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On the Exact Ground State Energy of Lieb and Wu

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The analytic properties of the ground state energy (f) for the one-dimensional half-filled Hubbard model are investigated as a function of the interaction (U). Lieb and Wu's exact expression

$$f(U)=-4\int_0^\infty \frac{J_0(\omega)J_1(\omega)}{\omega(1+\exp 2U\omega)}, \qquad U\geqq 0$$

is used. It is shown that the ground state energy is an infinitely many-valued function on the complex U plane and there are logarithmic branch points at $U=\pm i/n$ ($n=1, 2, \cdots$). So $U=0$ is the accumulation point of branch points of $f(U)$.

§ 1. Introduction

Analytic properties of the ground state energy of the many-body system are of great physical interest. In a recent paper Lieb and Wu[1)] gave the exact ground state energy of the one-dimensional Hubbard model. This model treats the electrons in the narrow band with interaction which acts only when two electrons are in the same atomic site. The Hamiltonian to be considered is

$$\mathcal{H}=-\sum_{\langle ij\rangle}\sum_{\sigma} c_{i\sigma}^{\dagger}c_{j\sigma}+4U\sum_{i=1}^{N_a} c_{i\uparrow}^{\dagger}c_{i\uparrow}c_{i\downarrow}^{\dagger}c_{i\downarrow}. \tag{1·1}$$

Here N_a is the number of atomic sites. Lieb and Wu obtained a set of the coupled-integral equations which gives the exact ground state energy at the thermodynamic limit. Their integral equations can be solved analytically when the band is half-filled, namely, the number of electrons is equal to that of atomic sites. In this paper we investigate the analytic properties of the ground state energy of the half-filled case and at the thermodynamic limit.

Let us define $f(U)$ and $g(U)$ as follows:

$f(U)=\lim_{N_a\to\infty} 1/N_a$ (lowest energy eigenvalue of (1·1) at the half-filled case),

$g(U)=\lim_{N_a\to\infty} 1/N_a$ (highest energy eigenvalue of (1·1) at the half-filled case).

According to the calculation of Lieb and Wu

$$f(U)=-4I(U), \qquad g(U)=2U+4I(U) \tag{1·2}$$

for $U\geqq 0$ and

$$f(U)=2U-4I(-U), \qquad g(U)=4I(-U) \tag{1·3}$$

for $U\leqq 0$. Here $I(U)$ is given by

$$I(U)=\int_0^\infty \frac{J_0(\omega)J_1(\omega)\,d\omega}{\omega(1+\exp 2U\omega)}\,,\qquad U\geqq 0\,. \tag{1·4}$$

The integration $I(U)$ can be analytically continued to the complex U plane from the positive real axis. It is clear that this integration has no singularities at Re $U>0$ because the integrand is analytic as a function of U and this integration is uniformly convergent in wider sense. Therefore singularities can exist on imaginary axis or the region Re $U<0$. In § 2 it will be shown that this function is analytic at Re $U<0$ and has infinite logarithmic branch points on imaginary axis.

§ 2. Lieb and Wu's ground state energy

Differential of (1·4) yields

$$\frac{dI}{dU}=-\int_0^\infty \frac{2e^{2U\omega}J_0(\omega)J_1(\omega)}{(e^{2U\omega}+1)^2}d\omega\,. \tag{2·1}$$

With the use of the relation

$$\frac{d}{d\omega}J_0^2(\omega)=-2J_0(\omega)J_1(\omega)$$

and the partial integration we obtain

$$(2·1)=\frac{U}{2}\int_0^\infty J_0^2(\omega)\frac{\sinh U\omega}{\cosh^3 U\omega}d\omega-\frac{1}{4}\,.$$

Therefore the third order derivative is

$$\frac{d^3I}{dU^3}=\int_0^\infty \frac{J_0^2(\omega)}{\cosh^2 U\omega}\omega\{(1-3\tanh^2 U\omega)+U\omega(-4\tanh U\omega+6\tanh^3 U\omega)\}\,d\omega\,.$$

At the limit $U\to 0+$ we can put $\cosh U\omega=1$ and $\tanh U\omega=0$. Then this integration is divergent because $J_0^2(\omega)$ decreases as $1/\omega$. So we have the following theorem. Theorem 1: d^3f/dU^3 diverges at the limit $U\to 0+$.

The following lemma is very useful for later discussions.

[Lemma 1]

$$\int_0^\infty \frac{J_0(\omega)J_1(\omega)}{\omega}e^{-2x\omega}d\omega=x\left[F\left(-\frac{1}{2},\frac{1}{2};1;-\frac{1}{x^2}\right)-1\right]. \tag{2·2}$$

Here F is the Gauss' hypergeometric function.

[Proof]*) One can easily prove the following formula:

$$J_0(\omega)J_1(\omega)=\left\{\sum_{i=0}^\infty \frac{(-1)^i}{(i!)^2}\left(\frac{\omega}{2}\right)^{2i}\right\}\left\{\sum_{j=0}^\infty \frac{(-1)^j}{j!(j+1)!}\left(\frac{\omega}{2}\right)^{2j+1}\right\}$$

$$=\sum_{n=0}^\infty \frac{(-1)^n(2n+1)!}{\{n!(n+1)!\}^2}\left(\frac{\omega}{2}\right)^{2n+1}.$$

*) The author is grateful to Dr. S. Inawashiro for suggesting this simple form of proof of the lemma, which was first derived by the author.

Then we have

$$\int_0^\infty \frac{J_0(\omega)J_1(\omega)}{\omega}e^{-2x\omega}d\omega=\sum_{n=0}^\infty \frac{(-1)^n(2n+1)!}{\{n!(n+1)!\}^2}\left(\frac{1}{2}\right)^{2n+1}\int_0^\infty \omega^{2n}e^{-2x\omega}d\omega$$

$$=\sum_{n=0}^\infty \frac{(-1)^n(2n+1)!!(2n-1)!!}{\{(n+1)!\}^2}\left(\frac{1}{2}\right)^{2(n+1)}\frac{1}{x^{2n+1}}$$

$$=x\left\{\sum_{n=1}^\infty \frac{\Gamma(n+\frac{1}{2})\Gamma(n-\frac{1}{2})}{(n!)^2\Gamma(\frac{1}{2})\Gamma(-\frac{1}{2})}\left(-\frac{1}{x^2}\right)^n\right\}=x\left\{F\left(-\frac{1}{2},\frac{1}{2};1;-\frac{1}{x^2}\right)-1\right\}. \quad \text{[Q.E.D.]}$$

We transform (1·4) as follows:

$$I(U)=\sum_{n=1}^\infty(-1)^{n-1}\int_0^\infty \frac{J_0(\omega)J_1(\omega)}{\omega}e^{-2nU\omega}d\omega\,.$$

Using (2·2) we have

$$I(U)=\sum_{n=1}^\infty(-1)^{n-1}nU\left\{F\left(-\frac{1}{2},\frac{1}{2};1;-\left(\frac{1}{nU}\right)^2\right)-1\right\}. \tag{2·3}$$

As is well known the function $F(-\frac{1}{2},\frac{1}{2};1;z)$ is an infinitely many-valued function and has logarithmic branch points at $z=1,\infty$. So we take a branch cut on real axis at $z\geqq 1$. The values of F at $|z|<1$ is given by an infinite series

$$F\left(-\frac{1}{2},\frac{1}{2};1;z\right)=1-\left(\frac{1}{2}\right)^2 z-\left(\frac{1\cdot 3}{2\cdot 4}\right)^2\frac{z^2}{3}-\cdots-\left(\frac{(2r-1)!!}{(2r)!!}\right)^2\frac{z^r}{2r-1}-\cdots. \tag{2·4}$$

Using the analytic continuation we define values of F at all over the complex plane of z.

Theorem 2: $I(U)$ has logarithmic branch points at $U=\pm i/n$, $n=1, 2, \cdots$.

[Proof] We take a positive arbitrary value ε and divide the series (2·3) as

$$I(U)=\sum_{n=1}^N(-1)^{n-1}nU\left\{F\left(-\frac{1}{2},\frac{1}{2};1;-\left(\frac{1}{nU}\right)^2\right)-1\right\}$$
$$+\sum_{n=N+1}^\infty(-1)^{n-1}nU\left\{F\left(-\frac{1}{2},\frac{1}{2};1;-\left(\frac{1}{nU}\right)^2\right)-1\right\}.$$

Here we choose N so that $N+1\geqq 1/\varepsilon>N$. Using the series (2·4) one can easily prove that the second term is convergent and has no singularity in the region

$$|U|>\varepsilon\,. \tag{2·5}$$

Then $f(U)$ has singularities only at $U=\pm i/n$ $(n=1,2,\cdots,N)$ in the region (2·5). Taking the limit $\varepsilon\to 0$ we obtain theorem 2. [Q.E.D.]

From this theorem we see that $U=0$ is the accumulation point of the branch points. So it is impossible to expand the ground state energy as an infinite power series of U around $U=0$. This means that the usual perturbation expansion is useless. But if we use (2·3) and (2·4) we have easily the power series expansion around $U=\infty$:

$$I(U)=\left(\frac{1}{2}\right)^2 \ln 2\cdot U^{-1}-\left(\frac{1\cdot 3}{2\cdot 4}\right)^2\frac{\zeta(3)}{3}\left(1-\frac{1}{2^2}\right)U^{-3}+\cdots$$

$$+(-1)^{r-1}\left(\frac{(2r-1)!!}{(2r)!!}\right)^2\frac{\zeta(2r-1)}{2r-1}\left(1-\frac{1}{2^{2r-2}}\right)U^{-2r+1}+\cdots. \qquad (2\cdot 6)$$

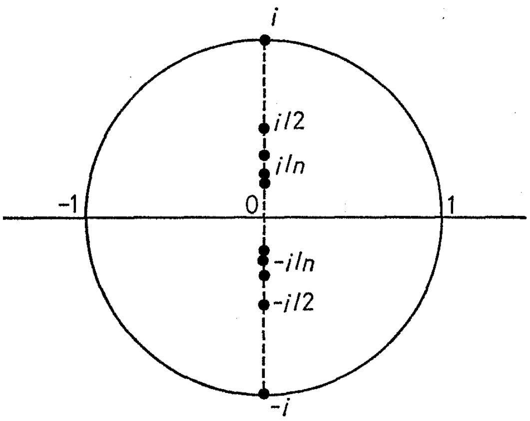

Fig. 1. The dots on the imaginary axis are logarithmic branch points. The series (2·6) converges at the outside of the unit circle.

Here ζ is Riemann's zeta function. It is clear that this series converges at $|U|>1$ because no singularity exists in this region. Harris and Lange[2] proposed the expansion of physical quantities by $1/U$ when U is sufficiently large. The fact that the expansion of the ground state energy by $1/U$ has a finite radius of convergence suggests that their method is useful. The function $f(U)$ is analytically continuable from Re $U>0$ to Re $U<0$. But there are many possible ways because this function has branch points on the imaginary axis. So let us take a branch cut on imaginary axis from i to $-i$.

Theorem 3: The analytic continuation of $f(U)$ for $U>0$ along the path which does not cross the imaginary axis at $|U|<1$ does not give the ground state energy but gives the highest energy at $U<0$.

[Proof] It is clear that we can use the expression (2·6) when the path of the analytic continuation is chosen as mentioned above. We can see easily that $I(U)$ is an odd function of U

$$I(U)=-I(-U). \qquad (2\cdot 7)$$

Comparing (1·3) and (2·7) we easily derive this theorem. [Q.E.D.]

§ 3. Discussion

It is commonly believed that the ground state energy can be written as

$$f(U)=A(U)+B(U)\cdot\log U. \qquad (3\cdot 1)$$

But theorem 2 shows that one cannot choose $A(U)$ and $B(U)$ as analytic functions of U at $U=0$. If A and B are analytic at $U=0$ we can choose a positive number ε so that in a region $|U|<\varepsilon$, A and B have no singularity. Then the righthand side of (3·1) has no singularity in the region $0<|U|<\varepsilon$. This fact is inconsistent with theorem 2.

In this paper we restricted ourselves to treat the half-filled case. In the case when the band is not halfly filled the integral equations are not analytically solved. So the investigation of the analytic properties of the ground state energy becomes a more difficult problem.[3]

Acknowledgement

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References

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