Small β expansion for infinite chain limit of one dimensional Hubbard model

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The one dimensional Hubbard model can be solved exactly. In the limit $N \to \infty$, the energy per particle remains finite and can be expressed as an integral. The small β expansion in this limit is investigated. Several elementary derivations are presented as well as a simple formula which can be used to generate both small and large beta expansions.

The one dimensional Hubbard model treats electrons on a lattice which repel when two of them are on the same site. Continued interest in the model is owed mainly to the fact that it describes a correlated system of particles which can be solved exactly for a finite number of sites. In fact, strongly correlated electrons in two dimensions are believed to be of great relevance for various properties of high-T_c superconductors. In the limit as $N \to \infty$, Lieb and Wu [1] obtained a set of coupled integral equations which can be used to solve for the energy per particle for the case in which the number of electrons is equal to that of atomic sites.

This article is intended to make accessible some very elementary techniques which can be used to expand a particular type of integral, which cannot be evaluated in closed form, in powers of small coupling and which also can be used to develop an expansion in inverse powers of the coupling. The techniques are quite general, and these kinds of manipulations ought to be applicable to other cases of physical interest.

The energy in this case is defined by an integral and it is the purpose of this paper to investigate some of its properties. In particular, the expansion of the energy for small β is developed, and it is found to agree with the results of other authors. Also, a new approach is described which leads directly to an equation from which both the small and large β expansions can be derived.

The Hamiltonian which describes the system is given by

$$H = -\beta \sum_{\substack{i=1 \\ \sigma=\uparrow,\downarrow}}^{N} (c_{i,\sigma}^{\dagger} c_{i+1,\sigma} + c_{i,\sigma}^{\dagger} c_{i-1,\sigma}) + U \sum_{i=1}^{N} n_{i,\uparrow} n_{i,\downarrow} ,$$

where all indices are taken modulo N, $c_{N+1,\sigma} = c_{1,\sigma}$. Further, $c^{\dagger}_{i,\sigma}(c_{i,\sigma})$ is the creation (annihilation) operator associated with the spin orbital $|i, \sigma\rangle$ located on the ith site and having spin $\sigma, n_{i,\sigma} = c^{\dagger}_{i,\sigma}c_{i,\sigma}$ is the occupation number operator associated with the same spinorbital, β designates the so-called resonance transfer integral, and $U = \gamma_{00}$ the one center Coulomb repulsion integral.

For the infinite chain, the analysis of Lieb and Wu leads to the following expression for the energy per particle

$$E = -4\beta \int_0^\infty \frac{J_0(x)J_1(x)}{x(1+\mathrm{e}^{\frac{Ux}{2\beta}})} \mathrm{d}x\,,$$

where J_0, J_1 are Bessel functions. Let $c = U/2\beta$, then the integration has no singularities when $\mathrm{Re}(c) > 0$ because the integrand is an analytic function of c, but singularities can exist on the imaginary axis, or the region $\mathrm{Re}(c) < 0$. Small β corresponds to large c and large β to small c. For simplicity, define the function $P(c)$ to be

$$P(c) = \int_0^\infty \frac{J_0(x)J_1(x)}{x(1+\mathrm{e}^{cx})} \mathrm{d}x\,. \tag{1}$$

Expansions for both small and large coupling regimes when $c > 0$ can be developed by first expanding the denominator of the integrand in an infinite series in powers of e^{-cx} as follows:

$$\int_0^\infty \frac{J_0(x)J_1(x)}{x(1+\mathrm{e}^{cx})} \mathrm{d}x = \int_0^\infty x^{-1}J_0(x)J_1(x)\sum_{k=1}^{\infty}(-1)^{k-1}\,\mathrm{e}^{-kcx}\,\mathrm{d}x\,.$$

For $c > 0$, the order of integration and summation can be interchanged, so the integral to be considered is

$$\int_0^\infty x^{-1}\,\mathrm{e}^{-kcx}\,J_0(x)J_1(x)\,\mathrm{d}x\,.$$

This expression can be expanded in either powers of c or inverse powers of c depending on the size of c and it is the latter case which will be of interest here. An equation will be derived from which a unified derivation of the expansions which pertain to both coupling regimes can be developed. The first step is to express the product of Bessel functions in a different way. The first way of doing this is along the lines of Takahashi [2], however an elementary derivation is possible.

THEOREM 1

$$J_0(x)J_1(x) = \sum_{n=0}^{\infty}\frac{(-1)^n(2n+1)!}{(n!(n+1)!)^2}\left(\frac{x}{2}\right)^{2n+1}. \tag{2}$$

Proof

Replace the Bessel functions by their infinite series representations which converge absolutely

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

Using the Cauchy product rule for two series this can be expressed as

$$J_0(x)J_1(x) = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!^2} \left(\frac{x}{2}\right)^{2n+1} \sum_{\nu=0}^{n} \binom{n}{\nu}^2 \frac{1}{\nu+1} .$$

To finish the proof, the finite sum on the right will be carried out.

LEMMA

$$\sum_{\nu=0}^{n} \binom{n}{\nu}^2 \frac{1}{\nu+1} = \frac{(2n+1)!}{(n+1)!^2} .$$

To prove this, integrate both sides of the binomial identity

$$\sum_{k=0}^{n} \binom{n}{k} t^k = (1+t)^n$$

from 0 to x to obtain

$$\sum_{k=0}^{n} \frac{1}{k+1} \binom{n}{k} x^k = \frac{1}{x(n+1)} ((1+x)^{n+1} - 1)$$

then multiplying both sides the binomial identity gives

$$\sum_{k=0}^{n} \frac{1}{k+1} \binom{n}{k} x^k \sum_{j=0}^{n} \binom{n}{j} x^j = \frac{1}{x(n+1)} ((1+x)^{2n+1} - (1+x)^n) .$$

The mth term of the Cauchy product on the series on the left is just the sum given in the lemma when $m = n$, and the coefficient of x^n on the right is just

$$\frac{1}{n+1} \binom{2n+1}{n+1} ,$$

which is the required result. □

Therefore, from the theorem we have the following expansion

$$x^{-1} J_0(x)J_1(x) = \sum_{n=0}^{\infty} \frac{(-1)^n (2n+1)!}{(n!(n+1)!)^2} x^{2n} .$$

It is straightforward to do the integral and obtain an expression which is valid for large c, or equivalently large β. This expansion will be written down toward the end.

The following theorem may be used to give another derivation of the large c expansion. In addition, it may also be used to rewrite the integrand in a form which is suitable for developing the small c, or large β, expansion. This is the form used by Misurkin and Ovchinnikov [3] in deriving their equation which is valid for small c.

Although simplified, this proof of theorem 1 follows Takahashi's development. The first proof of theorem 2 below depends largely on theorem 1 and therefore is not independent of Takahashi. However, a new and quite different proof can also be given which is somewhat elementary and independent of the first proof. In the second proof, the idea will be to convert the product of Bessel functions to a double integral.

THEOREM 2

$$J_0(x)J_1(x) = \frac{2}{\pi}\int_0^{\frac{\pi}{2}} J_1(2x\cos\varphi)\cos\varphi \, \mathrm{d}\varphi \,. \tag{3}$$

Proof 1

Using theorem 1, we have

$$\begin{aligned}
\frac{\pi}{2}J_0(x)J_1(x) &= \sum_{n=0}^{\infty} \frac{(-1)^n}{2^{2n+2}n!(n+1)!} x^{2n+1} \binom{2n+2}{n+1} \frac{\pi}{2} \\
&= \sum_{n=0}^{\infty} \frac{(-1)^n}{n!(n+1)!} x^{2n+1} \int_0^{\frac{\pi}{2}} \cos^{2n+2}\varphi \, \mathrm{d}\varphi \\
&= \int_0^{\frac{\pi}{2}} J_1(2x\cos\varphi)\cos\varphi \, \mathrm{d}\varphi \,.
\end{aligned}$$

Proof 2

An integral representation for the product $J_0(x)J_1(x)$ can be found by starting with the integral form of the Bessel functions [4] as follows

$$\begin{aligned}
J_0(x)J_1(x) &= \frac{1}{4\pi^2}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi} \mathrm{e}^{\mathrm{i}\varphi-\mathrm{i}x(\sin\theta+\sin\varphi)} \, \mathrm{d}\theta \, \mathrm{d}\varphi \\
&= \frac{1}{4\pi^2}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi} \mathrm{e}^{\mathrm{i}\varphi-2\mathrm{i}x\sin\frac{1}{2}(\theta+\varphi)\cos\frac{1}{2}(\theta-\varphi)} \, \mathrm{d}\theta \, \mathrm{d}\varphi \,.
\end{aligned} \tag{4}$$

Introduce new variables u and v defined by the equations

$$\theta - \varphi = 2u, \quad \theta + \varphi = 2v \,.$$

Since the integrand is unchanged if both u and v are increased by π or if u is increased by π while v is simultaneously decreased by π, the region of integration may be taken to be the rectangle for which $0 \leqslant u \leqslant \pi$, $-\pi \leqslant v \leqslant \pi$.

To prove this, it is easy to see that the square region of integration in (4) is rotated so that in the $u-v$ system, the vertices are on the coordinate axes. It will be shown that the contribution to the integral from the region to the left of the v axis is the same as that from the two triangles which would have to be added to the region to the right of the v axis to form the complete rectangular region bounded by $0 \leqslant u \leqslant \pi$ and $-\pi \leqslant v \leqslant \pi$. Consider first the integration over the top triangle to the left of the v-axis,

$$\int_{-\pi}^{0} \int_{0}^{u+\pi} \mathcal{K}(u,v)\, dv\, du\,,$$

where

$$\mathcal{K}(u,v) = e^{i(u+v)-2ix\cos u \sin v}\,.$$

Introducing the linear transformation $u = s-\pi, v = t+\pi$ this integral is transformed into

$$\int_{0}^{\pi} \int_{-\pi}^{s-\pi} \mathcal{K}(s-\pi, t+\pi)\, dt\, ds = \int_{0}^{\pi} \int_{-\pi}^{s-\pi} \mathcal{K}(s,t)\, dt\, ds\,.$$

The same technique can be applied to the remaining region, and since the absolute value of the Jacobian is 2, we have

$$\begin{aligned} J_0(x)J_1(x) &= \frac{1}{2\pi^2} \int_{0}^{\pi} \int_{-\pi}^{\pi} e^{-iu}\, e^{i(v-2x\cos u \sin v)}\, dv\, du \\ &= \frac{1}{\pi} \int_{0}^{\pi} e^{-iu} J_1(2x\cos u)\, du\,. \end{aligned}$$

Splitting this up into real and imaginary parts, it can be shown that the imaginary part vanishes, as can be seen by considering the part of the integral from $\pi/2$ to π. Setting $\tau + \pi = u$ and using $J_n(-t) = (-1)^n J_n(t)$ it is easy to see that

$$\int_{\frac{\pi}{2}}^{\pi} \cos u J_1(2x\cos u)\, du = \int_{0}^{\frac{\pi}{2}} \cos\tau\, J_1(2x\cos\tau)\, d\tau\,.$$

This completes the proof. □

Consequently, the second proof of theorem 2 gives another way of generating the small β expansion for the energy per particle. Simply substitute the infinite series representation for $J_1(2x\cos\varphi)$ and integrate term by term.

Using theorem 2, it is possible to transform the integral $P(c)$ into an elliptic integral of the second kind, which will generate the small β expansion, and also it provides the starting point for developing the large β expansion. To do this, consider the general integral defined by

$$\mathcal{I}(a,\lambda) = \int_{0}^{\infty} J_0(t)J_1(t)e^{-at}t^{\lambda}\, dt\,.$$

Replacing $J_0(t)J_1(t)$ by the expression derived in theorem 2, this becomes

$$\mathfrak{I}(a,\lambda) = \frac{2}{\pi}\int_0^{\frac{\pi}{2}} \mathrm{d}\varphi \cos\varphi \int_0^\infty J_1(2t\cos\varphi)\mathrm{e}^{-at}t^\lambda \,\mathrm{d}t\,.$$

Consider the generalized version of the second integral given by

$$\int_0^\infty \mathrm{e}^{-at}J_\nu(bt)t^\lambda \,\mathrm{d}t\,.$$

This will be written in terms of the hypergeometric function. Suppose that b is restricted so that $|b|<|a|$. If the integrand is expanded in powers of b, and we integrate term by term, we obtain

$$\int_0^\infty \mathrm{e}^{-at}J_\nu(bt)t^\lambda \,\mathrm{d}t = \sum_0^\infty \frac{(-1)^m \Gamma(\lambda+\nu+2m+1)}{m!\Gamma(\nu+m+1)a^{\lambda+\nu+2m+1}}\left(\frac{b}{2}\right)^{\nu+2m}.$$

The final series converges absolutely, since $|b|<|a|$, and so the process of term by term integration is justified. Expressing the right hand side in terms of the hypergeometric function gives

$$\int_0^\infty \mathrm{e}^{-at}J_\nu(bt)t^\lambda \,\mathrm{d}t = \left(\frac{b}{2a}\right)^\nu \frac{\Gamma(\lambda+\nu+1)}{a^{\lambda+1}\Gamma(\nu+1)}\,{}_2F_1 \times \left(\frac{\lambda+\nu+1}{2},\frac{\lambda+\nu+2}{2};\nu+1;\frac{-b^2}{a^2}\right).$$

This holds only when $\mathrm{Re}(a)>0$ and $|b|<|a|$ but as long as $\mathrm{Re}(a\pm \mathrm{i}b)>0$, which is the case here since b is strictly real, then both sides of this expression are analytic functions of b, and so the more extensive range of validity is obtained by analytic continuation to the complex plane. For the case of interest here, set $\nu=1$ and $\lambda=-1$ so that

$$\int_0^\infty J_1(2t\cos\varphi)\mathrm{e}^{-at}t^{-1}\,\mathrm{d}t = a^{-1}\cos\varphi\,{}_2F_1\left(\frac{1}{2},1;2;\frac{-4}{c^2}\cos^2\varphi\right).$$

Using the fact that

$${}_2F_1\left(\frac{1}{2},1;2;\frac{-r^2}{a^2}\right) = \frac{2a^2}{r^2}\left(\left(1+\frac{r^2}{a^2}\right)^{\frac{1}{2}}-1\right)$$

and replacing r^2 by $4\cos^2\varphi$ we have

$${}_2F_1\left(\frac{1}{2},1;2;\frac{-4}{a^2}\cos^2\varphi\right) = \frac{a}{2\cos^2\varphi}\left((a^2+4\cos^2\varphi)^{\frac{1}{2}}-a\right).$$

Substituting, we obtain the following remarkable form for $\mathfrak{I}(a,-1)$

$$\mathfrak{I}(a,-1) = \frac{1}{\pi}\int_0^{\frac{\pi}{2}} \mathrm{d}\varphi((a^2+4\cos^2\varphi)^{\frac{1}{2}}-a)\,.$$

This form for $\mathfrak{I}(a,-1)$ gives rise to the possibility of writing down a unified treatment for the expansions in both coupling regimes. Replacing a by kc the following expression for $P(c)$ can be written down

$$P(c) = \frac{1}{\pi}\sum_{k=1}^{\infty}(-1)^{k+1}\int_0^{\frac{\pi}{2}} \mathrm{d}\varphi(((kc)^2 + 4\cos^2\varphi)^{\frac{1}{2}} - kc). \tag{5}$$

It is now possible to write down an elementary derivation for the large c expansion by factoring $(kc)^2$ out of the square root and then expanding using the binomial theorem to obtain

$$\begin{aligned} P(c) &= \frac{1}{2c}\sum_{k=1}^{\infty}\frac{(-1)^{k-1}}{k} + \frac{1}{2}\sum_{m=2}^{\infty}\frac{(-1)^{m-1}}{2^{2m}}\binom{2m}{m}^2\frac{1}{2m-1}\sum_{k=1}^{\infty}\frac{(-1)^{k-1}}{k^{2m-1}}\frac{1}{c^{2m-1}} \\ &= \frac{\ln(2)}{2c} + \frac{1}{2}\sum_{m=2}^{\infty}\frac{(-1)^{m-1}}{2^{2m}}\binom{2m}{m}^2\frac{1}{2m-1}\left(1-\frac{2}{2^{2m-1}}\right)\zeta(2m-1)\frac{1}{c^{2m-1}}, \end{aligned}$$

where $\zeta(x)$ is the Riemann zeta function. This is just the expansion which can be found in Takahashi [2]. Replacing c by $5/2\beta$, the expansion in terms of β results

$$\begin{aligned} \mathcal{P}(\beta) &= \frac{\ln(2)}{5}\beta + \sum_{m=2}^{\infty}\frac{(-1)^{m-1}}{2^{4m}(2m-1)}\binom{2m}{m}^2 \\ &\quad\times\left(1-\frac{2}{2^{2m-1}}\right)\zeta(2m-1)\left(\frac{4}{5}\right)^{2m-1}\beta^{2m-1}, \end{aligned} \tag{6}$$

and it is easy to show that this series converges for values of $|\beta| \in [0, \frac{5}{4}]$.

If a multiplicative factor of -4β, which was neglected in writing (1), is included, an expansion of the Lieb–Wu energy per particle for the infinite chain for small β is obtained. In some ways, this is an improvement over the integral as far as performing calculations is concerned. For β in the interval $[0, \frac{5}{4}]$ one need only sum terms to get a value for the energy, however, outside this interval a summation technique must be applied and this is usually straightforward.

Equation (5) is of interest in its own right because it can be used to develop an asymptotic expansion for the energy per particle which holds in the opposite limit as β tends to infinity. This has not been examined rigorously in the literature.

References

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