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Effect of Electron Itineracy on Magnetism of $S = 1/2$ Ferromagnetic Ising Model

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Abstract *The effect of electron itineracy on the magnetism of S=1/2 ferromagnetic Ising model is investigated by introducing a hopping term. The electron Green's function method is used to deal with this Hamiltonian. Here emphasis is made on that the magnetization is caused by the difference between the filling of spin-up and spin-down electrons. This concept is in accordance with that of band structure theory. In the zero band width limit, our results are the same as obtained by spin Green's function method. However, our method achieves more detailed physical information. The spontaneous magnetization, Curie temperature, total energy, and specific heat are calculated and investigated in detail by the densities of states. Hopping term depresses the Curie temperature but remains the order-disorder transformation still to be second order transition. Above the transition point, the energy band is the same as that of tight binding system because exchange interaction has no effect anymore. While under the transition point, the energy band splits into two subbands due to exchange interaction.*

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Ising model, as a simplified case of Heisenberg model, is usually employed to study the properties of magnetic systems composed by local magnetic moments, especially for phase transition problems. There have been sophisticated methods to deal with Ising Hamiltonian such as the method of high-temperature series expansion,[1] the mean-field theory,[2] the mean-field renormalization group method,[3] and the variational cumulant expansion method.[4−7] All the methods manifest that the system consists of local spins, which belongs to an exchange model.

However, we usually meet such systems as 3d transition element magnetic metal, in which the electrons play roles of both itineracy and consisting of local spins, i.e., the magnetically active electrons are itinerant. Hubbard model,[8] as well as its simplified case Stoner model,[9] is usually utilized to deal with the magnetic problems of itinerant electron.[10−15] In these models, the magnetization is caused by the different band fillings of spin-up and spin-down itinerant electrons mainly due to an intra-atomic Coulomb interaction — a strong correlation effect. Therefore, we see that usually in considering the magnetism of itinerant electron, one uses Hubbard model. While in treating transition problem, he uses exchange model. It has not been seen that the electron point of view is utilized to treat the exchange model.

Since the Heisenberg exchange interaction is in fact Coulomb interaction between electrons, and the local spins are actually originated from electrons, the exchange model can also be treated from the viewpoint of electron. In this paper, Ising model is dealt with by electron Green's function method. Our aim is to introduce a hopping term to investigate the effect of electron itineracy on the magnetism of Ising model.

The spin-1/2 operator $\boldsymbol{S}_i$ of site i can be expressed by fermion operator: $\boldsymbol{S}_i = \psi_i^\dagger \boldsymbol{\sigma} \psi_i$, where $\boldsymbol{\sigma}$ is Pauli matrix and ψ_i is a two-component operator $\psi_i^\dagger = (c_{i\uparrow}^\dagger, c_{i\downarrow}^\dagger)$. In this way, Ising Hamiltonian reads

$$H_I = -\frac{J}{2} \sum_{(i,j)} S_i^z S_j^z = -\frac{J}{2} \sum_{(i,j)\sigma} \left(n_{i\sigma} n_{j\sigma} - n_{i\sigma} n_{j,-\sigma} \right). \quad (1)$$

Here J is the Heisenberg exchange interaction. Only the nearest neighbor interaction is considered. The Greek letter in subscript denotes spins. The physical significance of the Hamiltonian can be realized in two points of view. In viewpoint of spins, there is an exchange interaction between neighboring spins. If neighboring spins are parallel, the system has lower energy, and if they are antiparallel, it has higher energy, which determines the system to be ferromagnetic. In viewpoint of electrons, there is a Coulomb interaction between electrons at neighboring atoms. If the electrons' spin orients parallelly, the interaction is attractive. While if their spins are antiparallel, the interaction is repulsive. The interaction is related to electron occupation numbers. In this paper, we will adopt the latter one. For a model study we set $J = 1$. The unit of energy is J and that of temperature T is J/k_B, where k_B is Boltzmann constant. The system is assumed as a simple cubic (sc) lattice. The retarded Green's function is defined as $G_{lm}^{\alpha\beta} = \langle\langle c_{l\alpha}; c_{m\beta}^\dagger \rangle\rangle = -\mathrm{i}\theta(t-t')\langle c_{l\alpha} c_{m\beta}^\dagger + c_{m\beta}^\dagger c_{l\alpha} \rangle$. After applying the equation of motion[16,17] and decoupling approximation $\langle\langle n_{j\alpha} c_{l\alpha};\ c_{m\beta}^\dagger \rangle\rangle = n_{j\alpha} \langle\langle c_{l\alpha};\ c_{m\beta}^\dagger \rangle\rangle$, the Green's function can be solved as $G_{lm}^{\alpha\beta}(E) = \delta_{\alpha\beta}\delta_{lm}/[E + zJ(n_\alpha - n_{-\alpha})]$. Note that when $l \neq m$, $G_{lm}^{\alpha\beta}(E) = 0$. The electron cannot propagate from one site to another, which means that the

electrons are really localized. The energy level is

$$E = -zJ(n_\alpha - n_{-\alpha})\,. \tag{2}$$

The band occupation is evaluated by the spectral theorem.[17,18]

$$n_\alpha = \frac{\mathrm{i}}{2\pi N}\sum_l \int \mathrm{d}E \frac{G_{ll}^{\alpha\alpha}(E+\mathrm{i}0^+) - G_{ll}^{\alpha\alpha}(E-\mathrm{i}0^+)}{\mathrm{e}^{E/T}+1}\,. \tag{3}$$

The magnetization is defined as

$$m = n_\uparrow - n_\downarrow\,. \tag{4}$$

The result is

$$m = \tanh(zJm/2T)\,, \tag{5}$$

where $z = 6$ is the nearest neighbor number of sc lattice. Curie point should be $T_c = zJ/2 = 3$. The total energy of per site is

$$E_I/N = \langle H_I\rangle/N = -zJm^2/2\,. \tag{6}$$

Figure 1 shows electron occupation numbers and magnetization defined in Eqs. (3) and (4).

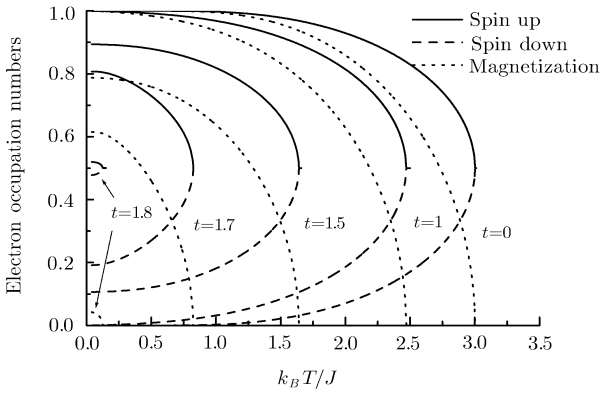

Fig. 1 Electron occupation numbers and magnetization vs. temperature for several hopping strengths.

The above results can also be obtained by spin Green's function method. If one defines $G_{lm} = \langle\langle S_l^+;\, S_m^-\rangle\rangle$ (or $G_{lm} = \langle\langle S_l^-;\, S_m^+\rangle\rangle$), he can achieve the energy spectrum Eq. (2) and magnetization $m = \langle S_i^z\rangle$ expressed by Eq. (5). Under the approximation $\langle S_i^z S_j^z\rangle \simeq \langle S_i^z\rangle\langle S_j^z\rangle$, the total energy is also Eq. (6). Therefore, the two ways using spin method and electron method are equivalent in the present simple case. In viewpoint of spin, as temperature rises, the spins have increasing thermo-motion and tend to orient arbitrarily. Order-disorder transition occurs when the statistical average of the spins in z direction is zero.

In the viewpoint of electron, a spin-down electron will be repulsed if there exists $n_\uparrow$ spin-up electrons at the nearest site and it feels repulsive energy $zJn_\uparrow$ due to z nearest neighbors. Similarly, a spin-up electron feels attracting energy $zJn_\downarrow$. Therefore, at zero temperature, there are two energy levels positioned at $E_{\downarrow,\uparrow} = \pm zJ$ with a gap $E_g = 2zJm$, see Fig. 2. Electrons occupy the lower level. As temperature rises, the two energy levels become closer. The occupation possibility of spin-up electron reduces and that of spin-down electron increases. At Curie point, the two sub-bands become identical. The electrons equally occupy the spin-up and spin-down levels.

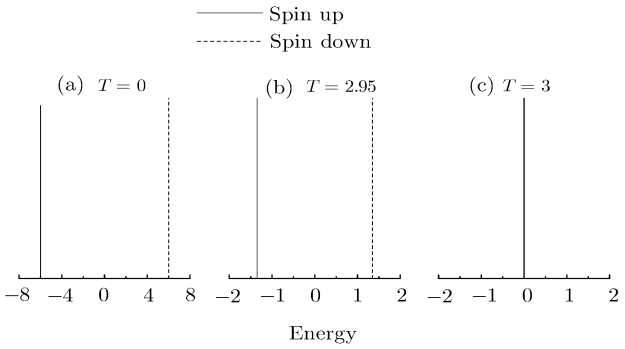

Fig. 2 Energy levels of ferromagnetic Ising model at three temperatures. The energy band is always symmetric with respect to $E = 0$, the Fermi energy.

Here we note that the energy gap is proportional to magnetization. This means that the decreasing tendency of the gap with increasing temperature is the same as the magnetization Eq. (5). The transition occurs because the two sub-bands have the same fillings. In one word, the magnetism can be explained by electrons with no need of the concept of local spin orientation.

It is obvious that compared with spin picture, the electron picture gives more physical details because it allows one to calculate more physical quantities such as electron occupation and densities of states (DOS) besides magnetization, Curie point, and total energy. We emphasize here that the local moment is caused by the difference of occupation of the states with spin-up and spin-down, Eq. (4). This conception is in accordance with the first-principle band calculation. What is more, with viewpoint of electron, we can introduce itineracy of electrons, which can hardly be done by spin viewpoint.

Now, a hopping term representing the itineracy of electron is added to Eq. (1),

$$H = -\frac{J}{2}\sum_{(i,j)\sigma}(n_{i\sigma}n_{j\sigma} - n_{i\sigma}n_{j,-\sigma}) + t\sum_{(i,j)\sigma} c_{i\sigma}^\dagger c_{j\sigma}\,. \tag{7}$$

This Hamiltonian can be termed as itinerant electron Ising model or tight binding Ising model. Only the nearest neighboring hoppings are considered. In derivation, the Green's function should be Fourier-transformed in three-dimensional space. Figure 1 shows the magnetization for various hopping strength. Figure 3 shows the DOS when hopping $t = 1$.

Compared with δ peaks in Fig. 2, the sub-bands in Fig. 3 extend into wide bands due to hopping effect. As temperature rises, the two sub-bands move closer and at Curie point they become identical. Because the sub-bands are wide, as temperature rises, they easily overlap. Electrons with spin-down also fill into the states under Fermi level. This results in the depress of Curie point. The stronger the hopping the lower the transition temperature.

Stronger hopping generates a wider energy band width, so that the filling of spin-up and spin-down two bands are closer. It is seen from Fig. 1 that for very strong hopping strength, even at zero temperature the electrons fill into both sub-bands.

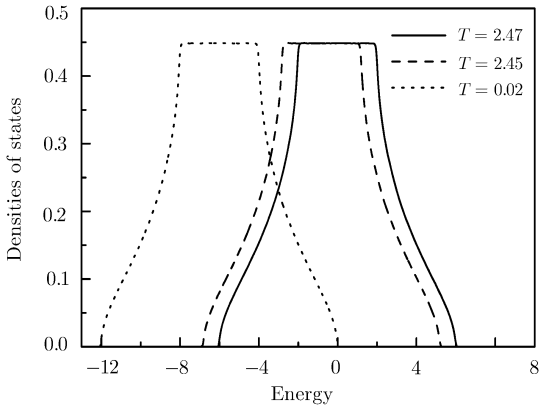

Fig. 3 Densities of states of ferromagnetic Ising model with hopping $t = 1$ at three temperatures (in the unit of J/k_B). Only the spin-up sub-band is depicted. The spin-down sub-band is always symmetric with respect to $E = 0$ and $T_c = 2.470$.

The energy band can also be realized in another point of view. Above Curie point, it is typical band of sc lattice, with band width $B = 2zt$,[19] as if there is no exchange interaction, see the solid line in Fig. 3. This is because when magnetization is zero, $n_\uparrow = n_\downarrow$, the attractive and repulsive interactions between neighboring sites are equal. Below Curie point, the exchange interaction results the splitting of the band into two sub-bands belonging to spin-up and spin-down, respectively. Figure 2 is a special case of Fig. 3 when band width is zero. The stronger the exchange interaction, the larger the splitting.

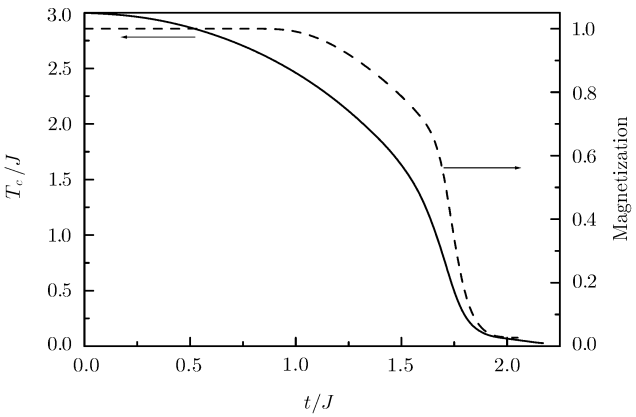

Fig. 4 Magnetization m at zero temperature and reduced Curie point T_c/J vs. hopping strength t/J.

At 0 K, because the half width of the sub-band is zt and the band centers are at $\pm zJ$, as $t/J < 1$, the two sub-bands do not overlap and the magnetization is 1, while as $t/J > 1$, the sub-bands start to overlap and the magnetization begin to drop. However, as t/J goes to infinite, the magnetization goes to infinitesimal but not zero since the sub-band centers are not the same. The m vs. t/J curve is shown is Fig. 4.

It is easily understood that stronger hopping and weaker exchange interaction depress transition temperature more. The transition temperature is determined by the competition between t and J. The T_c/J vs. t/J curve is plotted in Fig. 4. As t/J goes to infinity, T_c/J decreases but will not reach zero since at 0 K the two sub-bands are not the same.

The total energy is

$$\frac{E_0}{N} = \frac{\langle H\rangle}{N} = -\frac{1}{2}zJm^2 + \frac{1}{N}\sum_{(i,j)\sigma} t\langle c^\dagger_{i\sigma}c_{j\sigma}\rangle\,, \qquad (8)$$

where

$$\sum_{(i,j)\sigma} t\langle c^\dagger_{i\sigma}c_{j\sigma}\rangle = \sum_{\boldsymbol{k}}\Big[\frac{tz\gamma_{\boldsymbol{k}}}{\mathrm{e}^{(-zJm+z\gamma_{\boldsymbol{k}}t)/T}+1} + \frac{tz\gamma_{\boldsymbol{k}}}{\mathrm{e}^{(zJm+z\gamma_{\boldsymbol{k}}t)/T}+1}\Big]. \qquad (9)$$

It is composed by two parts: the ferromagnetic energy with the same form of Eq. (6) and the tight-binding energy. If $t = 0$, equation (8) goes back to Eq. (6). If $J = 0$, there is no magnetic energy and only the tight-binding energy is left. Note that in Eq. (8), t and J influence each other. Hopping influences the magnetic energy through its effect on magnetization m. The influence of exchange interaction on tight-binding energy is embodied in Eq. (9).

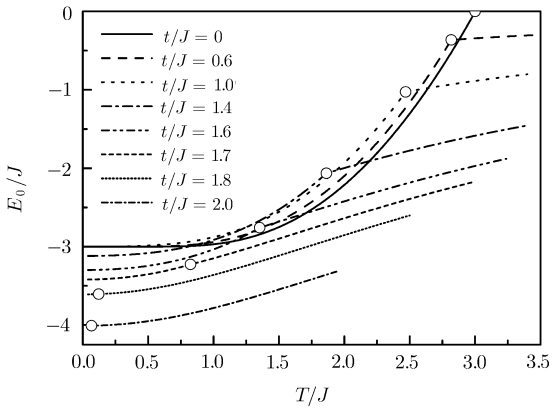

Fig. 5 Total energy vs. temperature T/J for several hopping strengths t/J. The open circles show the Curie points which are turning points of energy curves. For $t/J = 0$ curve, $T_c/J = 3$ above which the energy is zero.

Figure 5 shows the energy vs. temperature for various hopping strengths. Each curve shows a turning point at Curie point. Above Curie temperature, the energy is pure tight-binding one which can be obtained as one puts $m = 0$ in Eq. (8). The tight-binding energy always deceases with increasing hopping strength. From Fig. 5 we see that the total energy rises slightly below and near Curie point with increasing hopping strength until $t/J = 1.4$. This is because the hopping reduces the magnetization, see Fig. 1,

and therefore raises the magnetic energy, which results in the rise of total energy. As $t/J > 1.4$, the reduction of tight-binding energy overwhelms the increase of magnetic energy, so that the total energy begins to fall.

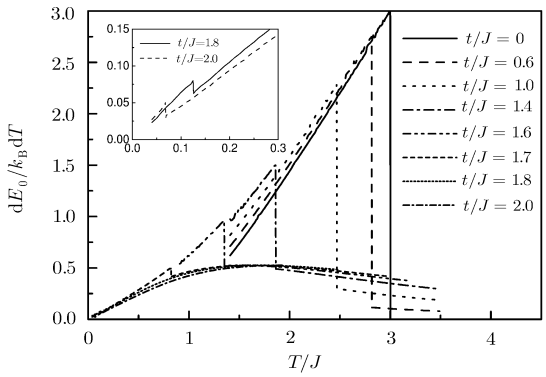

Fig. 6 Specific heat vs. T/J for several hoppings t/J. The curves for $t/J \leq 1.4$ are truncated at $T/J = 1.4$ in order to show clearly other curves. All curves go to zero when temperature approaches zero. The inner panel: enlarged curves for $t/J = 1.8$ and 2 to show the drops at Curie temperatures.

Figure 6 shows specific heat vs. temperature for various hopping strengths. The specific heat drops at Curie point. The stronger the hopping, the less the drop. At finite band width, the ferromagnetism-paramagnetism transition is still second-order transition.

To our knowledge, this is the first time to consider electron itineracy in Ising system. The itinerant Ising model, though in principle rather simple, nevertheless provokes a way to deal with itinerant electron magnetism induced by exchange effect rather than correlation effect. This model includes the minimum set of terms necessary for the description of such kind of systems. We think that the electron viewpoint gives more detailed physical information. It is now possible to calculate other properties such as transportation of electrons in the magnetic system in which the magnetism is mainly caused by exchange effect.

We should mention two discrepancies between Hubbard model and itinerant Ising model. One is that the magnetism of the former is due to the on-site Coulomb interaction, while that of the latter is due to the nearest neighbor Coulomb and exchange interactions. The second is that at zero band width the latter has a finite Curie point. While the former should not show magnetism as the system consists of isolated atoms.[20] This is because the interval of the spin-up and spin-down energy levels of the former is a constant independent of temperature. While those of the latter is proportional to magnetization, which is in turn dependent on temperature.

In conclusion, $S = 1/2$ ferromagnetic Ising model is dealt with by electron viewpoint so as to include the effect of electron itinerary. Hopping extends the energy band and depresses Curie point. Above T_c the exchange interaction has trivial effect and the system behaves as a typical tight-binding system. Below Curie point, the exchange interaction causes energy band split into two sub-bands. The lower the temperature, the larger the splitting. The total energy consists of magnetic energy and tight-binding energy, which interact with each other below Curie point.

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