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Magnetic phase transition of the one-dimensional Hubbard model under fixed chemical potential

Hirohito Kiwata

Department of Physics, Faculty of Science, Osaka University, Toyonaka, Osaka 560, Japan

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Abstract. We study the magnetic properties of the one-dimensional Hubbard model under fixed chemical potential. By using derivatives of the Lieb–Wu equation, the magnetization curve at zero temperature is obtained for various fixed band fillings and/or chemical potentials. As a well known result, in the case of the fixed band filling, there is only one second-order phase transition at magnetic saturation. On the other hand, when the chemical potential is fixed instead of the electron density, it is found that there is an additional phase transition in the magnetization curve.

Low-dimensional systems have drawn much attention for several decades. One of the reasons is that techniques for manufacturing materials of quasi-low-dimensional systems have developed and that properties which are characteristic to low-dimensional systems have been observed. Another reason is that one-dimensional systems are easy to handle and that exact solutions are obtained in some cases. The investigation of them is helpful to understand the nature of higher-dimensional systems. The one-dimensional Hubbard model is the simplest model for itinerant electrons on a lattice and has attracted much interest for a long time [1]. The one-dimensional Hubbard Hamiltonian in a magnetic field h is given as follows:

$$H = -\sum_{i,\sigma}\left(a_{i\sigma}^{\dagger}a_{i+1\sigma} + a_{i+1\sigma}^{\dagger}a_{i\sigma}\right) + U\sum_{i} n_{i\uparrow}n_{i\downarrow} - \frac{h}{2}\sum_{i}\left(n_{i\uparrow} - n_{i\downarrow}\right) - \mu\sum_{i}\left(n_{i\uparrow} + n_{i\downarrow}\right) \tag{1}$$

where $a_{i\sigma}^{\dagger}$ ($a_{i\sigma}$) is the creation (annihilation) operator of the electron with the spin σ at the ith site, $n_{i\sigma}$ the number operator $a_{i\sigma}^{\dagger}a_{i\sigma}$ and μ the chemical potential. For simplicity, the hopping integral is taken to be unity. The eigenvalue problem of this model is reduced to a set of integral equations (Lieb–Wu equation [2]) by means of the nested Bethe *ansatz* [3]. For the half-filling and singlet case, an explicit solution of the integral equations is derived as the closed form [2]. The magnetic properties of the one-dimensional Hubbard model have been investigated by several authors. The magnetization curve for the half-filled band has been obtained by Takahashi [4]. Shiba [5] calculated the zero-field magnetic susceptibility for arbitrary fillings, but for repulsive (positive) U only. Extending these works, the zero-field magnetic susceptibility at finite temperature is derived by Kawakami *et al* [6] by solving the thermodynamic Bethe *ansatz* equations [7]. The magnetization curve for several electron densities at negative U was studied by Woynarovich and Penc [8]. In

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this paper we study the magnetic properties of the one-dimensional Hubbard model with repulsive interactions. The magnetic properties of the positive-U Hubbard chain, which has no gap in the spin excitation [9, 10], are very different from those of the negative one, which has a gap.

Recently the technique for high-field magnetic measurement have been improved and various kinds of experiment have been done. In order to understand magnetic properties of low-dimensional systems, it is interesting to study the low-dimensional magnetic behaviour theoretically. It has been shown that there are additional phase transitions for the SU(M) quantum spin chain [11, 12]. In the present paper we calculate the magnetization curve for arbitrary fixed electron densities and/or chemical potential and show that there is a similar phase transition in the electron system.

We start by recalling the integral equations given by Lieb and Wu [2] for the ground state energy of the one-dimensional Hubbard model with fixed magnetization and fixed number of electrons:

$$2\pi\rho_1(k) = 1 + \cos k \int_{-B}^{B} \frac{8U\rho_2(\lambda)\,\mathrm{d}\lambda}{U^2 + 16(\sin k - \lambda)^2} \tag{2}$$

$$\int_{-Q}^{Q} \frac{8U\rho_1(k)\,\mathrm{d}k}{U^2 + 16(\lambda - \sin k)^2} = 2\pi\rho_2(\lambda) + \int_{-B}^{B} \frac{4U\rho_2(\lambda')\,\mathrm{d}\lambda'}{U^2 + 4(\lambda - \lambda')^2}. \tag{3}$$

The integration bounds B and Q are determined by

$$\int_{-Q}^{Q} \rho_1(k)\,\mathrm{d}k = \frac{N}{N_a} = n \tag{4}$$

$$\int_{-B}^{B} \rho_2(\lambda)\,\mathrm{d}\lambda = \frac{N_\downarrow}{N_a} \tag{5}$$

where N is the total number of electrons, N_a the number of lattice sites and $N_\downarrow$ the number of down-spin electrons. The energy per site ϵ and the magnetization per site m are given by

$$\epsilon(n, m) = \frac{E}{N_a} = -2\int_{-Q}^{Q} \cos k\rho_1(k)\,\mathrm{d}k \tag{6}$$

$$m = \frac{S^Z_{\text{total}}}{N_a} = \frac{1}{2}\int_{-Q}^{Q} \rho_1(k)\,\mathrm{d}k - \int_{-B}^{B} \rho_2(\lambda)\,\mathrm{d}\lambda. \tag{7}$$

Following Woynarovich and Penc's procedures [8], we can derive formulas for the magnetic field h and the magnetic susceptibility χ_m.

$$h = \left.\frac{\partial\epsilon}{\partial m}\right|_{n=\text{fixed}} = \frac{\epsilon_1(Q)\xi_{21}(B) - \epsilon_2(B)\xi_{11}(Q)}{D} \tag{8}$$

$$\chi_m^{-1} = \left.\frac{\partial^2\epsilon}{\partial m^2}\right|_{n=\text{fixed}} = \frac{1}{2D^2}\left\{\frac{v_1(Q)\xi_{21}(B)\xi_{21}(B)}{\rho_1(Q)} + \frac{v_2(B)\xi_{11}(Q)\xi_{11}(Q)}{\rho_2(B)}\right\} \tag{9}$$

where $D = \xi_{11}(Q)\xi_{22}(B) - \xi_{12}(Q)\xi_{21}(B)$ and our notation relies on Woynarovich and Penc [8]. The magnetic field h and the magnetic susceptibility χ_m depend on the electron

densities n in (4) and the magnetization m in (7) through the integration bounds Q and B. The chemical potential μ and the charge susceptibility χ_c are also given by

$$\mu = \left.\frac{\partial \epsilon}{\partial n}\right|_{m=\text{fixed}} = \frac{-\epsilon_1(Q)\{\xi_{21}(B) - 2\xi_{22}(B)\} + \epsilon_2(B)\{\xi_{11}(Q) - 2\xi_{12}(Q)\}}{2D} \tag{10}$$

$$\chi_c^{-1} = \left.\frac{\partial^2 \epsilon}{\partial n^2}\right|_{m=\text{fixed}} = \frac{1}{8D^2}\left\{\frac{v_1(Q)[\xi_{21}(B) - 2\xi_{22}(B)]^2}{\rho_1(Q)} + \frac{v_2(B)[\xi_{11}(Q) - 2\xi_{12}(Q)]^2}{\rho_2(B)}\right\}. \tag{11}$$

A detailed derivation can be found in [8], [13] and [14]. Using these equations (2)–(11), one can deal with various limiting cases analytically. In the case of $B \to \infty$, which corresponds to the singlet state, the zero-field magnetic susceptibility for arbitrary fillings is reproduced [5]. The case of the magnetic saturation corresponds to $B \to 0$. At the saturation field h_c, the spins of all electrons are aligned in the direction of the external field. One can determine the saturation field h_c as follows:

$$h_c(n) = \begin{cases} -(4/\pi)\cos(\pi n)\tan^{-1}\{(4/U)\sin(\pi n)\} \\ +(4/\pi)\sqrt{1+(U/4)^2}\tan^{-1}\{(4/U)\sqrt{1+(U/4)^2}\tan(\pi n)\} - Un \\ \qquad \text{for } 0 < n < \frac{1}{2} \\ -(4/\pi)\cos(\pi n)\tan^{-1}\{(4/U)\sin(\pi n)\} \\ -(4/\pi)\sqrt{1+(U/4)^2}\tan^{-1}\{(4/U)\sqrt{1+(U/4)^2}\cot\pi(n-\frac{1}{2})\} \\ +4\sqrt{1+(U/4)^2} - U + (U/\pi)\tan^{-1}\{\cot\pi(n-\frac{1}{2})\} \\ \qquad \text{for } \frac{1}{2} < n < 1. \end{cases} \tag{12}$$

This formula has already been derived by several authors [15, 16, 17]. At the saturation field h_c, the magnetic susceptibility $\chi_{m,c}$ and the chemical potential μ_c can also be calculated. They lead to

$$\chi_{m,c}(n)^{-1} = 2\pi\sin(\pi n)\left[\frac{2}{\pi}\tan^{-1}\left\{\frac{4}{U}\sin(\pi n)\right\}\right]^2 \tag{13}$$

$$\mu_c(n) = \begin{cases} \cos(\pi n)[(2/\pi)\tan^{-1}\{(4/U)\sin(\pi n)\} - 2] \\ -(2/\pi)\sqrt{1+(U/4)^2}\tan^{-1}\{(4/U)\sqrt{1+(U/4)^2}\tan(\pi n)\} + (U/2)n \\ \qquad \text{for } 0 < n < \frac{1}{2} \\ \cos(\pi n)[(2/\pi)\tan^{-1}\{(4/U)\sin(\pi n)\} - 2] \\ +(2/\pi)\sqrt{1+(U/4)^2}\tan^{-1}\{(4/U)\sqrt{1+(U/4)^2}\cot\pi(n-\frac{1}{2})\} \\ -2\sqrt{1+(U/4)^2} + (U/2) - (U/2\pi)\tan^{-1}\{\cot\pi(n-\frac{1}{2})\} \\ \qquad \text{for } \frac{1}{2} < n < 1. \end{cases} \tag{14}$$

For other values of Q and B, these integral equations are solved numerically. In order to obtain these quantities (4)–(11), the integral equations (2) and (3) are converted into matrix equations, so that the magnetic field dependence of the magnetization for various fixed densities and/or chemical potentials is calculated.

The magnetization curves for various values of the band filling at $U = 3$ are shown in figure 1. The magnetization saturates $m = n/2$ at the finite field h_c. Figure 2 shows the magnetic susceptibilities χ_m as a function of the magnetic field h for various fixed electron

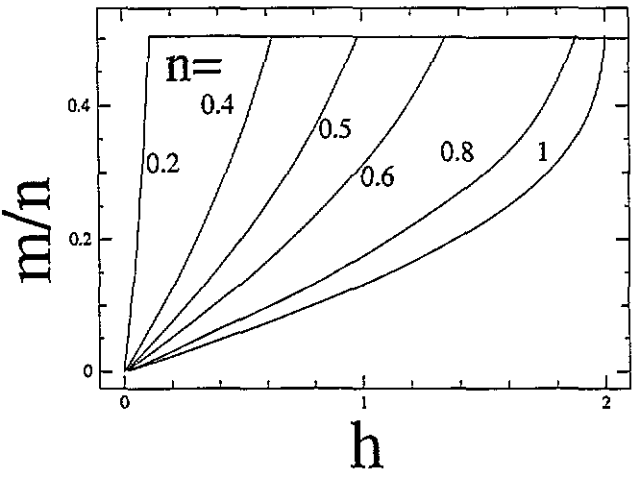

Figure 1. Magnetization curves of the one-dimensional Hubbard model with $U = 3$ for various fixed densities n.

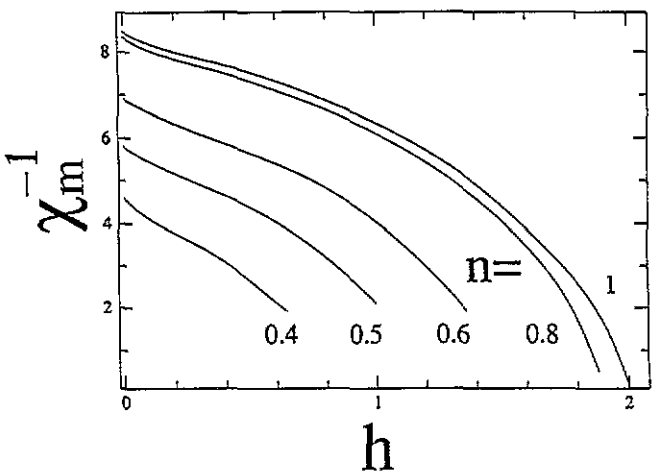

Figure 2. Magnetic susceptibilities of the one-dimensional Hubbard model with $U = 3$ for various fixed densities n.

densities. The susceptibility of the half-filling case is divergent at the magnetic saturation h_c [15].

So far, we have studied the magnetic properties with given electron densities. We now investigate those for fixed chemical potential instead of electron densities. The magnetization curves m versus h for various values of the chemical potential are shown in figure 3. Each curve consists of two parts, a broken curve and a solid one. The broken curve shows the magnetization versus the external magnetic field in the subspaces $N_\downarrow = 0$. In this case, the solution of the integral equations becomes

$$\rho_{1,N_\downarrow=0}(k) = \frac{1}{2\pi} \qquad \rho_{2,N_\downarrow=0}(\lambda) = 0. \tag{15}$$

We substitute the solution (15) into (6) and (7) and eliminate Q, which leads to the result

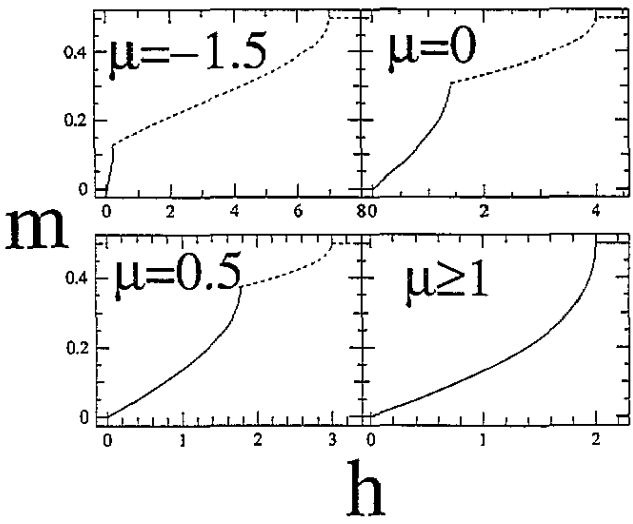

Figure 3. Magnetization of the one-dimensional Hubbard model with $U = 3$ for various chemical potentials μ. As the chemical potential becomes high, the critical field h_c shifts from left to right.

$$\epsilon_{N_\downarrow=0}(m) = -\frac{2}{\pi}\sin(2\pi m). \tag{16}$$

The magnetization as a function of the magnetic field in the chemical potential μ is

$$m = \frac{1}{2\pi}\cos^{-1}\{-\tfrac{1}{4}(2\mu + h)\}. \tag{17}$$

The solid curves in figure 3 are drawn by solving a set of integral equations (2), (3), (7) and (8) on the condition $N_\downarrow \neq 0$. As shown in figure 3, each curve has a cusp at a critical field $h_c = h_c(\mu)$, implying the field-induced phase transition at zero temperature. Since the magnetization curve is continuous, the phase transition is of second order. The critical field h_c as a function of the chemical potential is given by eliminating n from (12) and (14) (see figure 4). Since the ground state energy as a function of U is shown to be analytically continued at $U = 0$ for non-zero magnetization [18], the critical field h_c is also analytically continued at $U = 0$. In the case of the fixed chemical potential, the magnetization saturates at $h_s = 4 - 2\mu$.

We clarify the mechanism of this phase transition. Figure 5 shows schematically the configuration of the electrons in the magnetic field and the chemical potential. A circle denotes a site, an up arrow an up-spin electron and a down arrow a down-spin electron. In the first row, the magnetic field h is equal to zero and the chemical potentials are in the order of $\mu_1 < \mu_2 < \mu_3$. The number of electrons is obtained as a function of the chemical potential μ by solving $\mu = \mu(n)$. The higher the chemical potential is, the larger the number of the electrons is. In the second column of figure 5, the magnetic field dependence of the electron configuration is exhibited. As the magnetic field h becomes high, the spins of the electrons are overturned in the direction of the magnetic field h. This behaviour corresponds to the solid curve in figure 3. At h_c all of the spins are aligned. When the magnetic field is higher than h_c, the number of electrons with up spin increases and then becomes the half-filled one at h_s. This behaviour corresponds to the broken curve

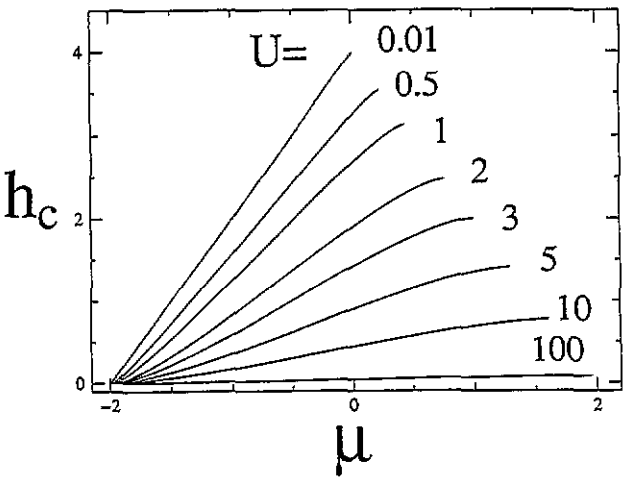

Figure 4. The critical magnetic field h_c as a function of the chemical potential μ for various values of U.

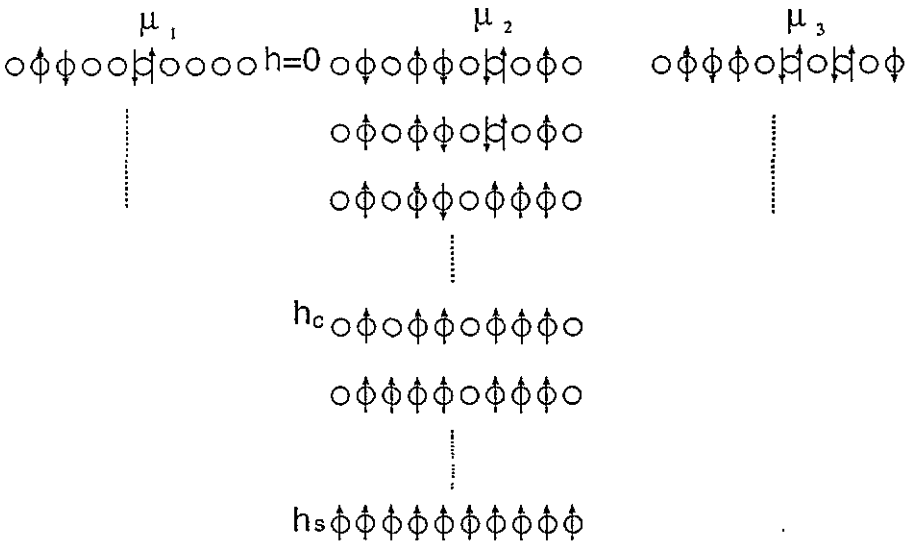

Figure 5. Schematic figure for the configuration of the electrons in the magnetic field and the chemical potential.

in figure 3. As the chemical potential increases, the value of the critical field h_c becomes large and this behaviour is found in figure 4. From figures 4 and 5, when the value of the chemical potential is less than -2 for each U, the magnetization curve consists of one part (broken curve). In the case where the value of the chemical potential is higher than the value of the right end of each curve in figure 4, the electron density is already half filled at $h = 0$, and the magnetization curve is the same as the half-filling one. As a result, it is found that there is an additional phase transition in the range of the μ curve in figure 4.

In summary, we have shown that the one-dimensional Hubbard model undergoes a phase transition in the finite-magnetic-field region. The transition is of second order with a cusp in the magnetization curve. An exact curve $H_c = H_c(U, \mu)$ is obtained from the Bethe *ansatz* solution. We ahve discussed the mechanism of this phase transition. In order to investigate the dimensional or model dependence of this phase transition, it is interesting to clarify the characteristic properties of the phase transition in higher dimensions and other models.

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