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Exact results for the excitonic phase

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Abstract. We construct exactly solvable models with arbitrary filling for any number of dimensions in which an excitonic phase arises. The ground-state and thermodynamic properties are investigated. There is a parameter region in the ground-state phase diagrams where an excitonic phase is sandwiched between an insulating phase and a semimetallic phase.

In 1961 Mott proposed that, under certain circumstances in a semimetal, holes and electrons can form excitons, and they then condense, thereby leading to an *excitonic phase* [1]. Since then this has been a subject of considerable experimental and theoretical interest [2]. For example, there is a recent proposal that a large droplet of a high-density excitonic phase can be stabilized in a suitably arranged quantum well structure where the electrons and holes are spatially separated [3]. To shed light on the excitonic phase, here we propose models in which an excitonic phase arises in certain parameter regions. Although our models involve some idealization of the real situations, they have the attractive feature of being exactly solvable. We shall obtain the ground-state and thermodynamic quantities explicitly. Some of Mott's proposals will be confirmed exactly. Thus it is possible that our model describes a universality class proposed by Mott. From our results one can gain much insight into the universal properties of an excitonic phase.

We begin by considering a two-band model with interband interactions described by the Hamiltonian

$$\mathcal{H} = \mathcal{H}_{\text{kin}} + \mathcal{H}_{\text{int}} \quad (1)$$

$$\mathcal{H}_{\text{kin}} = \sum_k \epsilon^{(v)}(k) c_k^{(v)\dagger} c_k^{(v)} + \sum_k \epsilon^{(c)}(k) c_k^{(c)\dagger} c_k^{(c)} \quad (2)$$

$$\mathcal{H}_{\text{int}} = -\frac{U}{N} \left(\sum_k c_k^{(c)\dagger} c_k^{(v)} \right) \left(\sum_{k'} c_{k'}^{(v)\dagger} c_{k'}^{(c)} \right) \quad (3)$$

where $c_k^{(v)}$ and $c_k^{(c)}$ are the fermion annihilation operators for the valence band, and the conduction band, and $\epsilon^{(v)}(k)$ and $\epsilon^{(c)}(k)$ are the energy dispersions of the valence band and the conduction band, respectively. The momentum vector \mathbf{k} takes values in the d -dimensional Brillouin zone. The interaction Hamiltonian \mathcal{H}_{int} represents the interaction between electrons in the conduction band and holes in the valence band. We impose the

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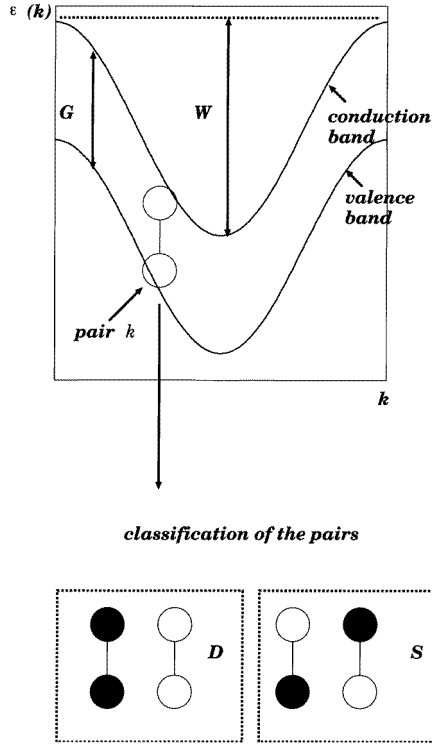


Figure 1. The band structure, and classification of the pairs.

constraint on the band structure that the valence band and the conduction band are ‘parallel’, i.e.

$$\epsilon^{(c)}(k) = \epsilon^{(v)}(k) + G \quad (4)$$

where G is independent of k (see figure 1). We set G and U positive and $\sim O(N^0)$, where N is the number of momentum points in the Brillouin zone. The spin degrees of freedom are neglected for simplicity, since we do not consider spin-related quantities here.

The main part of the diagonalization consists in two steps: (i) showing that the kinetic term \mathcal{H}_{kin} and the interaction term \mathcal{H}_{int} in (1), (2), and (3) act on different Hilbert spaces; (ii) reducing the problem to a quantum spin system which is exactly solvable.

For a fixed number of electrons, define sets \mathcal{S} and \mathcal{D} as follows (see figure 1): consider a pair which consists of a momentum point k in the valence band and in the conduction band. We denote the pair by k , where k takes values in the Brillouin zone. Denote the set of k s which are singly occupied as \mathcal{S} . The set \mathcal{D} consists of k s which are doubly occupied or empty. Note that $\mathcal{S} \cap \mathcal{D} = \emptyset$ and $\mathcal{S} \cup \mathcal{D} = \text{the Brillouin zone}$. The choice of \mathcal{S} and \mathcal{D} is not unique. Let us denote a realization of \mathcal{S} and \mathcal{D} by an index i . Introduce a Hilbert space spanned by the basis vectors

$$c_{l_1}^{(v)\dagger} \cdots c_{l_{N_e^v}}^{(v)\dagger} c_{m_1}^{(c)\dagger} \cdots c_{m_{N_e^c}}^{(c)\dagger} |0\rangle_{\mathcal{S}_i} \otimes (c_{k_1}^{(v)\dagger} c_{k_1}^{(c)\dagger})(c_{k_2}^{(v)\dagger} c_{k_2}^{(c)\dagger})(c_{k_3}^{(v)\dagger} c_{k_3}^{(c)\dagger}) \cdots (c_{k_M}^{(v)\dagger} c_{k_M}^{(c)\dagger}) |0\rangle_{\mathcal{D}_i} \quad (5)$$

where $l_1, \dots, l_{N_e^v}, m_1, \dots, m_{N_e^c}$, and $k_1, k_2, k_3, \dots, k_M$ take values in the Brillouin zone with $\{l_1, \dots, l_{N_e^v}, m_1, \dots, m_{N_e^c}\} = \mathcal{S}_i$, and $k_1, k_2, k_3, \dots, k_M \in \mathcal{D}_i$. Note that N_e^v (N_e^c) is the number of electrons in the valence (conduction) band in \mathcal{S}_i , and M is the number of doubly occupied pairs in \mathcal{D}_i . N_e^v , N_e^c , and M can be varied. Here the state $|0\rangle_{\mathcal{S}_i}$ is defined by $c_k^{(c)} |0\rangle_{\mathcal{S}_i} = 0$ ($k \in \mathcal{S}_i$) and $c_k^{(v)} |0\rangle_{\mathcal{S}_i} = 0$ ($k \in \mathcal{S}_i$). The state $|0\rangle_{\mathcal{D}_i}$ is defined by

$c_k^{(c)}|0\rangle_{\mathcal{D}_i} = 0$ ($k \in \mathcal{D}_i$) and $c_k^{(v)}|0\rangle_{\mathcal{D}_i} = 0$ ($k \in \mathcal{D}_i$). The direct sum of the Hilbert spaces with all the possible sets \mathcal{S}_j and \mathcal{D}_j is the Hilbert space that we consider, which is equivalent to the Hilbert space with a fixed number of electrons.

Let us introduce an operator \mathcal{P}^j which is a projection operator in the Hilbert space where \mathcal{S} and \mathcal{D} are fixed as \mathcal{S}_j and \mathcal{D}_j , and $\sum_j \mathcal{P}^j = \mathbf{1}$, where $\mathbf{1}$ is the identity operator. The Hamiltonian can be written as

$$\mathcal{H} = \left(\sum_j \mathcal{P}^j \right) \mathcal{H} \left(\sum_j \mathcal{P}^j \right) = \sum_j \mathcal{P}^j \mathcal{H} \mathcal{P}^j. \tag{6}$$

From relation (4), we have

$$\begin{aligned} \mathcal{P}^j \mathcal{H} \mathcal{P}^j &= \mathcal{P}^j \mathcal{H}_{\text{kin}} \mathcal{P}^j + \mathcal{P}^j \mathcal{H}_{\text{int}} \mathcal{P}^j \\ &= \mathcal{P}^j (\mathbf{1} \otimes \mathcal{H}_I) \mathcal{P}^j + G N_e^c + \mathcal{P}^j (\mathcal{H}_{\text{II}} \otimes \mathbf{1}) \mathcal{P}^j + \text{constant} \end{aligned} \tag{7}$$

where \mathcal{H}_I and \mathcal{H}_{II} are

$$\begin{aligned} \mathcal{H}_I &= - \sum_{k \in \mathcal{D}_j} \epsilon^{(v)}(k) c_k^{(v)} c_k^{(v)\dagger} + \sum_{k \in \mathcal{D}_j} \epsilon^{(c)}(k) c_k^{(c)\dagger} c_k^{(c)} \\ \mathcal{H}_{\text{II}} &= - \frac{U}{N} \left(\sum_{k \in \mathcal{S}_j} c_k^{(c)\dagger} c_k^{(v)} \right) \left(\sum_{k' \in \mathcal{S}_j} c_{k'}^{(v)\dagger} c_{k'}^{(c)} \right). \end{aligned} \tag{8}$$

Here the essential feature revealed is that the kinetic term and the interaction term act on different Hilbert spaces, i.e. ‘separation’ of the Hamiltonian. In the following we shall neglect the irrelevant constant term in the Hamiltonian.

Now we shall reduce the problem to diagonalization of a quantum spin system. Here the SU(2) algebra hidden in spinless fermions in the two-band system plays a crucial role (the hidden SU(2) algebra was used in [4–7] in different contexts). Let us define the ‘spin’ operators $\hat{S}_k^+ = \hat{S}_k^x + i\hat{S}_k^y$, $\hat{S}_k^- = \hat{S}_k^x - i\hat{S}_k^y$, and \hat{S}_k^z as $\mathcal{P}^j c_k^{(v)\dagger} c_k^{(c)} \mathcal{P}^j$, $\mathcal{P}^j c_k^{(c)\dagger} c_k^{(v)} \mathcal{P}^j$, and $\mathcal{P}^j \frac{1}{2} (c_k^{(v)\dagger} c_k^{(v)} - c_k^{(c)\dagger} c_k^{(c)}) \mathcal{P}^j$ respectively. The ‘total spin’ operator \hat{S}^α is

$$\sum_{k \in \mathcal{S}_j} \hat{S}_k^\alpha \quad (\alpha = x, y, z)$$

and $(\hat{S})^2$ is $(\hat{S}^x)^2 + (\hat{S}^y)^2 + (\hat{S}^z)^2$. The operators satisfy

$$[\hat{S}_k^l, \hat{S}_{k'}^m] = i \epsilon_{lmn} \hat{S}_k^n \delta_{kk'} \tag{9}$$

$$(\hat{S}_k^x)^2 + (\hat{S}_k^y)^2 + (\hat{S}_k^z)^2 = \frac{1}{2} \left(\frac{1}{2} + 1 \right) \tag{10}$$

where k and k' are in \mathcal{S}_j . Thus \hat{S}_k^x , \hat{S}_k^y , and \hat{S}_k^z ($k \in \mathcal{S}_j$) are the components of an $s = \frac{1}{2}$ quantum spin. Then we have

$$\mathcal{P}^j (\mathcal{H}_{\text{II}} \otimes \mathbf{1}) \mathcal{P}^j = \mathcal{P}^j (\mathcal{H}_{\text{spin}} \otimes \mathbf{1}) \mathcal{P}^j \tag{11}$$

where $\mathcal{H}_{\text{spin}}$ is given by

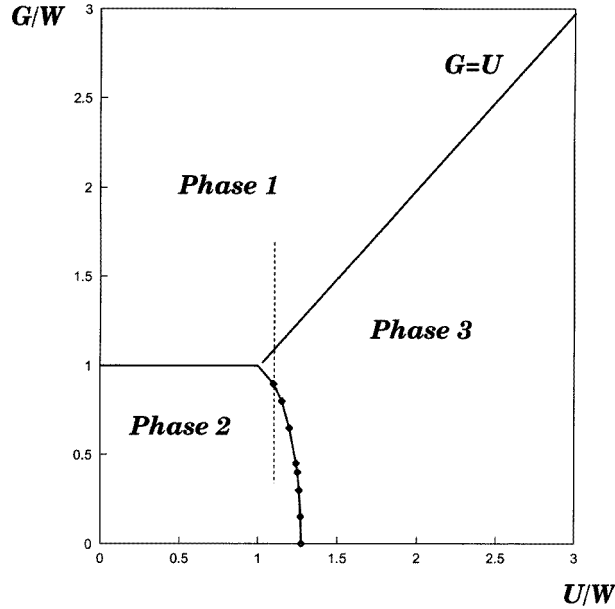
$$\begin{aligned} \mathcal{H}_{\text{spin}} &= - \frac{U}{N} \left(\sum_{k \in \mathcal{S}_j} \hat{S}_k^x - i\hat{S}_k^y \right) \left(\sum_{k' \in \mathcal{S}_j} \hat{S}_{k'}^x + i\hat{S}_{k'}^y \right) = - \frac{U}{N} (\hat{S}^x - i\hat{S}^y) (\hat{S}^x + i\hat{S}^y) \\ &= - \frac{U}{N} \{ (\hat{S})^2 - (\hat{S}^z)^2 - (\hat{S}^z) \}. \end{aligned} \tag{12}$$

Now we can identify k as a ‘site’ on which an $s = \frac{1}{2}$ quantum spin is defined. In the spin language, a spin is ‘up’, if the valence band part of the pair k is occupied, and a spin is

‘down’, if the conduction band part of the pair k is occupied. Note that, since k takes values in \mathcal{S}_j , all of the pairs considered are singly occupied. Now diagonalize $\mathcal{H}_{\text{spin}}$, which can be identified with a quantum spin Hamiltonian ($s = \frac{1}{2}$). Define $|S, S^z\rangle$ by an eigenstate of $(\hat{S})^2$ and \hat{S}^z which satisfies $(\hat{S})^2|S, S^z\rangle = S(S+1)|S, S^z\rangle$ and $\hat{S}^z|S, S^z\rangle = S^z|S, S^z\rangle$. The energy is specified by S and S^z (see (12)). There is, however, non-trivial degeneracy which is given by

$$\frac{(2S_{\text{max}})!(2S+1)}{(S_{\text{max}}-S)!(S_{\text{max}}+S+1)!}$$

where S_{max} is $N_{\mathcal{S}_j}/2$ and $N_{\mathcal{S}_j}$ is the number of elements in \mathcal{S}_j . This degeneracy plays a crucial role in the thermodynamic properties.



**Phase Diagram
at $T=0$ (Model A)**

Figure 2. The ground-state phase diagram of the one-dimensional two-band model (model A), where $\epsilon^{(c)}(k) = -(W/2)\cos k + W/2 + G/2$ and $\epsilon^{(v)}(k) = -(W/2)\cos k + W/2 - G/2$. The phase boundary between phase 2 and phase 3 was determined numerically. For example, an excitonic phase is sandwiched between a band insulator phase and a semimetallic phase for a range of G/W along the dashed line.

Let us consider a state

$$|S, S^z\rangle \otimes c_{p_1}^{(v)} c_{p_2}^{(v)} c_{p_3}^{(v)} \dots c_{p_L}^{(v)} c_{q_1}^{(c)\dagger} c_{q_2}^{(c)\dagger} c_{q_3}^{(c)\dagger} \dots c_{q_M}^{(c)\dagger} \prod_{k \in \mathcal{D}_j} c_k^{(v)\dagger} |0\rangle_{\mathcal{D}_j} \quad (13)$$

where L is the number of the holes in the valence band in \mathcal{D}_j , and M is the number of electrons in the conduction band in \mathcal{D}_j . From the ‘separation’ of the Hamiltonian (7) and the mapping to a quantum spin system (11), it can be seen that (13) is an eigenvector of

\mathcal{H} with an eigenvalue

$$-\frac{U}{N}[r^2 - (N_{S_j} + 1)r + N_e^c(N_{S_j} - N_e^c + 1)] + GN_e^c - \sum_{l=1}^L \epsilon^{(v)}(p_l) + \sum_{m=1}^M \epsilon^{(c)}(q_m) \quad (14)$$

where the r ($0 \leq r \leq N_{S_j}/2$, r : integer) are defined by $N_{S_j}/2 - S$. The total number of electrons is given by $N_{S_j} + 2M$. Varying the index j , \mathcal{H} is diagonalized completely.

Now let us consider the physical properties of the system in the thermodynamic limit ($N \rightarrow \infty$). For simplicity, we consider the half-filled case, namely, $N_{S_j} + 2M = N$. When the interaction is absent, the system is an insulator or a semimetal, depending on G .

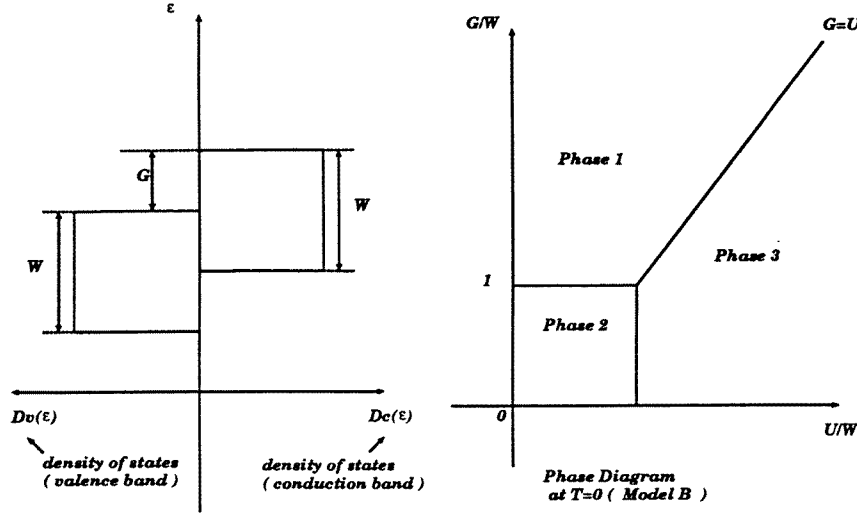


Figure 3. The density of states and the ground-state phase diagram of model B.

Let us consider the ground-state properties. The ground state is obtained by minimizing the energy (14). The competition between the kinetic term and the interaction term gives a rich phase diagram. We present the phase diagrams for two cases: (model A) a one-dimensional two-band model, as shown in figure 2; and (model B) a system with a constant density of states, which resembles that of the 2d systems (see figure 3). We find three different types of phase as shown in figures 2 and 3. Introduce the order parameter Δ [2] to characterize the phases:

$$\Delta = \sqrt{\frac{1}{N^2} \int dx \int dy \langle \psi^{(c)\dagger}(x) \psi^{(v)}(x) \psi^{(v)\dagger}(y) \psi^{(c)}(y) \rangle} \quad (15)$$

where the real-space field operators are

$$\psi^{(c)}(x) = \frac{1}{\sqrt{N}} \sum_k e^{ikx} c_k^{(c)}$$

and

$$\psi^{(v)}(x) = \frac{1}{\sqrt{N}} \sum_k e^{ikx} c_k^{(v)}.$$

The contents of the three phases are as follows.

Phase 1: $\Delta = 0$. The ground state is a band insulator as in the non-interacting case.

Phase 2: $\Delta = 0$. The ground state is a semimetal as in the non-interacting case.

Phase 3: $\Delta = \frac{1}{2}\sqrt{1 - (G/U)^2}$. The ground state is an excitonic phase.

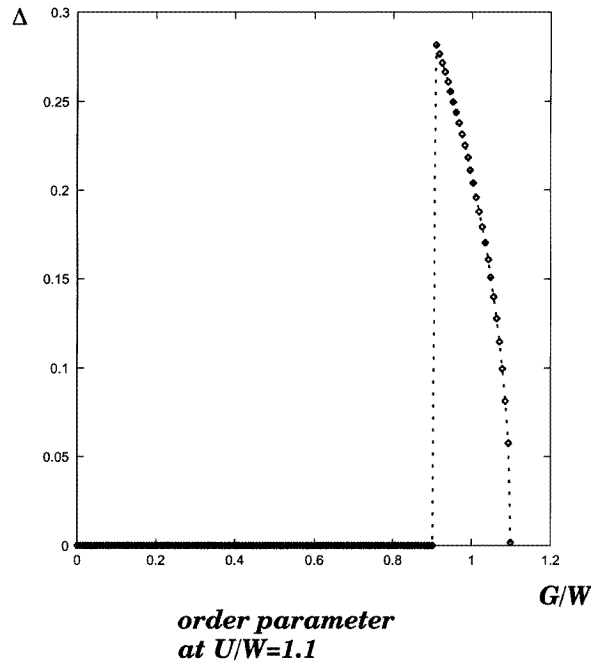


Figure 4. The order parameter of the ground state for $U/W = 1.1$ for model A. One can see that an excitonic phase is sandwiched between a band insulator phase and a semimetallic phase.

Note that there is a parameter region in model A where an excitonic phase is sandwiched between an insulating phase and a semimetallic phase, which is the picture proposed by Mott in 1961 [1] (see figures 2 and 4).

Next we consider the thermodynamic properties. For simplicity, let us take a system with flat bands ($\epsilon^{(c)} = \epsilon + G/2$, $\epsilon^{(v)} = \epsilon - G/2$). The grand partition function is

$$\mathcal{Z}_{\text{grand}} = \sum_{\substack{L, M \\ 0 \leq L+M \leq N}} \sum_{\substack{r; \text{ integer} \\ 0 \leq r \leq N_{S_j}/2}} \sum_{N_e^c=r}^{N_{S_j}-r} \mathcal{C} \exp(-\beta \mathcal{E}) \quad (16)$$

where \mathcal{C} and \mathcal{E} are defined by

$$\mathcal{C} = \frac{N!}{N_{S_j}! L! M!} \frac{N_{S_j}! (N_{S_j} - 2r + 1)}{r! (N_{S_j} - r + 1)!}$$

and

$$\begin{aligned} \mathcal{E} = & -\mu(N - L + M) + L(G/2 - \epsilon) + M(G/2 + \epsilon) + GN_e^c \\ & - \frac{U}{N} \{r^2 - (N_{S_j} + 1)r + N_e^c(N_{S_j} - N_e^c)\}. \end{aligned}$$

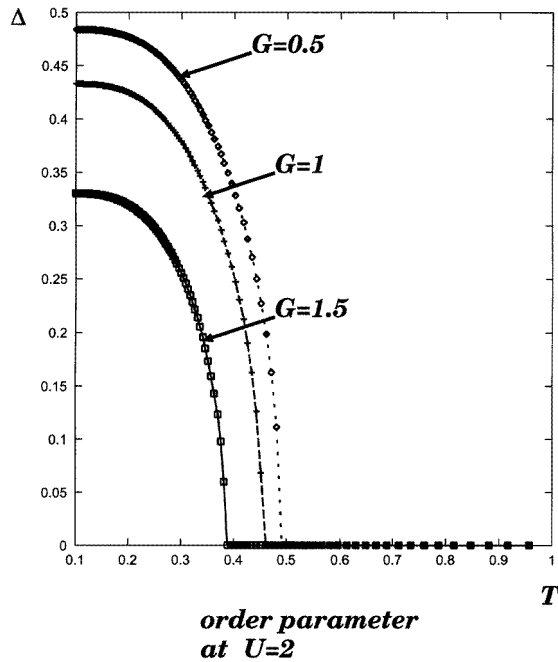


Figure 5. The temperature dependence of the order parameter for $U = 2$ for the flat-bands model.

In the thermodynamic limit ($N \rightarrow \infty$) the saddle-point method can be used. The chemical potential is set as $\mu = \epsilon$ and the system is half-filled. A direct calculation leads to analytic forms of the thermodynamic quantities. For example, $\Delta(T)$ is given by

$$\Delta(T) = 0.5 \sqrt{\left(\frac{y-1}{y+1}\right)^2 - \left(\frac{G}{U}\right)^2} \quad (17)$$

where y is the root of

$$\log x = \frac{1}{2} U T^{-1} (x-1)(x+1)^{-1} \quad (x \geq (1+U^{-1}G)(1-U^{-1}G)^{-1})$$

and, if there is no solution, $\Delta = 0$. The free energy $\Omega(T)$ per unit cell below T_c is given by

$$\Omega(T)/N = -2T(y+1) + 2T \frac{y}{y+1} \log y - \frac{1}{4} U \frac{(y-1)^2}{(y+1)^2} - \frac{1}{4} U^{-1} G^2 + \frac{1}{2} G. \quad (18)$$

As shown in figure 5, $\Delta(T) \sim (T_c - T)^\beta$ ($\beta = 1/2$) near the critical temperature, and the second-order phase transition occurs at a finite temperature. A more detailed study of the thermodynamic properties will be presented elsewhere.

In summary, we have constructed exactly solvable models where an excitonic phase arises in certain parameter regions. All of the eigenvalues and the eigenvectors were obtained explicitly. The ground-state phase diagrams have interesting structures. Mott's proposal that an excitonic phase is sandwiched between an insulating phase and a semimetallic phase was confirmed exactly. The thermodynamic properties were also discussed. We found that a second-order phase transition occurs at a finite temperature.

Although our results presented here are restricted to the cases where fully analytical treatments are possible, it is straightforward to analyse more general cases—for example, away from half-filling, and the thermodynamics for non-flat bands. For the more general cases, the essential features such as the critical exponent β and the topology of the ground-state phase diagram do not differ, and they seem to lie in the same universality class as the present case. They will be presented elsewhere.

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