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Low-Temperature Specific-Heat of One-Dimensional Hubbard Model

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Low-temperature specific heat per site (C) of one-dimensional Hubbard model is investigated by the method of non-linear integral equations. For the half-filled case we show $\lim_{H\to0}\lim_{T\to0} C/T=\pi I_0(\pi/2U)/(6I_1(\pi/2U))$, where T is temperature, H is magnetic field, U is the coupling constant, and I_0 and I_1 are modified Bessel functions. Although this equation yeilds $\lim_{T,H\to0} C/T=\pi/6$ in the limit $U\to0+$, the true value of $\lim_{T,H\to0} C/T$ at $U=0$ is $\pi/3$. This means that $\lim_{T,H\to0} C/T$ is a discontinuous function of U at $U=0$. This discontinuity disappears when the band is not half filled.

§ 1. Introduction

Low-temperature behavior of Hubbard model is interesting physically, and difficult to treat rigorously. The one-dimensional case of this model has been investigated by many physicists. Its thermodynamic potential density is difined by

$$\omega(U,T,A,H)=-T\lim_{N_a\to\infty}\{\ln(\mathrm{Tr}\exp(-T^{-1}(\mathcal{H}-A\sum_{i=1}^{N_a}(n_{i\uparrow}+n_{i\downarrow})))/N_a\},\tag{1·1a}$$

where $\mathcal{H}$ is the Hamiltonian:

$$\mathcal{H}=-\sum_{i=1}^{N_a}\sum_{\sigma}(c_{i\sigma}^{\dagger}c_{i+1\sigma}+c_{i+1\sigma}^{\dagger}c_{i\sigma})+4U\sum_{i=1}^{N_a}n_{i\uparrow}n_{i\downarrow}-\mu_0H\sum_{i=1}^{N_a}(n_{i\uparrow}-n_{i\downarrow}),$$

$$c_{N_a+1\sigma}\equiv c_{1\sigma}, \qquad n_{i\sigma}\equiv c_{i\sigma}^{\dagger}c_{i\sigma}.\tag{1·1b}$$

Here we have following symmetry relations through appropriate unitary transformations:

$$\begin{aligned}\omega(U,T,A,H)&=\omega(U,T,A,-H)=4U-2A+\omega(U,T,4U-A,H)\\&=\mu_0H-A+\omega(-U,T,\mu_0H-2U,\mu_0^{-1}(A-2U)).\end{aligned}\tag{1·2}$$

The first identity is obtained by changing up-spin and down-spin, the second by changing the creation and annihilation operators and the third by changing the creation and annihilation operators in the up-spin band. If we know the value of ω in the region $U\geq0$, $H\geq0$ and $A\leq2U$, we easily obtain the value of ω outside of this region through the relations (1·2). Then we restrict ourselves to calculate ω in this region. Other thermodynamic quantities such as energy and entropy per site (e, s), specific heat per site $(C_{H,A})$ and densities of up-spin and down-spin electrons $(n_\uparrow, n_\downarrow)$ are obtained by the differentiations of ω:

$$n_\uparrow + n_\downarrow = \frac{\partial\omega}{\partial A}, \qquad n_\uparrow - n_\downarrow = \frac{1}{\mu_0}\frac{\partial\omega}{\partial H}, \qquad e = -T^2\frac{\partial}{\partial T}\left(\frac{\omega}{T}\right) + \frac{\partial\omega}{\partial A}A,$$

$$S = -\frac{\partial\omega}{\partial T}, \qquad C_{H,A} = -T\frac{\partial^2\omega}{\partial T^2}, \qquad \chi = -\frac{\partial^2\omega}{\partial H^2}. \tag{1·3}$$

In a previous paper[1] the author derived a set of non-linear integral equations for the calculation of thermodynamic potential density ω. We used Bethe ansatz, which was first applied to this model by Lieb and Wu,[2] and some assumptions on the distributions of quasi-momenta k and parameters Λ on the complex plane. Recently Shiba and Pincus[3] calculated the energy levels of this model in the case of finite atomic numbers (such as six or five) and thermodynamic quantities. Their method is not useful to investigate the low-temperature properties of the model in the thermodynamic limit. For example, magnetic susceptibility of the finite system becomes zero or infinity in the limit of zero temperature. But this is not valid in the thermodynamic limit because magnetic susceptibility has finite values at $T=0$ in the half-filled state.[4),5)]

In the following sections we investigate the low-temperature behavior of this system, using the set of integral equations given in Ref. 1), and come to the conclusion that in the half-filled case low-temperature specific heat is proportional to temperature and coefficient is given analytically:

$$\lim_{H\to 0}\lim_{T\to 0} C/T = \pi I_0(\pi/2U)/(6I_1(\pi/2U)).$$

It should be noted that this is inversely proportional to the magnon velocity[6] at $T=0$:

$$v = 2I_1(\pi/2U)/I_0(\pi/2U),$$

and proportional to the magnetic susceptibility[5] at $T=0$:

$$\chi = \mu_0{}^2 I_0(\pi/2U)/(\pi I_1(\pi/2U)).$$

§ 2. Integral equations

The eigenvalue problem of one-dimensional Hubbard model described by the Hamiltonian (1·1b) can be treated by the method of Bethe's hypothesis. According to Lieb and Wu, we must solve a set of equations for N quasi-momenta k and M parameters Λ where N is the number of fermions and M is the number of down-spin fermions,

$$e^{ik_jN_a} = -\prod_{\alpha=1}^{M}\left(\frac{k_j - \Lambda_\alpha - 2iU}{k_j - \Lambda_\alpha + 2iU}\right), \qquad j=1,2,\cdots,N,$$

$$\prod_{j=1}^{N}\left(\frac{\Lambda_\alpha - k_j + iU}{\Lambda_\alpha - k_j - iU}\right) = -\prod_{\beta=1}^{M}\left(\frac{\Lambda_\alpha - \Lambda_\beta + 2iU}{\Lambda_\alpha - \Lambda_\beta - 2iU}\right), \qquad \alpha=1,2,\cdots,M.$$

In the previous paper[1] the author assumed that the k's and Λ's form bound states on the complex plane, and derived a set of non-linear integral equations for the distribution of the bound states at given temperature T, magnetic field H and chemical potential A:

$$\ln \zeta(k) = \kappa_0(k)/T + \int_{-\infty}^{\infty} s(\Lambda - \sin k) \ln((1+\eta_1'(\Lambda))/(1+\eta_1(\Lambda)))d\Lambda\,, \tag{2·1a}$$

$$\ln \eta_1(\Lambda) = s^* \ln(1+\eta_2(\Lambda)) - \int_{-\pi}^{\pi} dk \cos k\, s(\Lambda - \sin k) \ln(1+\zeta^{-1}(k)), \tag{2·1b}$$

$$\ln \eta_1'(\Lambda) = s^* \ln(1+\eta_2'(\Lambda)) - \int_{-\pi}^{\pi} dk \cos k\, s(\Lambda - \sin k) \ln(1+\zeta(k)), \tag{2·1c}$$

$$\ln \eta_n(\Lambda) = s^* \ln(1+\eta_{n-1}(\Lambda))(1+\eta_{n+1}(\Lambda)), \qquad n=2,3,\cdots, \tag{2·1d}$$

$$\ln \eta_n'(\Lambda) = s^* \ln(1+\eta_{n-1}'(\Lambda))(1+\eta_{n+1}'(\Lambda)), \qquad n=2,3,\cdots, \tag{2·1e}$$

$$\lim_{n\to\infty} \frac{\ln \eta_n}{n} = \frac{2\mu_0 H}{T}\,, \tag{2·1f}$$

$$\lim_{n\to\infty} \frac{\ln \eta_n'}{n} = \frac{4U-2A}{T}\,, \tag{2·1g}$$

where $s(\Lambda) \equiv \mathrm{sech}(\pi x/2U)/4U$, $f^*g \equiv \int_{-\infty}^{\infty} f(\Lambda - \Lambda')g(\Lambda')d\Lambda'$,

$$\kappa_0(k) = -2\cos k - 4\int_{-\infty}^{\infty} s(\Lambda - \sin k)(\mathrm{Re}\sqrt{1-(\Lambda - Ui)^2})d\Lambda\,. \tag{2·1h}$$

Function $\zeta(k)$ is the ratio of hole density and particle density of unbound quasi-momenta. Function $\eta_n(\Lambda)$ is that of n-th order bound state of Λ. Function $\eta_n'(\Lambda)$ is that of bound state of the $n\Lambda$'s and $2nk$'s. Thermodynamic potential per site is given by

$$\omega(T,A,H) = -T\int_{-\pi}^{\pi} \ln(1+\zeta^{-1}(k))\frac{dk}{2\pi} - T\sum_{n=1}^{\infty}\int_{-\infty}^{\infty} \ln(1+\eta_n^{-1}(\Lambda)) \times \mathrm{Re}\frac{1}{\sqrt{1-(\Lambda - nUi)^2}}\cdot\frac{d\Lambda}{\pi} \tag{2·2a}$$

$$= E_0 - A - T\left\{\int_{-\pi}^{\pi} \rho_0(k)\ln(1+\zeta(k))dk + \int_{-\infty}^{\infty} \sigma_0(\Lambda)\ln(1+\eta_1(\Lambda))d\Lambda\right\}, \tag{2·2b}$$

where E_0, $\rho_0(k)$, $\sigma_0(\Lambda)$ are the ground state energy per site, distribution function of the k's and that of the Λ's at $T=0$, $A=2U$, $\mu_0 H=0$, respectively:

$$\sigma_0(\Lambda) \equiv \int_{-\pi}^{\pi} s(\Lambda - \sin k)\frac{dk}{2\pi}\,, \tag{2·2c}$$

$$\rho_0(k) \equiv \frac{1}{2\pi} + \cos k\int_{-\infty}^{\infty} d\Lambda a_1(\Lambda - \sin k)\sigma_0(\Lambda), \tag{2·2d}$$

$$a_n(\Lambda) \equiv \frac{nU}{\pi(\Lambda^2 + (nU)^2)}\,, \tag{2·2e}$$

$$E_0 \equiv -2\int_{-\pi}^{\pi} \cos k\, \rho_0(k) dk\,. \qquad (2\cdot 2\text{f})$$

One should note that Eqs. (2·1) and (2·2) are valid only at $U \geq 0$, $A \leq 2U$ and $\mu_0 H \geq 0$. The other cases can be treated through Eqs. (1·2).

From Eqs. (2·1c), (2·1e) and (2·1g) we have

$$\ln(1+\eta_n') \geq 2n(2U-A)/T\,, \qquad n=1,2,3,\cdots.$$

At $2U-A \gg T$, we can replace $\ln \eta_n'$ by $\ln(1+\eta_n')$ in Eqs. (2·1c), (2·1e) and (2·1g) and obtain

$$\ln(1+\eta_n') = 2n(2U-A)/T + \int_{-\pi}^{\pi} a_n(\Lambda - \sin k) \ln(1+\zeta(k)) \cos k\, dk$$
$$+ O(\exp(-(2U-A)/T)), \qquad n=1,2,\cdots. \qquad (2\cdot 3\text{a})$$

Substituting case $n=1$ of this equation into (2·1a), we have

$$\kappa(k) = \kappa_0(k) + 2U - A + T\int_{-\pi}^{\pi} R(\sin k - \sin k') \ln(1+\exp(\kappa(k')/T)) \cos k' dk'$$
$$-T\int_{-\infty}^{\infty} s(\Lambda - \sin k) \ln(1+\exp(\varepsilon_1(\Lambda)/T)) d\Lambda + O(T\exp(-(2U-A)/T)),$$
$$(2\cdot 4\text{a})$$

where $R \equiv s * a_1$, $\kappa = T\ln\zeta$, $\varepsilon_1 = T\ln\eta_1$.

At $2U-A = O(T)$, function $\kappa(k)$ is always negative. Then the last term of (2·1c) is of the order of $T^{1/2}\exp(\kappa^{(0)}(\pi)/T)$ at low temperatures. Then we have

$$1+\eta_j' = (\mathrm{sh}\{(j+1)(2U-A)/T\}/\mathrm{sh}\{(2U-A)/T\})^2 + O(T^{1/2}\exp(\kappa^{(0)}(\pi)/T)),$$
$$(2\cdot 3\text{b})$$

where $\kappa^{(0)}$ is κ at zero temperature (hereafter we put (0) for the functions at zero temperature). Substituting this into (2·1a), we have

$$\kappa(k) = \kappa_0(k) + T\ln(2\,\mathrm{ch}\{(2U-A)/T\}) - T\int_{-\infty}^{\infty} s(\Lambda - \sin k)$$
$$\times \ln\left(1+\exp\frac{\varepsilon_1(\Lambda)}{T}\right) d\Lambda + O(T^{3/2}\exp(\kappa^{(0)}(\pi)/T)). \qquad (2\cdot 4\text{b})$$

At $\mu_0 H \gg T$, we have

$$\ln(1+\eta_n) = a_{n-1}^* \ln(1+\eta_1) + 2(n-1)\mu_0 H/T\,, \qquad n=2,3,\cdots. \qquad (2\cdot 3\text{c})$$

Substituting this into (2·1b), we have

$$\varepsilon_1(\Lambda) = TR^* \ln(1+\exp(\varepsilon_1(\Lambda)/T)) + \mu_0 H - T\int_{-\pi}^{\pi} dk \cos k\, s(\Lambda - \sin k)$$
$$\times \ln(1+\exp(-\kappa(k)/T)) + O(T\exp(2\mu_0 H/T)). \qquad (2\cdot 4\text{c})$$

Equations (2·4a) and (2·4c) are transformed as follows:

$$\kappa(k) = -2\cos k - A - \mu_0 H - T\int_{-\infty}^{\infty} a_1(\sin k - \Lambda)\ln(1+\exp(-\varepsilon_1(\Lambda)/T))d\Lambda\,, \tag{2·5a}$$

$$\varepsilon_1(\Lambda) = T\int_{-\infty}^{\infty} a_2(\Lambda-\Lambda')\ln(1+\exp(-\varepsilon_1(\Lambda')/T))d\Lambda'$$
$$-T\int_{-\pi}^{\pi} a_1(\Lambda - \sin k)\ln(1+\exp(-\kappa(k)/T))\cos k\,dk + 2\mu_0 H\,. \tag{2·5b}$$

From Eq. (2·2a) we have

$$\omega(T, A, H) = -T\int_{-\pi}^{\pi} \ln(1+\exp(-\kappa(k)/T))\frac{dk}{2\pi}\,. \tag{2·5c}$$

Here we have neglected the terms which are of the order of $e^{-2\mu_0 H/T}$ or $e^{-(4U-2A)/T}$. Equations (2·4) or (2·5) are useful to obtain thermodynamic potential at $2U - A \gg T$ and $2\mu_0 H \gg T$.

As shown in Fig. 1, (A, H) plane is devided into several regions by the low-temperature properties. The number of fermions per site n has the following properties at zero temperature:

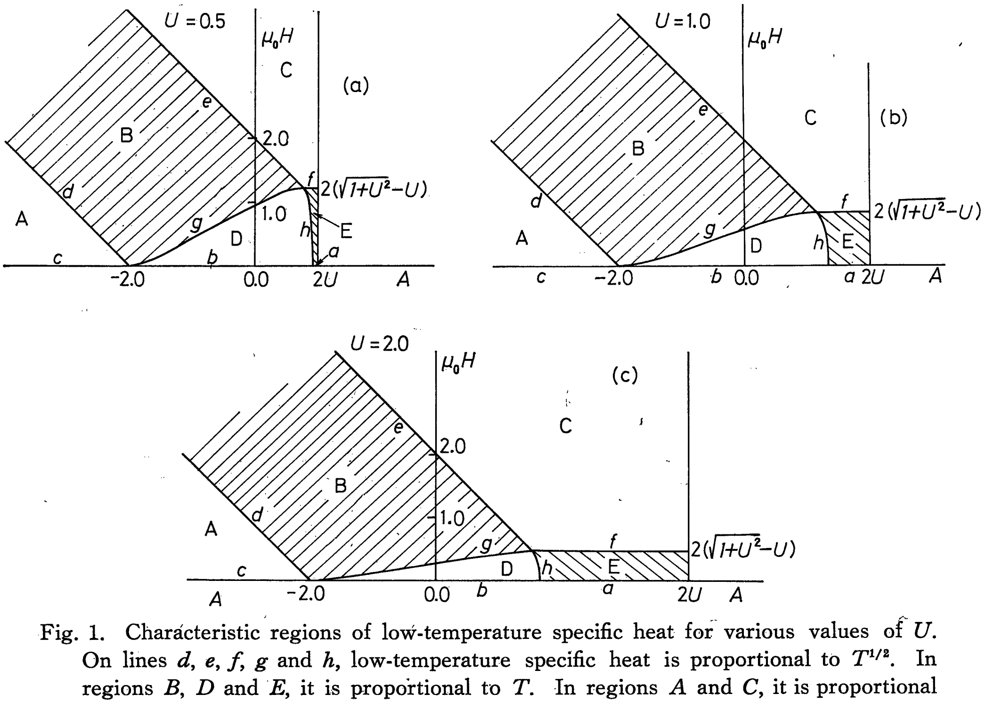

Fig. 1. Characteristic regions of low-temperature specific heat for various values of U. On lines d, e, f, g and h, low-temperature specific heat is proportional to $T^{1/2}$. In regions B, D and E, it is proportional to T. In regions A and C, it is proportional to $T^{-3/2}\exp(-\alpha/T)$.
a) $U=0.5$
b) $U=1.0$
c) $U=2.0$

$$n=1 \quad \text{at regions } C \text{ and } E,$$
$$0<n<1 \quad \text{at regions } B \text{ and } D,$$
$$n=0 \quad \text{at region } A.$$

On lines a, b and c, magnetization is zero.

§ 3. Case $\mu_0 H \gg T$

a) $A \leq -2-\mu_0 H$ (*Region A*)

In this region, density of fermions is zero at zero temperature. From Eq. (2·5a), we have

$$\kappa(k) = -2\cos k - A - \mu_0 H - T\exp(-2\mu_0 H/T).$$

Substituting this into (2·5c), we obtain

$$\omega(T,A,H) = -\pi^{-1}T^{3/2}\int_0^\infty \ln\left(1+\exp\left(\frac{2+A+\mu_0 H}{T}\right)e^{-x^2}\right)dx.$$

b) $\varepsilon_1^{(0)}(0) \geq 0$, $A > -2-\mu_0 H$ (*Region B*)

Here the number of fermions per site, n, satisfies $1>n>0$. At zero temperature all fermions have up-spin. From Eq. (2·5c) we have

$$\omega(T,A,H)-\omega(0,A,H) = -T\int_{-\pi}^{\pi}\ln(1+\exp(-|\kappa(k)|/T))\frac{dk}{2\pi}$$
$$-\int_{-Q}^{Q}\delta\kappa(k)\frac{dk}{2\pi},$$

where Q and $-Q(Q>0)$ are zeroes of $\kappa^{(0)}(k)$. From Eqs. (2·5a) and (2·5b) we obtain

$$\delta\kappa = -T\int_{-\infty}^{\infty} a_1(\sin k - \Lambda)\ln(1+\exp(-\varepsilon_1(\Lambda)/T))d\Lambda,$$

$$\varepsilon_1(\Lambda) = -2\int_{-Q}^{Q} a_1(\Lambda-\sin k)\cos^2 k\, dk + 2\mu_0 H + O(T^2) + O(T^{3/2}\exp(-\varepsilon_1^{(0)}/T)).$$

Then we have

$$\omega(T,A,H) = \omega(0,A,H) - \frac{T^2}{2\pi}\frac{1}{2\sin Q}\cdot\frac{\pi^2}{3}$$
$$-T^{3/2}2g(0)\sqrt{\frac{2}{\varepsilon_1^{(0)\prime\prime}(0)}}\int_0^\infty \ln(1+\exp(-\varepsilon_1^{(0)\prime\prime}(0)/T)\cdot e^{-x^2})dx,$$

where

$$g(\Lambda) = \int_{-Q}^{Q} a_1(\Lambda-\sin k)\frac{dk}{2\pi}.$$

c) $\mu_0 H \geq 2(\sqrt{1+U^2}-U)$, $A \geq 2-\mu_0 H$ (*Region C*)

At zero temperature, density of fermion is one, and all fermions have up-spin. Substituting Eq. (2·5a) into Eq. (2·5c), we have

$$\omega(T,A,H) = -A-\mu_0 H - T\int_{-\pi}^{\pi} \ln(1+\exp(\kappa(k)/T))\frac{dk}{2\pi}$$
$$-T\int_{-\infty}^{\infty} 2\left(\mathrm{Re}\,\frac{1}{\sqrt{1-(\Lambda-Ui)^2}}\right)\ln(1+\exp(-\varepsilon_1(\Lambda)/T))d\Lambda\,. \qquad (3\cdot1)$$

From Eqs. (2·5a) and (2·5b), we obtain

$$\kappa(k) = -2\cos k - A - \mu_0 H - O(T^{3/2}\lambda),$$
$$\varepsilon_1(\Lambda) = -4\,\mathrm{Re}(\sqrt{1-(\Lambda-Ui)^2}-U) + 2\mu_0 H + O(T^{3/2}\lambda) + O(T^{3/2}\mu),$$
$$\lambda \equiv \exp(-(4(\sqrt{1+U^2}-U)-2\mu_0 H)/T), \qquad \mu = \exp((2-A-\mu_0 H)/T).$$

Substituting these into Eq. (3·1), we have

$$\omega(T,A,H) = -A-\mu_0 H - \pi^{-1}T^{3/2}\int_0^{\infty}\ln(1+\mu e^{-x^2})dx$$
$$-4T^{3/2}(\sqrt{1+U^2}-U)(1+U^2)^{-1/4}\int_0^{\infty}\ln(1+\lambda e^{-x^2})dx\,. \qquad (3\cdot2)$$

On the boundary of this region we have

$$\omega = \begin{cases} -A-\mu_0 H - \pi^{-1}T^{3/2}\zeta\left(\frac{3}{2}\right)\left(1-\frac{1}{\sqrt{2}}\right)\frac{\sqrt{\pi}}{2} & \text{at } \mu_0 H = 2(\sqrt{1+U^2}-U), \\ -A-\mu_0 H - 4T^{3/2}(\sqrt{1+U^2}-U)(1+U^2)^{-1/4}\zeta\left(\frac{3}{2}\right)\left(1-\frac{1}{\sqrt{2}}\right)\frac{\sqrt{\pi}}{2} & \\ & \text{at } A = 2-\mu_0 H. \end{cases} \qquad (3\cdot3)$$

d) $\varepsilon_1^{(0)}(0)<0$, $\kappa^{(0)}(\pi)>0$ (*Region D*)

From Eq. (2·5c), we have

$$\omega(T,A,H)-\omega(0,A,H) = -\frac{\pi T^2}{6\kappa'(Q)} + \int_{-Q}^{Q}\frac{dk}{2\pi}\delta\kappa(k). \qquad (3\cdot4)$$

Function $\delta\kappa(k)$ is determined by

$$\delta\kappa(k) = \int_{-B}^{B} a_1(\sin k-\Lambda)\delta\varepsilon_1(\Lambda)d\Lambda - \frac{\pi^2 T^2}{6\varepsilon_1'(B)}\{a_1(\sin k-B)+a_1(\sin k+B)\}, \qquad (3\cdot5a)$$

$$\delta\varepsilon(\Lambda) + \int_{-B}^{B} a_2(\Lambda-\Lambda')\delta\varepsilon(\Lambda')d\Lambda' = \int_{-Q}^{Q} dk\cos k\, a_1(\sin k-\Lambda)\delta\kappa(k)$$
$$-\frac{\pi^2 T^2\cos Q}{6\kappa'(Q)}\{a_1(\sin Q-\Lambda)+a_1(\sin Q+\Lambda)\}$$

$$+\frac{\pi^2T^2}{6\varepsilon_1'(B)}\{a_2(B-\Lambda)+a_2(B+\Lambda)\}, \tag{3·5b}$$

where Q and B are zeroes of $\kappa^{(0)}(k)$ and $\varepsilon_1^{(0)}(\Lambda)$, respectively. From these equations we obtain

$$\omega(T,A,H)-\omega(0,A,H)=-\frac{\pi^2T^2}{3}\left[\frac{\sigma_1^{(0)}(B)}{\varepsilon_1^{(0)\prime}(B)}+\frac{\rho^{(0)}(Q)}{\kappa^{(0)\prime}(Q)}\right]+O(T^3), \tag{3·6a}$$

where $\rho^{(0)}(k)$ and $\sigma_1^{(0)}(\Lambda)$ are the distribution functions of k and Λ at zero temperature and determined by

$$\rho_1^{(0)}(k)=\frac{1}{2\pi}+\cos k\int_{-B}^{B}a_1(\Lambda-\sin k)\sigma_1^{(0)}(\Lambda)d\Lambda, \tag{3·6b}$$

$$\sigma_1^{(0)}(\Lambda)+\int_{-B}^{B}a_2(\Lambda-\Lambda')\sigma_1^{(0)}(\Lambda')d\Lambda'=\int_{-Q}^{Q}a_1(\Lambda-\sin k)\rho^{(0)}(k)dk. \tag{3·6c}$$

The equations for $\sigma_1^{(0)}$ and $\varepsilon_1^{(0)\prime}$ are written as

$$\sigma_1^{(0)}(\Lambda)-\int_{|\Lambda|>B}R(\Lambda-\Lambda')\sigma_1^{(0)}(\Lambda')d\Lambda'=\int_{-Q}^{Q}s(\Lambda-\sin k)\rho^{(0)}(k)dk, \tag{3·6d}$$

$$\varepsilon_1^{(0)\prime}(\Lambda)-\int_{|\Lambda|>B}R(\Lambda-\Lambda')\varepsilon_1^{(0)\prime}(\Lambda')d\Lambda'=\int_{-Q}^{Q}s(\Lambda-\sin k)\kappa^{(0)\prime}(k)dk. \tag{3·6e}$$

The right-hand sides of these equations are

$$\exp\left(-\frac{\pi|\Lambda|}{2U}\right)(2U)^{-1}\int_{-Q}^{Q}dk\exp\left(-\frac{\pi\sin k}{2U}\right)\rho^{(0)}(k)$$

and

$$\mathrm{sign}(\Lambda)\exp\left(-\frac{\pi|\Lambda|}{2U}\right)(2U)^{-1}\int_{-Q}^{Q}dk\exp\left(-\frac{\pi\sin k}{2U}\right)\kappa^{(0)\prime}(k)$$

at $|\Lambda|\gg1$, U. Then we have

$$\frac{\sigma_1^{(0)}(B)}{\varepsilon_1^{(0)\prime}(B)}=\frac{\int_{-Q}^{Q}dk\exp(\pi\sin k/2U)\rho^{(0)}(k)}{\int_{-Q}^{Q}dk\exp(\pi\sin k/2U)\kappa^{(0)\prime}(k)}+O(B^{-2})$$

and

$$\omega(T,A,H)-\omega(0,A,H)=-\frac{\pi^2T^2}{3}\left\{\frac{\rho^{(0)}(Q)}{\kappa^{(0)\prime}(Q)}+\frac{\int_{-Q}^{Q}dk\exp(\pi\sin k/2U)\rho^{(0)}(k)}{\int_{-Q}^{Q}dk\exp(\pi\sin k/2U)\kappa^{(0)\prime}(k)}\right.$$
$$\left.+O(\{\ln(\mu_0H)\}^{-2})\right\}, \tag{3·7}$$

when μ_0H is very small. From this equation we obtain

$$\lim_{H\to0}\lim_{T\to0}C_{A,H}/T=\frac{2\pi^2}{3}\left\{\frac{\rho^{(0)}(Q)}{\kappa^{(0)\prime}(Q)}+\frac{\int_{-Q}^{Q}dk\exp(\pi\sin k/2U)\rho^{(0)}(k)}{\int_{-Q}^{Q}dk\exp(\pi\sin k/2U)\kappa^{(0)\prime}(k)}\right\}. \tag{3·8}$$

e) $2(\sqrt{1+U^2}-U)>\mu_0 H\gg T$, $\kappa^{(0)}(\pi)\leq 0$ (*Region E*)

From Eq. (2·2b) we have

$$\omega(T,A,H)-\omega(0,A,H)=-2T^{3/2}\rho_0(\pi)\sqrt{\frac{2}{-\kappa(\pi)}}\int_0^\infty \ln\left(1+\exp\left(\frac{\kappa(\pi)}{T}\right)\cdot e^{-x^2}\right)dx$$
$$-T\int_{-\infty}^{\infty}\sigma_0(\Lambda)\ln\left(1+\exp\left(-\frac{|\varepsilon_1(\Lambda)|}{T}\right)\right)d\Lambda-T\int_{|\Lambda|>B}\sigma_0(\Lambda)\delta\varepsilon_1(\Lambda)d\Lambda+O(T^4),\tag{3·9}$$

where $\delta\varepsilon\equiv\varepsilon-\varepsilon^{(0)}$. From Eq. (2·4b) we have

$$\delta\varepsilon(\Lambda)-\int_{|\Lambda'|>B}R(\Lambda-\Lambda')\delta\varepsilon_1(\Lambda')d\Lambda'$$
$$=-\pi^2T^2(R(\Lambda-B)$$
$$+R(\Lambda+B))/(6\varepsilon_1'(B))$$
$$+O((B-B')^2),$$

where B and B' are zeroes of ε_1 and $\varepsilon_1^{(0)}$, respectively. Summing the second and the third terms of r.h.s. of (3·9), we have

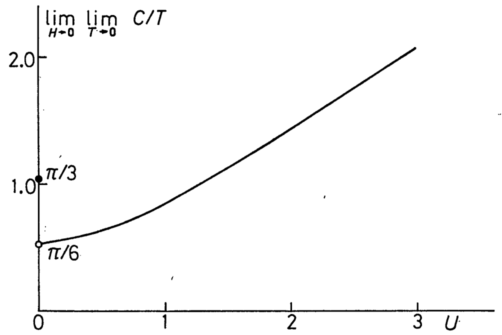

Fig. 2. Coefficient of T-linear low-temperature specific heat in the half-filled case ($A=2U$), and $\mu_0 H=0$.

$$-\frac{\pi^2T^2}{3}\frac{\sigma_1^{(0)}(B)}{\varepsilon^{(0)\prime}(B)}+O(T^3),\tag{3·10}$$

where $\sigma_1^{(0)}$ and $\varepsilon_1^{(0)\prime}$ are determined by

$$\sigma_1^{(0)}(\Lambda)-\int_{|\Lambda'|>B}R(\Lambda-\Lambda')\sigma_1^{(0)}(\Lambda')d\Lambda'=\sigma_0(\Lambda),\tag{3·11a}$$

$$\varepsilon_1^{(0)\prime}(\Lambda)-\int_{|\Lambda'|>B}R(\Lambda-\Lambda')\varepsilon_1^{(0)\prime}(\Lambda')d\Lambda'=2\int_{-\pi}^{\pi}s(\Lambda-\sin k)\sin k\,dk\,.\tag{3·11b}$$

At $|\Lambda|\gg\max.(1,1/U)$, r.h.s. of (3·11a) and (3·11b) are $(2U)^{-1}I_0(\pi/2U)e^{-\pi|\Lambda|/2U}$ and $\mathrm{sign}(\Lambda)\cdot 2\pi U^{-1}I_1(\pi/2U)e^{-\pi|\Lambda|/2U}$, respectively. Then we have

$$\frac{\sigma_1^{(0)}(B)}{\varepsilon_1^{(0)\prime}(B)}=\frac{I_0(\pi/2U)}{4\pi I_1(\pi/2U)}+O(B^2)$$

and

$$\omega(T,A,H)-\omega(O,A,H)=-2T^{3/2}\rho_0(\pi)\sqrt{\frac{2}{-\kappa^{(0)\prime}(\pi)}}$$
$$\times\int_0^\infty \ln(1+\exp(\kappa^{(0)}(\pi)/T)e^{-x^2})-\frac{\pi T^2}{12}\cdot\frac{I_0(\pi/2U)}{I_1(\pi/2U)}$$
$$+O((\ln\mu_0 H)^{-2})+O(T^3).\tag{3·12}$$

The coefficient of T-linear specific heat at $A=2U$ is

$$\lim_{H\to 0}\lim_{T\to 0} C_{A,H}/T=\frac{\pi}{6}\cdot\frac{I_0(\pi/2U)}{I_1(\pi/2U)}.$$

This value is shown in Fig. 2 as a function of U.

§ 4. Case $\mu_0 H=O(T)$

a) $\kappa^{(0)}(\pi)\leq 0$ (*near line a*)

From Eqs. (2·1) we have

$$\ln\eta_1(\Lambda)=s*\ln(1+\eta_2(\Lambda))-\frac{2}{T}\int_{-\pi}^{\pi}dk\cos^2 k\, s(\Lambda-\sin k)+O\left(T^{1/2}\exp\frac{\kappa^{(0)}(\pi)}{T}\right),$$

$$\ln\eta_n(\Lambda)=s*\ln(1+\eta_{n-1}(\Lambda))(1+\eta_{n+1}(\Lambda)),\qquad n=2,3,\cdots,$$

$$\lim_{n\to\infty}\frac{\ln\eta_n}{n}=\frac{2\mu_0 H}{T}.$$

Thus Eq. (2·2b) can be written as follows:

$$\omega(T,A,H)=E_0-A-2T^{3/2}\rho_0(\pi)\sqrt{\frac{2}{-\kappa^{(0)\prime\prime}(\pi)}}\int_0^\infty\ln\left(1+\exp\frac{\kappa^{(0)}(\pi)}{T}\cdot e^{-x^2}\right)dx$$
$$-\frac{T^2}{2}\cdot\frac{I_0(\pi/2U)}{I_1(\pi/2U)}C\left(\frac{2\mu_0 H}{T}\right)+O(T^4),\tag{4·1}$$

where $C(y)$ is determined by

$$C(y)=\int_{-\infty}^{\infty}e^{-\pi x/2}\ln(1+\eta_1(x))dx,$$

$$\ln\eta_1(x)=-e^{-\pi x/2}+\int_{-\infty}^{\infty}\frac{1}{4}\operatorname{sech}\frac{\pi(x-x')}{2}\ln(1+\eta_2(x'))dx',$$

$$\ln\eta_n(x)=\int_{-\infty}^{\infty}\frac{1}{4}\operatorname{sech}\frac{\pi(x-x')}{2}\ln(1+\eta_{n-1}(x'))(1+\eta_{n+1}(x'))dx',$$
$$n=2,3,\cdots,$$

$$\lim_{n\to\infty}\frac{\ln\eta_n}{n}=y.\tag{4·2}$$

b) $\kappa^{(0)}(\pi)>0$ (*near line b*)

From Eq. (2·2b) we have

$$\omega(T,A,H)-\omega(0,A,H)=\int_{-Q}^{Q}\frac{dk}{2\pi}\delta\kappa(k)-\frac{\pi}{12}\cdot\frac{T^2}{\kappa^{(0)\prime}(Q)}+O(T^3).\tag{4·3}$$

The equation for $\delta\kappa\equiv\kappa-\kappa^{(0)}$ is

$$\delta\kappa(k)-\int_{-Q}^{Q}R(\sin k-\sin k')\delta\kappa(k')\cos k'dk'$$

$$= -T\int_{-\infty}^{\infty} s(\Lambda - \sin k)\ln(1+\eta_1(\Lambda))d\Lambda$$

$$+\frac{\pi^2 T^2}{6\kappa^{(0)'}(Q)}(R(\sin k - \sin Q) + R(\sin k + \sin Q)) + O(T^4). \quad (4\cdot4)$$

After some calculations we obtain

$$\omega(T,A,H) - \omega(0,A,0) = -\frac{\pi^2 T^2 \rho^{(0)}(Q)}{3\kappa^{(0)'}(Q)} - 2\pi T^2 C\left(\frac{2\mu_0 H}{T}\right)$$

$$\times\left(\int_{-Q}^{Q}\exp\left(\frac{\sin k}{U}\right)\rho^{(0)}(k)dk \Big/ \int_{-Q}^{Q}\exp\left(\frac{\sin k}{U}\right)\kappa^{(0)'}(k)dk\right) + O(T^3), \quad (4\cdot5)$$

where $\rho^{(0)}$, $\kappa^{(0)}$ and $C(y)$ are defined in Eqs. (3·6) and (4·2). Functions similar to $C(y)$ defined in (4·2) appeared in the investigation of the low-temperature specific heat of Heisenberg-Ising ring at $|\Delta|\leq 1$.[7] From the result of numerical calculation in Ref. 7) we conjecture

$$C(0) = \pi/6 \quad \text{and} \quad C''(0) = 1/2\pi. \quad (4\cdot6)$$

If these equations are true, we obtain

$$\lim_{T\to 0}\lim_{H\to 0} C/T = \lim_{H\to 0}\lim_{T\to 0} C/T,$$

$$\lim_{T\to 0}\lim_{H\to 0}\chi = \lim_{H\to 0}\lim_{T\to 0}\chi.$$

§5. Discussions and summary

From the theory of non-interacting fermions, thermodynamic potential per site at $U=0$ is

$$\omega(T,A,H) = \frac{1}{2\pi}\left\{\int_{-\pi}^{\pi}\ln(1+\exp(-2\cos k - \mu_0 H - A/T))dk\right.$$

$$\left. + \int_{-\pi}^{\pi}\ln(1+\exp(-2\cos k + \mu_0 H - A/T))dk\right\}. \quad (5\cdot1)$$

From this equation we obtain

$$\lim_{H\to 0}\lim_{T\to 0} C/T = \pi/3$$

at $A=2U=0$ and $\mu_0 H=0$. This value differs from $\lim_{U\to 0}\lim_{H\to 0}\lim_{T\to 0} C/T = \pi/6$. One can interpret this discontinuity of the coefficient of T-linear specific heat at $U=0$ as follows. In the half-filled case at $U>0$ one-particle excitation spectrum has a energy gap $-\kappa^{(0)}(\pi) = 2U - 2 + 4\int_0^\infty d\omega\, J_1(\omega)/\omega(1+e^{2U\omega})$. Then this excitation does not contribute to the coefficient of T-linear specific heat. But at $U=0$, gap is zero and this excitation does contribute to the coefficient. In the case $n<1$ one finds no such discontinuity, because both magnon excitation and one-particle excitation contribute to the coefficient of T-linear specific heat.

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