_i\}}$, and making use of the equality

$$\sum_{\mathbf{k}^{(1)},\dots,\mathbf{k}^{(j)}} \prod_{n=1}^{j} f(\mathbf{k}^{(n)}) = (-1)^{j} j! \sum_{p_{1},\dots,p_{j} \in \pi_{j}} \prod_{n=1}^{j} \frac{1}{p_{n}!} \left(\frac{\mathcal{F}_{n}}{n} \right)^{p_{n}},$$
(17)

where π_i denotes the set of integers $\{p_n | n=1,\ldots,j\}$ such that $\sum_{n=1}^{j} np_n = j$ and $\mathcal{F}_n = -\sum_{\mathbf{k}} [f(\mathbf{k})]^n$, one gets

$$Z_{1} = Z_{0} \sum_{j=1}^{N/2} (-1)^{j} \sum_{l=j}^{\infty} \frac{1}{2\pi} \int_{-\pi}^{\pi} d\zeta (\tau e^{i\zeta})^{2l} \sum_{p_{1}, \dots, p_{j} \in \pi_{j}} \prod_{n=1}^{j} \frac{1}{p_{n}!} \left\{ -\frac{1}{n} \sum_{\mathbf{k}} \left[G(\mathbf{k}, e^{-i\zeta}) \right]^{n} \right\}^{p_{n}},$$

$$(18)$$

with $G(\mathbf{k},z) \equiv x \{\cosh[z\varphi(\mathbf{k})] - 1\} + y \{\cosh[z\varphi(\mathbf{k})] - 1\}$. After performing the integral, the partition function Z_N is

obtained as

$$\frac{Z_{\mathcal{N}}}{Z_{0}} = 1 + \sum_{j=1}^{\mathcal{N}/2} (-\tau^{2})^{j} \sum_{p_{1}, \dots, p_{j} \in \pi_{j}} \prod_{n=1}^{j} \frac{1}{p_{n}!} \left[\frac{g_{n}(\tau)}{n} \right]^{p_{n}},$$
(19)

where $\mathcal{G}_n(z) \equiv -(1/z^2) \sum_{\mathbf{k}} [G(\mathbf{k}, z)]^n$. In the thermodynamic limit $\mathcal{N} \to \infty$, expression (19) can be further simplified by use of a known identity for partition polynomials in number theory, 8 and reads

$$Z_{\mathcal{N}} = Z_0 \exp(\mathcal{N}\mathcal{B}), \qquad (20)$$

with $\mathcal{B} = \mathcal{N}^{-1} \sum_{\mathbf{k}} \ln[1 + G(\mathbf{k}, \tau)].$

We now turn to the study of the free energy. In the thermodynamic limit the free energy per site

$$f = \lim_{N \to \infty} -\frac{1}{\beta N} \ln Z_N = -\frac{1}{\beta} (\ln z_0 + \beta).$$

In such a limit the sum over $\mathbf{k} \in \mathcal{D}$ turns into a convergent integral,

$$\lim_{N\to\infty}\frac{1}{N}\sum_{\mathbf{k}\in\mathcal{D}}\longrightarrow\frac{1}{(2\pi)^d}\int_0^{2\pi}d\vartheta_1\cdots\int_0^{2\pi}d\vartheta_{d-1}\int_0^{\pi}d\vartheta_d.$$

For the sake of simplicity we focus our attention on the

$$n_0 \sim -\frac{1}{\beta} \left\{ \frac{\partial}{\partial \omega} \ln \frac{z_0}{1+\lambda} + \frac{1}{(4\pi\tau)^{d/2}} \zeta \left[\frac{d}{2}, 1, -\lambda e^{2\tau d} \right] \frac{\partial}{\partial \omega} \ln \lambda \right\},$$

 $\zeta(s,1,-z)$ denoting the Lerch zeta function, which, for s=1 (i.e., d=2), reduces to ln(1+z). In this case one can easily solve Eq. (22) at T=0, and the chemical potential is found to be discontinuous for U > 16|t| in $n_0 = 1$. The ground-state energy u is then obtained as $u = (\partial f/\partial \beta)_{T=0} + \mu n_0$. As it turns out to be piecewise linear, u is given in Table I for different ranges of values of n_0 . In particular, one can notice that u is minimum for $1/\pi < n_0 < 1 - 1/\pi$, and that the value U = 16|t| is critical, in that for fixed filling $(1 - \gamma < n_0 < 1 + \gamma)$, with $\gamma = \max\{1/\pi - U/16\pi |t|, 0\}$) the ground-state energy changes through it, passing from a quadratic to a linear dependence on U. The order parameter responsible for this behavior is the double-occupancy expectation value, namely, $\mathcal{P} = (\partial f/\partial U)_{T=0}$, which at $n_0 = 1 - \gamma$ becomes different from zero, whereas from $n_0 = 1 + \gamma$ on it goes like n_0-1 . This implies that the model exhibits a metal-insulator (Mott) transition. Figure 1 shows a plot of u vs U at half filling $(n_0=1)$ together with the corresponding curve derived for the 1D Hubbard model from

TABLE I. Ground-state energy versus band filling.

Range n ₀	u/8 t
$0 \le n_0 < 1/\pi$	$-n_0$
$1/\pi \le n_0 < 1 - 1/\pi$	$-1/\pi$
$1-1/\pi \le n_0 < 1-\gamma$	$-1 + n_0$
$1-\gamma \le n_0 < 1+\gamma$	$(U/16 t)(n_0-1)-\pi\gamma^2$
$1+\gamma \le n_0 < 1-1/\pi$	$(U/8 t -1)(n_0-1)$
$1 + 1/\pi \le n_0 < 2 - 1/\pi$	$(U/8 t)(n_0-1)-1/\pi$
$2-1/\pi \le n_0 < 2$	$(U/8 t)(n_0-1)-(2-n_0)$

particular choice $\rho = \pm 1$, whereby \mathcal{B} can be conveniently expressed as a power series both in the variable $\lambda = (1-R)/(1+R)$, $R = \sqrt{1-2(x+y)}$, and in τ :

$$\mathcal{B} = -\sum_{m=1}^{\infty} \frac{(-1)^m}{m} \lambda^m \{ [I_0(2m\tau)]^d - 1 \}$$

$$= \sum_{k=1}^{\infty} c_k^{(d)} \frac{\tau^{2k}}{2k} \beta_{2k} (-\lambda) , \qquad (21)$$

where $I_{\nu}(z)$ is a modified Bessel function of the first kind, the coefficients $c_k^{(d)}$ are defined by

$$[I_0(2z)]^d - 1 \equiv \sum_{k=1}^{\infty} c_k^{(d)} z^{2k},$$

and $\beta_n(\alpha)$ are the Apostol polynomials, 9 related to the Lerch zeta function. 10

The free energy per site is given by the above expressions once ω is suitably chosen. Indeed, one has to fix the total electron occupation number, namely, the ratio $n_0 = \langle N_e \rangle / \mathcal{N}$. This is done here following the customary convention of choosing the chemical potential as a solution to the equation $n_0 \equiv \partial f / \partial \omega$. For instance, in the low-temperature limit $(\beta \rightarrow \infty)$

$$\left. \frac{\partial}{\partial \omega} \ln \lambda \right\},$$
 (22)

the exact solution. 11,12

In conclusion, it is worth pointing out that the solution presented, besides constituting an interesting example of an exactly solvable system, provides, on one hand, a promising starting point for working out perturbatively (e.g., in the parameter $t - \Delta t$) solutions of the general-

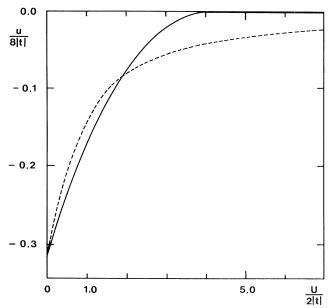


FIG. 1. Ground-state energy u/8|t| vs U/2|t| at $n_0=1$ for d=2. The dashed curve represents the same quantity for the 1D Hubbard model as given in Ref. 12.

ized KSSH model (1); on the other hand, as the partition function Z_N is given exactly also for finite \mathcal{N} , it can provide a reference test for numerical calculations on a nontrivial quantum system. Finally, work is at present in progress on the problem of studying the solution of the same model within the Fermi-linearization approximation scheme. ¹³ This can be done rather easily in that the underlying dynamical (super)algebras are the same. The exact solution discussed here can then become an excellent testing ground for the fermionic mean-field approach.

¹S. Kivelson, W. P. Su, J. R. Schrieffer, and A. J. Heeger, Phys. Rev. Lett. **58**, 1899 (1987).

²For a discussion of the relevance of the bond-charge repulsion term, see, D. Baeriswyl, P. Horsch, and K. Maki, Phys. Rev. Lett. **60**, 70 (1988); J. T. Gammel and D. K. Campbell, *ibid.* **60**, 71 (1988); S. Kivelson, W. P. Su, J. R. Schrieffer, and

- A. J. Heeger, ibid. 60, 72 (1988).
 - ³J. E. Hirsch, Physica (Amsterdam) **158C**, 326 (1989).
- ⁴J. Friedel, P. Lenghart, and G. Leman, J. Phys. Chem. Solids 25, 781 (1964).
 - ⁵D. J. Klein, Phys. Rev. B 8, 3452 (1973).
- ⁶Y. Hasegawa, P. Lederer, T. M. Rice, and P. B. Wiegman, Phys. Rev. Lett. **63**, 907 (1989).
- ⁷D. C. Mattis, *The Theory of Magnetism I* (Springer-Verlag, Berlin, 1981), Chap. 6.
- ⁸J. Riordan, *Combinatorial Identities* (Wiley, New York, 1968), Chap. 5, p. 183, Eq. (21).
 - ⁹T. M. Apostol, Pacific J. Math. 1, 161 (1951).
- ¹⁰E. T. Wittaker and G. N. Watson, *A Course of Modern Analysis* (Cambridge Univ. Press, London, 1952), 4th ed.
- ¹¹E. H. Lieb and F. Y. Wu, Phys. Rev. Lett. **20**, 1445 (1968). ¹²W. D. Langer and D. C. Mattis, Phys. Lett. **36A**, 139 (1971).
- ¹³A. Montorsi and M. Rasetti, Mod. Phys. Lett. B 4, 613 (1990).