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Equivalence of the Dimer Resonating-Valence-Bond Problem to the Quantum Roughening Problem

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A geometric mapping of dimers on a square lattice onto surfaces of a 3D crystal is constructed. The mapping transforms the dimer-RVB (resonating valence band) problem to the quantum roughening problem: Low-energy excitations correspond to the crystal surface fluctuations; holes are represented by screw dislocations. A phase diagram is discussed and the existence of a quantum-limit state with gapless excitations is demonstrated using the results obtained previously for the roughening problem.

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Recently the quantum dimer problem was discussed[1] as a candidate for a system having a quantum-liquid ground state.[2] Although a number of approaches have been developed[3,4] to solve the problem, the physics contained in it remains far from being clear. Two main (and mutually related) questions to be answered are the following: (a) Is the ground state ordered or disordered? (b) Is there a gap in the low-energy excitation spectrum? Here I consider the dimer problem on a square lattice and show that it can be mapped exactly onto the roughening problem for a specially chosen 3D crystal. (For dimers on a hexagonal lattice such a mapping also exists, see Fig. 1.) The possibility of this mapping seems to be very attractive since our understanding of the roughening problem is far deeper than of the dimer one. The constructed mapping is purely geometric, so the method can be applied to both quantum and classical versions of the dimer problem. The ordered (crystalline) and disordered (liquid) states of the dimer problem are identified with the smooth and the rough states of a fluctuating surface in the 3D crystal roughening problem (respectively). Thus low-energy excitations of the dimer problem are found: They correspond to long-wavelength fluctuations of the corresponding crystal surface (compare with "resonons"[4]).

For quantum dimers on a square lattice Rokhsar and Kivelson[4] demonstrated the existence of "topological sectors" described by two winding numbers. In a recent work[5] Ioffe and Larkin introduced dipole momenta of dimers and found a conservation law for the density of dipoles. Within the approach presented here these results acquire a clear meaning. Both the winding numbers and the macroscopic dipole momentum correspond to the average slope of a crystal surface obviously conserved by all local Hamiltonians.

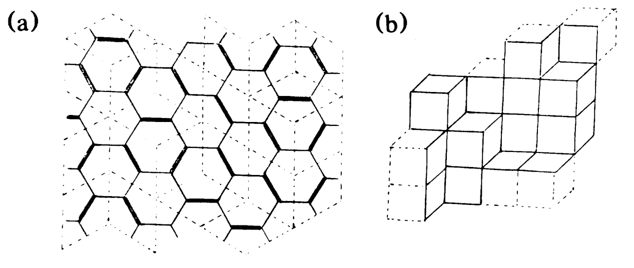

FIG. 1. Mapping of dimers on a hexagonal lattice to a surface of a cubic crystal. (a) A hexagonal lattice with dimers covered by 60° rhombi. (b) A piece of a surface of a 3D cubic crystal corresponding to the rhombic tiling. The broken lines show faces of cubes which are either invisible or absent in the tiling (a).

Let us start by constructing *a mapping of planar dimer configurations onto surfaces of a 3D crystal.* It is well known that any configuration of dimers can be equivalently represented as a tiling of the square lattice by 2×1 dominos covering adjacent plaquettes. It will be convenient for us to work with dominos instead of dimers. First of all, we define a 3D crystal such that a certain class of its surfaces is in one-to-one correspondence with planar configurations of dominos. As a basic constituent of the crystal we use the polytope shown in Fig. 2(a): Its triangular faces are perpendicular to the basal (x,y) plane, while other (rectangular) faces form the 45° angle with it. Identical polytopes are arranged in 2D layers parallel to the basal plane. The layers are placed one upon another as shown in Fig. 2(b). Polytopes in odd layers are related with those in even ones by the 90° rotation around the z axis and a proper shift. Notice that the surfaces of adjacent layers are mutually complementary and touch each other perfectly (an empty space between neighboring layers is shown in Fig. 2 only for convenience). A unit cell of a crystal so defined can be chosen as any pair of adjacent polytopes having a common face.

Let the whole space be tiled periodically as described above. Choose an arbitrary infinite surface having a one-to-one projection on the basal plane. Remove all polytopes which are strictly above the surface and view the boundary of the region containing all remaining polytopes along the z axis (or project this boundary on the basal plane). Clearly, we obtain a tiling of the plane by dominos, since all triangular faces project into segments, while rectangular faces project into the 2×1 dominos. Thus we see that any surface everywhere transverse to the z direction generates a domino configuration in the basal plane.

Now, we are going to show that this transformation is

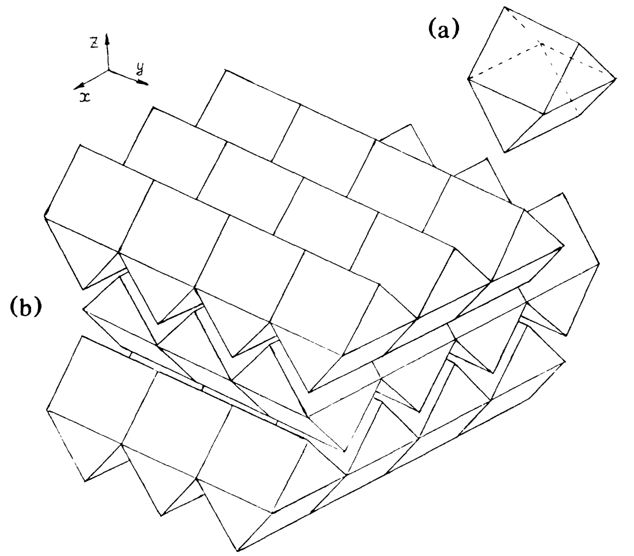

FIG. 2. (a) The basic polytope. (b) A 3D crystal consisting of basic polytopes arranged in layers. A separation of the layers is introduced for clarity.

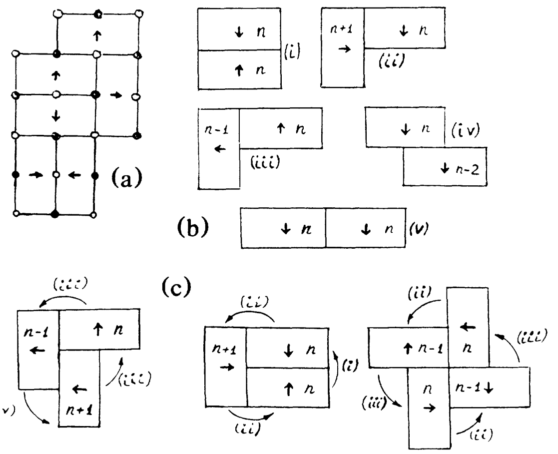

FIG. 3. (a) Arrows are placed on dominos so that they point from white vertices to black ones on horizontal dominos and from black vertices to white ones on vertical dominos. (b) Five rules defining a relation of integer numbers on neighboring dominos. (c) Three (of twelve) minimal closed paths to be considered for verifying the self-consistency of the rules (b).

reversible, i.e., that each configuration of dominos can be viewed as a projection of a crystal surface described above. As a first step we place *arrows* on the dominos. Consider odd and even (white and black) sublattices of the basic square lattice.[1] These two lattices generate an arrow on each domino according to the rule which is clear from Fig. 3(a). After corresponding polytopes will be constructed the geometric meaning of the arrows will be revealed: The arrows will indicate the steepest downward directions on the faces of the polytopes.

Next, we attribute *integer numbers* to arrowed dominos. These numbers will have a geometric meaning of a number of a layer which the corresponding polytope belongs to (see Fig. 2). The numbers are calculated recursively: After the number is known for some domino it can be found for all its neighbors using the rules (i)-(v) connecting the numbers on adjacent dominos [see Fig. 3(b)]. Clearly, given a number for one domino, all other dominos in the plane can be reached step by step using these rules, so, finally, all dominos receive their numbers. The only thing we have to check is the self-consistency of this procedure. Imagine that we go along a closed path and each time when coming from a domino to a neighboring one we calculate a new number using the rules shown in Fig. 3(b). Is it possible that after returning to the domino we started with we find a number different from that which we had at the beginning? To make sure that this cannot happen one has to consider only circular paths of minimal size, because any other path can be decomposed into a number of minimal ones. Minimal paths can include three or four dominos; hence their number is finite: In total there are twelve such paths [as an example, three of them are shown in Fig. 3(c)]. Therefore, the absence of a contradiction can be verified by inspecting all of these twelve paths. After doing this we find that the integer numbers can be attributed to arrowed dominos *unambiguously*.

Finally, starting from any domino configuration we arrive at arrowed and numbered dominos. If the numbers and arrows are taken as indicating the polytopes' layer labels and the directions of slopes of their faces (respectively), then the construction of a crystal surface becomes straightforward (see an example in Fig. 4). Note that the only freedom in the described procedure is related with the choice of black and white colors of the two sublattices used to put arrows on dominos. Two possible orientations of arrows yield two different crystal surfaces which are mirror images of each other, where the mirror plane is parallel to the basal plane.

Now, after the mapping is obtained, we can view the Hamiltonian for dimers[4] on the basis of the roughening problem language. The "kinetic" term $\sum -J(|\parallel\rangle\langle = | + \mathrm{H.c.})$ describes a polytope sticking to (removing from) the surface, depending on the orientations of the arrows on the dominos corresponding to the dimers in the brackets. The "potential" term $\sum V(|\parallel\rangle\langle\parallel| + | = \rangle\langle = |)$ gives an energy of an atomic step. This term provides equal amplitudes for both orientations of arrows on the dominos.

Let us discuss a phase diagram of the problem by making use of the results[6] found for the quantum roughening problem. It is convenient to introduce in the Hamiltonian two new terms relevant for the roughening problem:

$$\sum_{\text{dimers}} \mu_x(|\leftarrow\rangle\langle\leftarrow| - |\rightarrow\rangle\langle\rightarrow|) + \mu_y(|\uparrow\rangle\langle\uparrow| - |\downarrow\rangle\langle\downarrow|)\,.$$

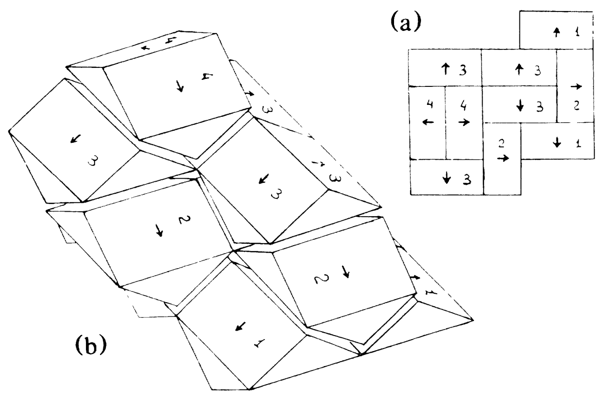

FIG. 4. (a) Dominos arrowed and numbered according to the rules shown in Figs. 3(a) and 3(b). (b) The corresponding piece of a 3D crystal. A geometric meaning of numbers and arrows is clear: They correspond to layer numbers and slopes of rectangular faces.

Here vertical (horizontal) arrows correspond to horizontal (vertical) dominos [see Fig. 3(a)]. These terms guide the orientation of the crystal surface representing the ground state of dimers. The phase diagram in the (μ_x,μ_y) plane consists of regions corresponding to (a) *rational* and (b) *irrational* slopes. In the regions of type (a) the surface is always smooth;[6] i.e., there is a gap in the spectrum of its long-wavelength fluctuations. Therefore, dimers form not a liquid but a crystal (spin Peierls) state. However, if the quantum parameter $\lambda = J/V$ is large, the gap becomes exponentially small as a function of λ, while the correlation length becomes exponentially large. In this case the surface can behave as a rough one (and dimers as a quantum liquid) at sufficiently large (but microscopic) length and time scales. Rational slopes always occupy regions of a positive measure in the (μ_x,μ_y) plane since the energy of an atomic step is nonzero.

As for the regions of type (b), they correspond to a rough state of the surface. Their measure is positive and, moreover, they can dominate the phase diagram in the strong quantum limit $\lambda \gg 1$.[6,7] Very often the regions (a) and (b) interpenetrate each other forming a complex fractal structure. The roughness of the surface implies that *a true quantum-liquid state of dimers is formed in this part of the phase diagram.* Since the energy of a step on a rough surface is zero, the spectrum of excitations is gapless.[8] Therefore, fluctuations of the surface are described by a massless scalar field: $S = \int dt\, d^2r[(\partial_t h)^2 - c^2(\nabla h)^2]$, thus yielding a linear spectrum of excitations: $\omega = c\,|\mathbf{k}|$.

Up to now only close-packed dimers were considered. Since doped states containing holes (vertices not covered by dimers) are also of interest, let us make some remarks on them. In a domino configuration a hole is represented by an empty square plaquette. One can easily make sure that in the 3D crystal picture empty squares correspond to *screw dislocations* having Burgers "charge" ±1. What is the effect of holes on the ground state? It is well known that dislocations act to destroy a smooth state, so in the presence of a sufficiently large amount of dislocations the system can favor a rough state even if it lives in a region of type (a) of the phase diagram. In the dimer language this conclusion means that holes can stabilize a quantum-liquid state even if it is unstable for the undoped systems.

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[7] In this case the measure of the regions of type (a) is exponentially small in λ: The interval of parameters μ_x,μ_y corresponding to some rational slope can be estimated as a characteristic energy of a step, which becomes exponentially small when $\lambda \to \infty$. Therefore, the regions of type (b) occupy most of the phase diagram.

[8] An experimental evidence for the existence of a quantum rough surface state with gapless excitations is given by the observation of crystallization waves on the solid-liquid interface of ^{4}He: K. O. Keshishev, A.Ya. Parshin, and A. V. Babkin, Pis'ma Zh. Eksp. Teor. Fiz. **30**, 63 (1979) [JETP Lett. **30**, 56 (1979)].