



## **Exact many-electron ground states on the diamond Hubbard chain**

Zsolt Gulácsi, Arno P. Kampf, Dieter Vollhardt

## Angaben zur Veröffentlichung / Publication details:

Gulácsi, Zsolt, Arno P. Kampf, and Dieter Vollhardt. 2007. "Exact many-electron ground states on the diamond Hubbard chain." *Physical Review Letters* 99 (2): 026404. https://doi.org/10.1103/physrevlett.99.026404.

Nutzungsbedingungen / Terms of use:

## **Exact Many-Electron Ground States on the Diamond Hubbard Chain**

Zsolt Gulácsi, 1,2 Arno Kampf, 1 and Dieter Vollhardt 1

<sup>1</sup>Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute for Physics, University of Augsburg, D-86135 Augsburg, Germany

<sup>2</sup>Department of Theoretical Physics, University of Debrecen, H-4010 Debrecen, Hungary (Received 30 March 2007; published 13 July 2007)

Exact ground states of interacting electrons on the diamond Hubbard chain in a magnetic field are constructed which exhibit a wide range of properties such as flat-band ferromagnetism and correlation-induced metallic, half-metallic, or insulating behavior. The properties of these ground states can be tuned by changing the magnetic flux, local potentials, or electron density.

DOI: 10.1103/PhysRevLett.99.026404 PACS numbers: 71.10.Fd, 71.27.+a

Condensed matter systems with macroscopic degeneracies react very sensitively on internal or external perturbations and thus give rise to fascinating emergent behavior. Well-known examples are electrons in a magnetic field in two dimensions [1] and spins on lattices with geometric frustration [2]. Dispersionless ("flat") electronic bands in solids also lead to macroscopic degeneracies. Recent advances in nanotechnology allow for the possibility to design simple structures, which have flat single-electron bands, i.e., when electronic correlations are neglected [3-6]. The controlled setup of optical lattices for cold atoms using standing wave laser light fields also allows one to realize a variety of lattice models of interacting fermions and bosons [7,8]. The ability to generate flat bands by changing external parameters such as a gate voltage or a magnetic field would make even a direct manipulation of macroscopically degenerate systems possible. For example, the understanding of ferromagnetism in organic compounds [5] could be improved, and the tuning of instabilities or the switching between different phases would permit direct applications in spintronics.

Most exact flat-band results concern flat *lowest*-energy bands, and provide solutions for ground states or the low temperature thermodynamics [8,9]. For such a case Mielke and Tasaki proved that ferromagnetism is stabilized at or near half-filling [10]. Lieb's ferrimagnetism emerges on a bipartite lattice with a macroscopically degenerate energy level exactly in the middle of the spectrum [11]. For the more general case, when the interaction leads to an effective flat band above a dispersive band, exact results were derived for the periodic Anderson model [12], by exact diagonalization of small clusters and *ab initio* band-structure calculations [5], or analytically for the two-particle problem [6].

In this Letter we concentrate on one of the simplest lattice electron models, the Hubbard model on a diamond chain, as found, e.g., in azurite. In the diamond chain flat bands occur already in the one-electron picture. External potentials or a magnetic field can give rise to additional flat bands. For selected parameter sets, and by appropriately tuning local potentials or the magnetic flux, we construct

exact many-body ground states on the diamond chain, which are either insulating or conducting and fully or partially spin polarized. Our results thus open new routes for the design of spin-valve devices and gate induced ferromagnetism.

Figure 1 shows the diamond chain, whose sites are denoted by  $\mathbf{i} + \mathbf{r}_s$ , where  $\mathbf{i}$  and  $\mathbf{r}_s$  (with sublattice index s = 1, 2, 3 and  $\mathbf{r}_3 = \mathbf{0}$ ) denote the unit cells and the three sites inside, respectively. The Bravais vector of the chain is  $\mathbf{a}$ ; periodic boundary conditions along the chain are assumed. Given N electrons their density is  $n = N/(3N_c)$ , where  $N_c$  is the number of unit cells. The Hamiltonian for the diamond Hubbard chain has the form

$$\hat{H} = \sum_{\mathbf{k},\sigma} \sum_{s,s'=1}^{3} M_{s,s'}(\mathbf{k}) \hat{c}_{s,\mathbf{k},\sigma}^{\dagger} \hat{c}_{s',\mathbf{k},\sigma} + \hat{H}_{U},$$

$$\hat{H}_{U} = U \sum_{\mathbf{i}} \sum_{s=1}^{3} \hat{n}_{\mathbf{i}+\mathbf{r}_{s},\uparrow} \hat{n}_{\mathbf{i}+\mathbf{r}_{s},\downarrow},$$
(1)

where the kinetic and the interaction part are written in **k** space and position space, respectively. Here and in the following sums or products over **k** and **i** extend over the  $N_c$  vectors enumerating the unit cells,  $\hat{c}_{\mathbf{j},\sigma}^{\dagger}$  creates an electron with spin  $\sigma$  at site **j**, the local density is given by  $n_{\mathbf{j},\sigma} = \hat{c}_{\mathbf{j},\sigma}^{\dagger} \hat{c}_{\mathbf{j},\sigma}$ , and  $\hat{c}_{s,\mathbf{k},\sigma}$  is the Fourier transformed sublattice operator. The elements of the symmetric matrix  $M_{s,s'}(\mathbf{k})$  in the kinetic energy are

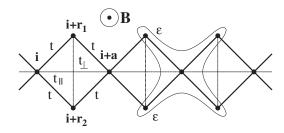


FIG. 1. Diamond Hubbard chain. The cross-shaped region depicts a localized (Wannier) eigenfunction for  $t_{\perp}=t_{\parallel}=0$  and flux  $\delta=\pi/2$  (see text).

$$M_{1,1} = M_{2,2} = \epsilon,$$
  $M_{3,3} = 2t_{\parallel} \cos ak,$   $M_{1,2} = t_{\perp},$   $M_{(s=1,2),3} = 2t \cos\{[ak + (-1)^s \delta]/2\}.$  (2)

Here, t,  $t_{\perp}$ ,  $t_{\parallel}$  denote the hopping matrix elements to nearest neighbors (NN) and to next NN sites (perpendicular and parallel to  ${\bf a}$ ), respectively. A Peierls phase factor  $\exp({\rm i}\delta/2)$  with  $\delta=2\pi\Phi/\Phi_0$  accounts for a perpendicular magnetic field  ${\bf B}$ ,  $\Phi$  is the flux threading the unit cell, and  $\Phi_0=hc/e$  is the flux quantum. Choosing the vector potential  ${\bf A}\parallel{\bf a}$  in the field dependent hopping amplitudes  $t_{{\bf j},{\bf j}'}({\bf B})=t_{{\bf j},{\bf j}'}(0)\exp[({\rm i}2\pi/\Phi_0)\int_{\bf j}^{{\bf j}'}{\bf A}\cdot d{\bf l}]$  the magnetic field does not alter  $t_{\perp}$  and  $t_{\parallel}$ . The on site potential  $\epsilon$  acts on the sublattices s=1,2. U is the on site Hubbard repulsion. Below energies will be in units of 2t.

The diagonalization of the kinetic energy part in Eq. (1) leads to a cubic eigenvalue equation for the band dispersion  $E(\mathbf{k})$ . With  $P_1 = (1 + t_\perp^2) + \cos\delta\cos ak$  and  $P_0 = t_\perp[\cos\delta + \cos ak + t_\perp(\epsilon - 2t_\parallel\cos ak)]$  the dispersion  $E_\nu(\mathbf{k})$  ( $\nu = 1, 2, 3$ ) is determined by

$$X^{3} + X^{2}(\epsilon - 2t_{\parallel}\cos ak) - XP_{1} = P_{0}, \tag{3}$$

with  $X=E-\epsilon$ . Depending on the choice of  $t_{\perp}$ ,  $t_{\parallel}$ , the magnetic field, and the potential  $\epsilon$ , the single-electron band structure contains one, two, or even three exactly flat bands (Fig. 2). It should be stressed that these bands lose their meaning as soon as the interaction is switched on.

Vidal *et al.* recently presented a detailed study of two electrons on the diamond Hubbard chain in the limit  $t_{\perp} = t_{\parallel} = \epsilon = 0$  [6]. They showed that for half a flux quantum per unit square ( $\delta = \pi/2$ ) the excited singlet eigenstates are localized if U = 0, but become delocalized for U > 0. Apparently, the interaction U is able to induce subtle correlations leading to conducting states, which led them [6] to speculate that such a delocalization also holds for a finite electron density.

Here we construct exact many-particle ground states for quite general cases and thereby also resolve some of the issues raised in [6]. The strategy for deducing exact ground states was described before in the context of the periodic Anderson model [12], but has not yet been applied to Hubbard models. The key steps are to first cast the Hamiltonian in positive semidefinite form and then to construct an explicit eigenstate with minimal energy.

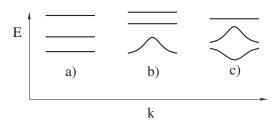


FIG. 2. Single-electron band structure. (a)  $t_{\perp} = t_{\parallel} = 0$ ,  $\delta = \pi/2$ . (b)  $\epsilon = -t_{\perp} + t_{\perp}^{-1}/2$ ,  $\delta = \pi$ ; the upper flat bands are degenerate for  $t_{\perp}t_{\parallel} = 1/4$ . (c)  $t_{\parallel} = 0$ ,  $\epsilon t_{\perp} \cos \delta = t_{\perp}^2 - \cos^2 \delta$ .

Solution I. Flat-band ferromagnetism.—We start with localized ground states for densities  $n \le 1/3$ ,  $t_{\perp} = t_{\parallel} = 0$ , and  $\delta = \pi/2$  ("Aharonov-Bohm cage" [6]), in which case Eq. (3) provides three flat single-electron bands with energies  $E_2 = \epsilon$ ,  $E_{2\pm 1} = (\epsilon \mp \sqrt{\epsilon^2 + 4})/2$  [see Fig. 2(a)]. Introducing the canonical fermionic operators  $\hat{C}_{\nu,i,\sigma}$ ,

$$\hat{C}_{2\pm 1, \mathbf{i}, \sigma} = \frac{1}{\sqrt{2}} [F_{\pm} \hat{Q}_{\mathbf{i}\sigma}^{(+)} \mp 2F_{\mp} \hat{c}_{\mathbf{i}, \sigma}], \quad \hat{C}_{2, \mathbf{i}, \sigma} = \frac{\hat{Q}_{\mathbf{i}\sigma}^{(-)}}{2}, \quad (4)$$

with  $F_{\pm}^2=1\mp\epsilon/\sqrt{\epsilon^2+4}$ ,  $\hat{Q}_{\mathbf{i}\sigma}^{(\pm)}=\hat{Q}_{\mathbf{i}\sigma}^{(1)}(\mp\delta)\pm\hat{Q}_{\mathbf{i}\sigma}^{(2)}(\pm\delta)$ , and  $\hat{Q}_{\mathbf{i}}^{(l=1,2)}(\delta)=e^{-\mathrm{i}\delta/2}\hat{c}_{\mathbf{i}+\mathbf{r}_l,\sigma}+e^{+\mathrm{i}\delta/2}\hat{c}_{\mathbf{i}-\mathbf{a}+\mathbf{r}_l,\sigma}$ , the Hamiltonian can be written in the form

$$\hat{H} = \sum_{\mathbf{i},\sigma} \sum_{\nu=1}^{3} E_{\nu} \hat{C}^{\dagger}_{\nu,\mathbf{i},\sigma} \hat{C}_{\nu,\mathbf{i},\sigma} + \hat{H}_{U}. \tag{5}$$

Since  $\hat{C}_{\nu,\mathbf{i},\sigma}^{\dagger}\hat{C}_{\nu,\mathbf{i},\sigma}$  and  $\hat{H}_U$  in Eq. (5) are positive semi-definite operators, the ground state of  $N \leq N_c$  electrons at U > 0 is obtained by filling up the eigenstates as

$$|\Psi_g^{\rm I}(N)\rangle = \prod_{i=1}^N \hat{C}_{3,i,\sigma_i}^{\dagger}|0\rangle, \tag{6}$$

 $|0\rangle$  denotes the vacuum. The ground-state energy is  $E_g^{\rm I} =$  $E_3N$ . The operators  $\hat{C}^{\dagger}_{\nu,\mathbf{i},\sigma}$  create electrons in localized Wannier eigenstates; an example of their structure (for  $\nu =$ 3) is shown in Fig. 1. For n = 1/3 one obtains a unique, fully saturated ferromagnetic ground state. For n < 1/3only the Wannier states with a spatial overlap have the same spin. The (degenerate) ground states hence consist of ferromagnetic clusters of arbitrary spin orientation. When the density is increased to n = 1/3 the clusters touch and the degeneracy is lifted. Since  $\hat{H}_U|\Psi_g^I(N)\rangle = 0$  and the kinetic part of  $\hat{H}$  is diagonal in real space, the ground state (6) is localized. This is an explicit realization of Mielke-Tasaki's flat-band ferromagnetism [10]. Since the lowest single-electron band is flat only for  $\delta = \pi/2$  and dispersive for  $\delta = 0$ , the system is most probably conducting; we here encounter a metal-insulator transition as a function of magnetic field.

Solution II. Correlated half-metal.—The results of Ref. [6] suggest that itinerant states are easier to realize at  $\delta \neq \pi/2$ . To investigate this point we analyze a group of solutions for flux  $\delta = \pi$ , density  $n \geq 4/3$ , hopping  $t_{\perp}$ ,  $t_{\parallel} > 0$ , and local potential  $\epsilon = 1/(2t_{\perp}) - t_{\perp}$ . Then the bare band structure consists of two upper flat bands  $E_1$ ,  $E_2$ , and a lower dispersive band  $E_3(\mathbf{k})$  [Fig. 2(b)]. For simplicity we discuss here only the case  $t_{\perp}t_{\parallel} = 1/4$ , which implies  $E_1 = E_2 = \epsilon + t_{\perp}$  and  $E_3 = \epsilon - t_{\perp} - (1 - \cos ak)/(2t_{\perp})$ . Electrons in the dispersive single-electron band are created by the fermionic operators

$$\hat{C}_{\mathbf{k},\sigma} = \frac{\hat{c}_{2,\mathbf{k},\sigma} - \hat{c}_{1,\mathbf{k},\sigma}}{\sqrt{2}R_{\mathbf{k}}} + \frac{\sqrt{1 - \cos ak}}{2t_{\perp}R_{\mathbf{k}}}\hat{c}_{3,\mathbf{k},\sigma}, \quad (7)$$

with  $R_k = \sqrt{1 + (1 - \cos ak)/(4t_\perp^2)}$ . Defining noncanoni-

cal fermionic operators [13] as

$$\hat{A}_{\mathbf{i},\sigma} = \sqrt{t_{\parallel}} [\hat{c}_{\mathbf{i},\sigma} - \hat{c}_{\mathbf{i}+\mathbf{a},\sigma} - 2t_{\perp} e^{i(\delta/2)} (\hat{c}_{\mathbf{i}+\mathbf{r}_{\perp},\sigma} - \hat{c}_{\mathbf{i}+\mathbf{r}_{\perp},\sigma})],$$

Eq. (1) is transformed into positive semidefinite form as

$$\hat{H} = \sum_{\mathbf{i},\sigma} \hat{A}_{\mathbf{i},\sigma} \hat{A}_{\mathbf{i},\sigma}^{\dagger} + U\hat{P} + E_g^{II}, \tag{8}$$

 $E_g^{\rm II} = (\epsilon + U + t_\perp)N - N_c[3U + 4t_\perp + 1/t_\perp]$  is the ground-state energy. For the positive semidefinite operator  $\hat{P} = \sum_{{\bf j}=1}^{3N_c} (\hat{n}_{{\bf j},\uparrow} \hat{n}_{{\bf j},\downarrow} - \hat{n}_{{\bf j},\uparrow} - \hat{n}_{{\bf j},\downarrow} + 1)$  in Eq. (8) to assume its minimum eigenvalue 0 there must be at least one electron at each site. For  $N = 4N_c$  electrons (n = 4/3) the ground state then has the form

$$|\Psi_{g}^{\mathrm{II}}(4N_{c})\rangle = c \left[\prod_{\mathbf{i}} \hat{A}_{\mathbf{i},-\sigma}^{\dagger} \hat{A}_{\mathbf{i},\sigma}^{\dagger}\right] \hat{F}_{\sigma}^{\dagger} |0\rangle, \tag{9a}$$

$$= \prod_{\mathbf{k}} \left[ \hat{C}_{\mathbf{k},-\sigma}^{\dagger} \prod_{s=1}^{3} \hat{c}_{s,\mathbf{k},\sigma}^{\dagger} \right] |0\rangle. \tag{9b}$$

Here  $\hat{F}^{\dagger}_{\sigma} = \prod_{\mathbf{i}} [\hat{c}^{\dagger}_{\mathbf{i}+\mathbf{r}_{\mathbf{s}_{\mathbf{i},1}},\sigma} \hat{c}^{\dagger}_{\mathbf{i}+\mathbf{r}_{\mathbf{s}_{\mathbf{i},2}},\sigma}]$ , where the sublattice indices  $s_{\mathbf{i},1}$ ,  $s_{\mathbf{i},2}$  are arbitrary but not equal, creates two electrons with spin  $\sigma$  on arbitrary sites of each unit cell, c is a normalization factor. Since  $\hat{A}^{\dagger}_{\mathbf{i},\sigma}$  creates one more spin  $\sigma$  electron in each unit cell, every lattice site is occupied by a spin  $\sigma$  electron. The electrons with spin  $-\sigma$  are spatially extended, but they are localized in the thermodynamic limit. This is inferred from the long-distance behavior of the ground-state expectation value of the hopping term  $\Gamma_{\mathbf{r},-\sigma} = \langle \hat{c}^{\dagger}_{\mathbf{j},-\sigma} \hat{c}_{\mathbf{j}+\mathbf{r},-\sigma} + \mathrm{H.c.} \rangle$ . With  $\mathbf{j} = \mathbf{i} + \mathbf{r}_1$ , r/a = m, and  $N_c \to \infty$  one finds  $\Gamma_{m,-\sigma} = [(-1)^m \exp(-m/\xi_{-\sigma})]/\sqrt{1+1/t_{\perp}}$ . The one-particle localization length

$$\xi_{-\sigma} = -\{\ln[1 + (2t_{\perp})^2 - (2t_{\perp})\sqrt{(2t_{\perp})^2 + 2}]\}^{-1} \quad (10)$$

is finite; it increases almost linearly with  $1/t_{\perp}$ . The ground state is given by

$$|\Psi_g^{II}(4N_c + \Delta N)\rangle = \prod_{\alpha=1}^{\Delta N} \hat{c}_{n_\alpha, \mathbf{k}_\alpha, -\sigma}^{\dagger} |\Psi_g^{II}(4N_c)\rangle, \qquad (11)$$

where  $n_{\alpha}$  can take the values s=1,2,3. Since the operators  $\hat{c}_{n_{\alpha},\mathbf{k}_{\alpha},-\sigma}^{\dagger}$  add plane-wave-type states to  $|\Psi_{g}^{\mathrm{II}}(4N_{c})\rangle$  the ground state now contains genuinely itinerant spin  $-\sigma$  electrons [14]. This, together with the fact that  $\delta\mu(N)=0$  [15] for  $1<\Delta N< N_{c}$  implies that the ground state  $|\Psi_{g}^{\mathrm{II}}(4N_{c}+\Delta N)\rangle$  is conducting. The net magnetization decreases linearly with increasing electron density.  $|\Psi_{g}^{\mathrm{II}}(4N_{c}+\Delta N)\rangle$  remains the ground state up to  $\Delta N=N_{c}$  (n=5/3), where it becomes nonmagnetic. For densities 4/3 < n < 5/3 the ground state therefore corresponds to a *correlation-induced half-metal*. Namely, while the  $3N_{c}$  electrons with spin  $\sigma$  are completely immobile and  $N_{c}$  electrons with spin  $-\sigma$  are confined to their localized Wannier function, only the  $\Delta N-\sigma$  electrons are itinerant, leading to a low carrier-density metallic behavior

with a low spin polarization. Since the conduction through this correlated half-metal involves only electrons of one spin species, such a system may, in principle, serve as a spin-valve device, if contacted by metallic reservoirs [16,17]. Bearing in mind that at U=0 the electronic states at the Fermi level are dispersionless and hence localized, we find that a finite, repulsive Hubbard interaction can induce a localization-delocalization transition towards a half-metal. This is an explicit example for the correlation-induced conducting state conjectured by Vidal  $et\ al.$  [6]. At fixed magnetic field it can be realized by tuning the sublattice potential  $\epsilon$ . Similar solutions at  $\delta=\pi$  can be deduced also at  $t_\parallel t_\perp < 1/4$ , when the two upper flat bands are nondegenerate.

Solution III.—We now construct exact ground states for more general values of the magnetic flux,  $\delta \in (-\pi/2, +\pi/2)$ , including zero flux, for electron densities  $n \ge 5/3$ . In particular, we will show that, by switching on a magnetic field, a nonmagnetic ground state may turn into a nonsaturated ferromagnet. We note that this occurs in the absence of any Zeeman coupling to the spin and is only due to the Peierls factor in the kinetic energy. Specifically we select the parameters  $t_{\parallel}=0$ ,  $t_{\perp}<0$ ,  $b\equiv-\cos\delta/t_{\perp}$ ,  $\epsilon=b-b^{-1}$ . In the noninteracting case one obtains a band structure with one upper flat band at  $E_1=\epsilon+1/b$ , and two lower dispersive bands at  $E_{2,3}=\epsilon-b/2\pm(b^2/4+t_{\perp}^2+\cos\delta\cos ak)^{1/2}$  [Fig. 2(c)]. Defining the noncanonical fermionic operators [13]

$$\hat{A}_{\pm,\mathbf{i},\sigma} = \frac{1}{\sqrt{2b}} \times \begin{cases} b\hat{c}_{\mathbf{i}+\mathbf{a},\sigma} - \hat{c}_{\mathbf{i}+\mathbf{r}_2,\sigma} e^{i(\delta/2)} - \hat{c}_{\mathbf{i}+\mathbf{r}_1,\sigma} e^{-i(\delta/2)} \\ b\hat{c}_{\mathbf{i},\sigma} - \hat{c}_{\mathbf{i}+\mathbf{r}_2,\sigma} e^{-i(\delta/2)} - \hat{c}_{\mathbf{i}+\mathbf{r}_1,\sigma} e^{i(\delta/2)} \end{cases}$$

the ground-state energy follows as  $E_g^{\rm III} = (U+b)N - N_c(3U+4/b+2b)$  and the Hamiltonian in positive semi-definite form is

$$\hat{H} = \sum_{\alpha = +} \sum_{\mathbf{i}, \sigma} \hat{A}_{\alpha, \mathbf{i}, \sigma} \hat{A}^{\dagger}_{\alpha, \mathbf{i}, \sigma} + U \hat{P} + E_g^{\text{III}}.$$
 (12)

III.a. Field induced localized ferromagnetism at n = 5/3.—For  $N = 5N_c$  the ground state has the general form

$$|\Psi_g^{\text{III}}(5N_c, \delta)\rangle = \hat{G}^{\dagger}\hat{E}^{\dagger}(\delta)|0\rangle,$$
 (13)

where  $\hat{G}^{\dagger} = \hat{G}_{\uparrow}^{\dagger} \hat{G}_{\downarrow}^{\dagger}$ , with  $\hat{G}_{\sigma}^{\dagger} = \prod_{\alpha=\pm} \prod_{i} \hat{A}_{\alpha,i,\sigma}^{\dagger}$ , inserts two electrons with spin  $\sigma$  and two electrons with spin  $-\sigma$  in each unit cell. The first term of the Hamiltonian (12) therefore annihilates the ground state (13) since  $\hat{A}_{\alpha,i,\sigma}^{\dagger} \hat{G}^{\dagger} = 0$ . In order to fulfill also  $\hat{P}\hat{G}^{\dagger} \hat{E}^{\dagger}(\delta)|0\rangle = 0$ , the operator  $\hat{E}^{\dagger}(\delta)$  requires a special form, which depends on the properties of  $\hat{G}^{\dagger}$ : For zero flux  $(\delta=0)$   $\hat{G}^{\dagger}$  creates a double occupancy on each site of the s=3 sublattice, where the diamonds touch, thereby blocking any electron motion along the chain. The operator  $\hat{E}^{\dagger}(\delta=0)$ , which adds one more electron to each unit cell, can therefore place electrons only on sublattices s=1,2, i.e.,  $\hat{E}^{\dagger}(0)=\prod_{i}(\alpha_{i}\hat{c}_{i+r_{i},\sigma_{i+1}}^{\dagger}+\beta_{i}\hat{c}_{i+r_{2},\sigma_{i+2}}^{\dagger})$  with arbitrary numerical co-

efficients  $\alpha_i$ ,  $\beta_i$  and spins  $\sigma_{i,1}$ ,  $\sigma_{i,2}$ . Altogether the ground state is localized and nonmagnetic with a high spin degeneracy and has the form

$$|\Psi_g^{\rm III}(5N_c,0)\rangle = \left[\prod_{{\bf i},\sigma} \hat{c}_{{\bf i},\sigma}^{\dagger}(\hat{c}_{{\bf i}+{\bf r}_1,\sigma}^{\dagger} + \hat{c}_{{\bf i}+{\bf r}_2,\sigma}^{\dagger})\right] \hat{E}^{\dagger}(0)|0\rangle.$$

For finite flux  $(\delta \neq 0)$   $\hat{G}^{\dagger}$  no longer creates a double occupancy on each site of the s=3 sublattice, thus allowing electrons to move. To provide eigenvalue zero for the first two terms of  $\hat{H}$ , (12),  $\hat{E}^{\dagger}(\delta \neq 0)$  must be chosen such that it introduces one electron with *fixed* spin (say,  $\uparrow$ ) on each site of the s=3 sublattice, i.e.,  $\hat{E}^{\dagger}(\delta \neq 0)=\prod_{\bf i}\hat{c}^{\dagger}_{{\bf i}+{\bf r}_3,\uparrow}$ . As a consequence there will be one  $\uparrow$  spin electron on all sites; i.e., these electrons are immobile  $(N_{\uparrow}=3N_c,N_{\downarrow}=2N_c)$ . For  $\delta \neq 0$  the ground state for  $N=5N_c$  is therefore a nonsaturated ferromagnet independent of  $\delta$  and with a finite one-particle localization length  $\xi_{\downarrow}$  (the proof proceeds as in [14]).

III.b. Field induced itinerant ferromagnetism and insulator-metal transition at 5/3 < n < 2.—The properties of the ground state at  $\delta = 0$  remain valid even for  $N = 5N_c + \Delta N$  with  $1 < \Delta N < N_c$  since the ground state is now  $|\Psi_g^{\rm III}(N,\delta=0)\rangle = [\prod_{i=1}^{\Delta N}(\alpha_i'\hat{c}_{i+\mathbf{r}_1,\sigma_{i,1}}^{\dagger} + \beta_i'\hat{c}_{i+\mathbf{r}_2,\sigma_{i,2}}^{\dagger})] \times |\Psi_g^{\rm III}(5N_c,0)\rangle$ . The product is over  $\Delta N$  arbitrary sites; the coefficients  $\alpha_i'$ ,  $\beta_i'$  and spins  $\sigma_{i,1}$ ,  $\sigma_{i,2}$  are arbitrary. Thus, at  $\delta = 0$  one obtains again a localized ground state. For finite flux the ground state is instead

$$|\Psi_g^{\rm III}(N > 5N_c, \delta)\rangle = \prod_{\alpha=1}^{\Delta N} \hat{c}_{n_\alpha, \mathbf{k}_\alpha, -\sigma}^{\dagger} |\Psi_g^{\rm III}(5N_c, \delta)\rangle. \quad (14)$$

Since the ground state now contains plane-wave-type contributions and  $\delta\mu(5N_c+\Delta N)=0$  for  $\Delta N>1, |\Psi_g^{\rm III}(N>5N_c,\delta)\rangle$  corresponds to a conducting, nonsaturated ferromagnetic state with only mobile spin  $-\sigma$  electrons and a magnetization  $M \propto (1-\Delta N/N_c)$ . Hence the magnetic field induces an insulator-metal transition. In the metallic state the net magnetic moment decreases linearly with increasing density.

Solution III therefore has the following properties: At zero magnetic field,  $t_{\parallel}=0$ , and a sublattice potential  $\epsilon=t_{\perp}-t_{\perp}^{-1}$ , but otherwise arbitrary  $t_{\perp}<0$ , U>0, it represents a localized nonmagnetic ground state over a continuous range of densities  $n \geq 5/3$ . By contrast, at finite magnetic field and the potential  $\epsilon=t_{\perp}/\cos\delta-\cos\delta/t_{\perp}$ , but otherwise for the same parameters, a nonsaturated, ferromagnetic ground state is obtained. This state is localized at n=5/3, but gapless for n>5/3. For the latter density the majority spin  $(\sigma)$  electrons are immobile and only the minority spin  $(-\sigma)$  electrons are itinerant. Therefore, by varying the magnetic field and the sublattice potential one can tune from a localized, nonmagnetic ground state in the density range  $n \geq 5/3$  to a nonsaturated ferromagnet, which is insulating at n=5/3 and gapless for n>5/3.

In summary, by constructing exact ground states on the diamond Hubbard chain in a magnetic field we showed that this one-dimensional structure displays remarkably complex physical properties which originate from flat single-electron bands. The selected solutions describe flat band ferromagnetism, correlated half-metal behavior with spin-valve features, and insulator-metal transitions. These properties do not depend on the Zeeman interaction [18]. The virtue of tuning fundamentally different ground states through external magnetic fields or site-selective potentials thereby points to new possibilities for the design of electronic devices, which can switch between insulating or conducting and ferromagnetic or nonmagnetic states.

We thank K. Byczuk for discussions. Support by the Hungarian Scientific Research Fund through Contract No. OTKA-T48782, the Alexander von Humboldt Foundation, and the Deutsche Forschungsgemeinschaft through SFB 484 is gratefully acknowledged.

- [1] The Quantum Hall Effect, R. E. Prange and S. M. Girvin (Springer, New York, 1990).
- [2] R. Moessner and A. Ramirez, Phys. Today 59, No. 2, 24 (2006).
- [3] H. Ishii, T. Nakayama, and J. I. Inoue, Phys. Rev. B 69, 085325 (2004).
- [4] H. Tamura, K. Shiraishi, T. Kimura, and H. Takayanagi, Phys. Rev. B 65, 085324 (2002).
- [5] R. Arita, Y. Suwa, K. Kuroki, and H. Aoki, Phys. Rev. Lett. 88, 127202 (2002); Y. Suwa, R. Arita, K. Kuroki, and H. Aoki, Phys. Rev. B 68, 174419 (2003).
- [6] J. Vidal, B. Doucot, R. Mosseri, and P. Butaud, Phys. Rev. Lett. 85, 3906 (2000).
- [7] D. Jaksch, C. Bruder, J. I. Cirac, C. W. Gardiner, and P. Zoller, Phys. Rev. Lett. 81, 3108 (1998).
- [8] C. Wu, D. Bergman, L. Balents, and S. Das Sarma, arXiv:cond-mat/0701788.
- [9] O. Derzhko, A. Honecker, and J. Richter, arXiv:cond-mat/0703295.
- [10] A. Mielke and H. Tasaki, Commun. Math. Phys. 158, 341 (1993); H. Tasaki, Commun. Math. Phys. 242, 445 (2003).
- [11] E. H. Lieb, Phys. Rev. Lett. 62, 1201 (1989); S.-Q. Shen,Z.-M. Qiu, and G.-S. Tian, *ibid.* 72, 1280 (1994).
- [12] Z. Gulácsi and D. Vollhardt, Phys. Rev. Lett. 91, 186401 (2003); Phys. Rev. B 72, 075130 (2005).
- [13] While the fermionic identity  $(\hat{A}_{\mathbf{i},\sigma})^2 = 0$  holds, the anti-commutator is noncanonical:  $\{\hat{A}_{\mathbf{i},\sigma},\hat{A}_{\mathbf{j},\sigma}^{\dagger}\} \neq \delta_{\mathbf{i},\mathbf{j}}$ .
- [14] This is proved by calculating  $\Gamma_{\mathbf{r},-\sigma}$ . For  $|\mathbf{r}/\mathbf{a}| \gg 1$ ,  $\Delta N = 1$ , s = 1, one finds  $\Gamma_{\mathbf{r},-\sigma}/\Gamma_{\mathbf{r},-\sigma}^{(1)} = 1 [2 + (1 \cos ak)/t_{\perp}]^{-1}$ .  $\Gamma_{\mathbf{r},-\sigma}^{(1)}$  is the plane wave result and k is the momentum of the electron added above n = 4/3.
- [15] Here  $\delta \mu(N) = E_g^{\text{II}}(N+1) 2E_g^{\text{II}}(N) + E_g^{\text{II}}(N-1)$  and  $E_g^{\text{II}}(N)$  defined below Eq. (8).
- [16] B. Dieny, Phys. Rev. B 43, 1297 (1991).
- [17] Density functional theory recently predicted also half-metallic behavior for an organometallic wire; see V. V. Maslyuk *et al.*, Phys. Rev. Lett. **97**, 097201 (2006).
- [18] A Zeeman coupling alters only solution I for n < 1/3, where one would obtain a ferromagnetic solution.