Average partition function of an electron in random binary alloy

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We compute the average partition function for an electron moving in a random binary alloy system. A coherent state representation variational (CSRV) method is applied to the single-band tight-banding model Hamiltonian. The results are compared with the exact solution in one-dimensional Anderson's model. The partition function goes over smoothly to the Lifshitz tail in the low-temperature limit and to the result of mean-field theory in the high-density limit. This CSRV method gives the exact results in periodic and very-high-density limit and approaches virtual-crystal theory in small-β limit.

I. INTRODUCTION

The nature of electronic states in a binary alloy with two atomic species A and B distributed at random on a regular space lattice, has drawn a lot of attention. In this paper we are interested in computing the average partition function of an electron moving in a random alloy. This partition function is averaged over the random configurations. The electronic density of states of the random binary alloy may be found as the inverse Laplace transform of this average partition function. Gross[1] has computed the average partition function of an electron moving in a Gaussian random potential by path integral formulation. It is interesting to use the coherent state representation variational (CSRV) method which is closely related to the Feynman path integral formalism to the binary random alloy which is under extensive investigation by other methods. This paper is arranged as follows: I formulate the problem in Sec. II and apply this formalism to Anderson's model in Sec. III. In Sec. IV the exact solution of the one-dimensional Anderson's model is given, and finally, I compare the CSRV results with the exact ones, analytically and numerically.

II. FORMULATION BY THE CSRV METHOD

Let us take the single-band tight-binding model Hamiltonian in a random alloy which has been under extensive study. For a specific configuration of the alloy, the model Hamiltonian is given by

$$\mathcal{H}_{nm} = \epsilon_n \delta_{nm} + h_{nm} \ . \tag{1}$$

The diagonal elements may be regarded as random atomic levels which assume one of the two possible values ϵ_A or ϵ_B, depending on whether an atom of type A or B occupies the site n. The hopping integrals h_{nm} are assumed to be independent of the alloy configuration. In other words, the elements of ϵ_n are diagonal but random, whereas those of h_{nm} are off-diagonal but translationally invariant (i.e., h_{nm} depends only on the distance from site m to site n).

We shall use the coherent state representation variational (CSRV) method which was developed by Luttinger,[2] to deal with the simple liquidlike disordered system and its diamagnetism[3]; Lu has applied this method to the repulsive[4] and attractive[5] Frisch-Lloyd disordered model.[6] Let us reformulate the CSRV method in the discrete representation and briefly describe the method by introducing the set of functions $\Psi(P, Q; l)$ defined as

$$\Psi(P, Q; l) = e^{iPl}\chi(l - Q) \tag{2}$$

for a discrete lattice point l. P and Q are c numbers and χ is the normalized function

$$(\chi, \chi) = \sum_l |\chi(l)|^2 = 1 \ .$$

We formulate this theory in one dimension for simplicity and it can be extended to the three-dimensional case trivially. In order to satisfy periodic boundary conditions, we take

$$P = 2\pi \frac{m}{Na}, \quad Q = na,$$

where $m = 0, \pm1, \pm2, \ldots, n = 0, \pm1, \pm2, \ldots,$ a is the lattice length, and N is the total number of lattice points. It can be easily shown that the set of functions $\Psi(P, Q; l)$ is overcomplete and does not form an orthonormal set[2], and the trace of any reasonable operator $\hat{B}$ is given by

$$\mathrm{Tr}(\hat{B}) = \frac{1}{N} \sum_P \sum_Q [\Psi(P, Q), \hat{B}\Psi(P, Q)] . \tag{3}$$

with arbitrary but normalized χ.[7]

Therefore, the partition function of the random alloy system is given by

$$\vartheta(\beta) = \mathrm{Tr}(e^{-\beta\mathcal{H}}) = \frac{1}{N} \sum_P \sum_Q [\Psi(P, Q), e^{-\beta\mathcal{H}}\Psi(P, Q)] .$$

By the Jensen's inequality for convex functions, we have

$$\vartheta(\beta) \geq \frac{1}{N}\sum_{P,Q} e^{-\beta(\Psi,\mathcal{H}\Psi)}$$

and

$$(\Psi,\mathcal{H}\Psi)=\sum_l \epsilon_l |\chi(l-Q)|^2 + \sum_{l\neq l'} e^{iP(l-l')}\chi^*(l-Q)\chi(l'-Q)h_{ll'} .$$

We can express the random ϵ_l as follows:

$$\epsilon_l = n_l\epsilon + \epsilon_B ,$$

where $\epsilon=\epsilon_A-\epsilon_B$ and

$$n_l=\begin{cases}1 & \text{if } A \text{ atom is at } l \text{ site}\\ 0 & \text{if } B \text{ atom is at } l \text{ site}\end{cases} .$$

ϑ is the configuration-dependent partition function. Let us calculate the configuration average to obtain the average partition function:

$$z(\beta)\equiv\langle\vartheta(\beta)\rangle \geq \frac{1}{N}\sum_{P,Q}\left\langle \exp\left[-\beta\left(\sum_l \epsilon_l|\chi(l-Q)|^2+\sum_{l\neq l'} e^{iP(l-l')}\chi^*(l-Q)\chi(l'-Q)h_{ll'}\right)\right]\right\rangle .$$

The configuration average is defined by

$$\langle f(n_l)\rangle = \sum_{\{n_l\}} f(n_l)\Big/\sum_{\{n_l\}}' 1 .$$

The prime of the summation means we sum over all the $\{n_l\}$ configurations with the constraint $\sum_l n_l = N_A$. In order to relax this restriction, we may use the canonical ensemble average which is defined as follows:

$$\langle f(n_l)\rangle = \sum_{\{n_l\}} f(n_l)\, e^{-\mu\sum_l n_l}\Big/\sum_{\{n_l\}} e^{-\mu\sum_l n_l} .$$

By the canonical ensemble average, the average partition function becomes

$$z(\beta)\geq \frac{1}{N}\sum_{P,Q}\left[(p_A e^{-\beta\epsilon_A|\chi(l-Q)|^2}+p_B e^{-\beta\epsilon_B|\chi(l-Q)|^2})\exp\left(-\beta\sum_{l'} e^{iP(l-l')}\chi^*(l-Q)\chi(l'-Q)h_{ll'}\right)\right] .$$

Because of the requirement $\langle\sum_l n_l\rangle = N_A$, we have $p_A=N_A/N=(e^{\mu}+1)^{-1}$; that is, $p_A/p_B=e^{\mu}$. After the configuration average, the system is translationally invariant, so we can let $l+Q\to l$ and $l'+Q\to l'$ and sum over Q. We then obtain

$$z(\beta)\geqq \sum_P \exp\left(\sum_l \ln(p_A e^{-\beta\epsilon_A|\chi(l)|^2}+p_B e^{-\beta\epsilon_B|\chi(l)|^2})-\beta\sum_{l\neq l'} e^{iP(l-l')}\chi^*(l)\chi(l')h_{ll'}\right) .$$

If we take the nearest-neighbor interaction approximation with

$$h_{ll'}=h(\delta_{l,l'+a}+\delta_{l,l'-a}) , \tag{4}$$

then

$$z(\beta)\geqq \sum_P \exp\left(\sum_l[\ln(p_A e^{-\beta\epsilon_A\chi^2(l)}+p_B e^{-\beta\epsilon_B\chi^2(l)}) - \beta\alpha\cos(Pa)]\right) , \tag{5}$$

where we assume $\chi(l)$ is real for simplicity and α is defined as

$$\alpha = 2h\sum_l \chi(l)\chi(l-a) . \tag{6}$$

Next, we sum over P, and in order to carry out this sum simply, we assume this is a very long chain with N approaching infinity. Then the partition function of a one-dimensional random alloy system per unit lattice point can be written as

$$z(\beta)\geqq I_0(\beta\alpha)\exp\left(\sum_l \ln(p_A e^{-\beta\epsilon_A\chi^2(l)}+p_B e^{-\beta\epsilon_B\chi^2(l)})\right) , \tag{7}$$

where I_0 is the Bessel function of an imaginary argument of order zero. Let us call the right-hand side of the expression $z_v(\beta)$; thus $z(\beta)\geq z_v(\beta) \equiv \exp\{W[\chi(l)]\}$.

The criterion for choosing the best $\chi(l)$ is that one which will make the above inequality as strong as possible. The stationary condition with the normalization constraint is

$$\delta\left(W[\chi(l)]-\lambda_0\sum_l\chi(l)^2\right)\Big/\delta\chi(l)=0 . \tag{8}$$

From this condition we obtain a self-consistent nonlinear difference equation as the follows:

$$h\frac{I_1(\beta\alpha)}{I_0(\beta\alpha)}[\chi(l+a)+\chi(l-a)] - \frac{\epsilon p e^{-\beta\epsilon\chi^2(l)}}{pe^{-\beta\epsilon\chi^2(l)}+(1-p)}\chi(l)=\lambda\chi(l) , \tag{9}$$

where we set $\epsilon_A=\epsilon$ and $\epsilon_B=0$, $p_A=p$, and $\lambda_0/\beta=\lambda$.

If we assume $\chi(l)$ is a very slowly varying function, then Eq. (9) becomes a Schrödinger-type equation with self-consistent potential:

$$aG(\alpha)\chi''(l)+\left(2G(\alpha)-\frac{\epsilon p e^{-\beta\epsilon\chi^2(l)}}{pe^{-\beta\epsilon\chi^2(l)}+(1-p)}\right)\chi(l)=\lambda\chi(l)\ , \tag{10}$$

where $G(\alpha)=hI_1(\beta\alpha)/I_0(\beta\alpha)$.

Making use of the boundary $\chi(L)=\chi'(L)=0$, Eq. (10) can be integrated exactly:

$$\chi'(l)=\left(\frac{\lambda-2G}{a^2G}\chi^2(l)-\frac{1}{\beta aG}\ln[pe^{-\beta\epsilon\chi^2(l)}+(1-p)]\right)^{1/2}\ . \tag{11}$$

If β is small, that is, in the high-temperature case, the approximate solution of λ and $\chi(l)$ is given by

$$\lambda\simeq 2G-p\epsilon+\tfrac{1}{2}\beta(p-p^2)\epsilon^2\chi^2(0)\ , \tag{12}$$

$$\chi(l)\simeq\chi(0)\,\mathrm{sech}(kl)\ , \tag{13}$$

where $k^2=(p-p^2)\beta\epsilon^2\chi^2(0)/2a^2G$ and $\chi(0)$ can be determined by the normalization condition given by the following equation:

$$1=\frac{2\chi^2(0)}{a}\left(\frac{2a^2G}{(p-p^2)\beta\epsilon^2\chi^2(0)}\right)^{1/2}\times\tanh\left[\left(\frac{(p-p^2)\beta\epsilon^2\chi^2(0)}{2a^2G}\right)^{1/2}\left(\frac{Na}{2}\right)\right]\ . \tag{14}$$

For small β, $\chi(0)$ is approximately given by

$$\chi(0)\sim 1/\sqrt{N}\ .$$

Therefore the lower bound of the average partition function is

$$z_v\simeq I_0(\beta\alpha)e^{-\beta p\epsilon}$$

which can also be obtained directly from Eq. (7). This result implies that in the high-temperature limit, the virtual crystal picture is a good approximation. In the virtual crystal picture[8] the random system is represented by a virtual ordered system which replaces the random atomic levels by the averaged level $\tilde{\epsilon}=p_A\epsilon_A+p_B\epsilon_B$.

The other limit is the low-temperature case, that is, $\beta\to\infty$. For this case, we expect the wave function will be localized in a large region, that is, the $\chi(l)$ is not zero only inside this big well of width b. Therefore the partition function is given by

$$z_v(\beta)\simeq(2\pi\beta\alpha)^{-1/2}\exp\left\{\beta\left[2|h|-|h|\left(\frac{\pi a}{b}\right)^2+\frac{\ln(1-p)}{\beta}\left(\frac{b}{a}\right)\right]\right\}\ . \tag{15}$$

Maximizing the exponent, we obtain

$$b=\left(\frac{2\pi^2|h|a^3\beta}{-\ln(1-p)}\right)^{1/3}\ . \tag{16}$$

Therefore,

$$z_v\cong(4\pi\beta|h|)^{1/2}\exp\left[\beta(2|h|)-3\left(\frac{\pi^2}{4}|h|[\ln(1-p)]^2\right)^{1/3}\beta^{1/3}\right]\ . \tag{17}$$

From the inverse Laplace transform, this partition function will give the famous Lifshitz's tail spectrum[9] which starts from the band bottom edge $-2|h|$.

Another interesting case is the high-density limit for $N_A\to N$; for this case Eq. (7) becomes

$$z_v(\beta)\to I_0(\beta\alpha)e^{-\beta\epsilon}\ .$$

This is just the partition function for a pure A atom crystal in tight-binding approximation, because the exact partition function for a pure A atom crystal is given by

$$z_A(\beta)=\sum_k e^{-\beta\epsilon(k)}=\frac{a}{2\pi}\int_{BZ}dk\,e^{-\beta(\epsilon_A+2h\cos ka)}=I_0(2\beta h)e^{-\beta\epsilon_A}\ . \tag{18}$$

Therefore, if we choose $\chi(l)=1/\sqrt{N}$ as an extended state in our CSRV method, α will equal $2h$. This proves the CSRV method will give the exact result in the periodic limit.

III. APPLICATION TO ANDERSON'S MODEL WITH $\epsilon_A=0$ AND $\epsilon_B\to\infty$

The formulation of the previous section can be applied to the so-called Anderson's model of substitutional binary random alloy with $\epsilon_A=0$ and $\epsilon_B\to\infty$.[10-12] In fact, the problem of the one-dimansional Anderson's model can be solved exactly and it is interesting to compare the results of the CSRV method and the exact solution.

In one dimension the system is divided by B atoms randomly. Let us assume there is some range of n lattice sites on which the effective wave function $\chi(l)$ is not equal to zero and $\chi(l)=0$ on all the complementary regions of lattice points. The region where $\chi(l)\neq 0$ is empty of B atoms. The partition function of the one-dimensional Anderson's model of the random alloy which satisfies Eq. (7) is

$$z(\beta)\geq I_0(2\beta hB)p_A^n\ , \tag{19}$$

where $B=\sum_{l=1}^{n-1}\chi(l)\chi(l+1)$.

Because I_0 is an even, montonically increasing function, the best $\chi(l)$ must be the one which makes B maximum subject to the constraint

$\sum_l^n \chi^2(l) = 1$ for some given n. By variational principle,

$$d\left(B - \lambda \sum_{l=1}^{n} \chi^2(l)\right)\Big/ d\chi(m) = 0 \ . \tag{20}$$

This yields the set of equations

$$\chi(m-1) - \lambda\chi(m) + \chi(m+1) = 0, \text{ for } m = 1, 2, \ldots, n \ .$$

The eigenvalues and the eigenfunctions are given by

$$\lambda_s = 2\cos\left[\left(\frac{s}{n+1}\right)\pi\right] , \quad \text{for } s = 1, 2, \ldots, n.$$

$$\chi^{(s)}(m) = \chi^{(s)}(1)\sin\left[m\left(\frac{s}{n+1}\right)\pi\right] \ ,$$

Because B can be expressed in the form $\frac{1}{2}(\chi, A\chi)$, where A is given by an $n \times n$ matrix with $A_{km} = (\delta_{k,m+1} + \delta_{k,m-1})$, by the property of orthogonal transformation we can easily see $B = \frac{1}{2}\lambda_s$. Therefore, the maximum value of B is just one-half the maximum eigenvalue $\lambda_s^{\max} = \cos(\pi/n+1)$, hence the best $z_v(\beta)$ for a given n can be written as

$$z_v(\beta) = p_A^n I_0\left[2\beta h \cos\left(\frac{\pi}{n+1}\right)\right] \ . \tag{21}$$

Now we maximize $z_v(\beta)$ by choosing the best value of n, then the $z_v(\beta)$ will provide the best approximation to the exact result. In the large-β limit, by using the asymptotic representation of I_0, we have the best n as

$$n \sim \left(\frac{2\pi|h|}{-\ln p}\right)^{1/3} \beta^{1/3} \tag{22}$$

and

$$z_v(\beta) \simeq (4\pi\beta h)^{-1/2} e^{2|h|\beta - d\beta^{1/3}} \ , \tag{23}$$

where $d = 3[\frac{1}{4}\pi^2 |h| (\ln p)^2]^{1/3}$. Therefore, the Lifshitz tail will come out in the low-lying spectrum again, starting from $-2|h|$ which is the band bottom of the corresponding crystal system.

The previous work can be extended to the three-dimensional case trivially; we just write down the results:

$$z_v(\beta) = \prod_{i=1}^{3} I_0(\beta\alpha_i) \prod_l \left(p_A e^{-\beta\epsilon_A \chi^2(l)} + p_B e^{-\beta\epsilon_B \chi^2(l)}\right) , \tag{24}$$

where $\alpha_i = 2h\sum_{\vec{l}} \chi(\vec{l})\chi(\vec{l} + \vec{a}_i)$. $\vec{a}_i$ is the primitive lattice vector; for $\beta \to \infty$ we also obtain the Lifshitz tail in the three-dimensional case.[9,13]

IV. EXACT SOLUTION FOR ONE-DIMENSIONAL ANDERSON'S MODEL

The Anderson's model can be solved exactly in the one-dimensional case. Let us assume there are N lattice points divided by N_B B atoms into $N_B - 1$ intervals and there are ν_1 A atoms in the first interval and ν_2 A atoms in the second interval and so on, such that $\nu_1 + \nu_2 + \ldots + \nu_{N_B - 1} = N_A$. Any fixed set of $\{\nu_i\}$ corresponds to a fixed configuration of the random alloy and the energy level of the ν_j interval is denoted by $\epsilon_{n_j}(\nu_j)$.

The cumulative density of states (integrated density of states) $N(E, \{\nu_j\})$ is defined by

$$N(E, \{\nu_j\}) = \sum_j \sum_{n_j} \Theta(E - \epsilon_{n_j}(\nu_j)) \ , \tag{25}$$

where we sum over all the intervals and all the energy levels for a specified interval. The configuration-averaged cumulative density of states can be done by assuming canonical distribution for ν_j, i.e., the probability distribution of $\{\nu_j\}$ is given by

$$P(\{\nu_j\}) = \sum_{j=1}^{K} p_B e^{-\mu\nu_j} \ , \tag{26}$$

where $K = N_B - 1$, the "chemical potential" μ is determined by the requirement $\langle \sum_{i=1}^{K} \nu_j \rangle = N_A$, as $e^{-\mu} = p_A$. It is very convenient to calculate $N(E, \{\nu_j\})$ by relaxing the constraint $\sum_{j=1}^{K} \nu_j = N_A$ and using Eq. (26):

$$\begin{aligned} N(E) &\equiv \langle N(E, \{\nu_j\}) \rangle \\ &= \sum_{j=1}^{K} \sum_{n_j} \left(\sum_{\nu_1} \sum_{\nu_2} \cdots P(\{\nu_j\}) \Theta(E - \epsilon_{n_j}(\nu_j)) \right) \\ &= N p_B^2 \sum_{\nu=1}^{\infty} e^{-\mu\nu} \sum_n \Theta(E - \epsilon_n(\nu)) \ , \end{aligned} \tag{27}$$

where the $\epsilon_n(\nu)$ are the eigenvalues of the Anderson's model Hamiltonian within the interval of νA atoms, and is given by

$$\epsilon_n(\nu) = 2h\cos\left(\frac{n}{\nu+1}\pi\right) \ . \tag{28}$$

Therefore the density of states per unit lattice can be written as

$$\begin{aligned} g(E) &\equiv \frac{1}{N}\frac{dN(E)}{dE} \\ &= p_B^2 \sum_{\nu=1}^{\infty} \sum_{n=1}^{\nu} p_A^{\nu} \delta\left(E - 2h\cos\left(\frac{n}{\nu+1}\pi\right)\right) \ , \end{aligned} \tag{29}$$

and the average partition function per unit lattice is the Laplace transform of $g(E)$ is obtained as follows:

$$z(\beta) = p_B^2 \sum_{\nu=1}^{\infty} \sum_{n=1}^{\nu} p_A e^{-2\beta h \cos[n\pi/(\nu+1)]} \ . \tag{30}$$

From (29) we can find that the density of states is symmetric about $E = 0$ and confined between $-2|h|$ and $+2|h|$.

V. COMPARISON BETWEEN CSRV METHOD AND THE EXACT SOLUTION AND DISCUSSIONS

In this section I try to compare the results of the CSRV method and the exact solution in the one-dimensional Anderson's model; comparisons were made in several limiting regions and I also compare them numerically.

(1) The high-temperature or $\beta \to 0$ limit. In this limit, Eq. (30) can be reduced to

$$z(\beta) \to (1-p_A)^2 \sum_{\nu=1}^{\infty} p_A^{\nu} \nu = p_A .$$

On the other hand, for the CSRV result, I use the fact that $I_0(0)=1$. The variational partition function given by the CSRV method is

$$z_v(\beta) \to p_A^n .$$

It is obvious that the best value of n which will maximize $z_v(\beta)$ is $n=1$. Hence it is shown in the high-temperature limit that the CSRV method is exact.

(2) For the high-density limit, that is, $p_A \to 1$. In this limit the CSRV method should work well because this approximation method in some sense is a mean-field theory. In the high-density case, the averaged mean-field picture is very close to the exact one. For $p_A \to 1$, we can see the large ν term in Eq. (30) will dominate. Therefore we can just approximate Eq. (30) by

$$z(\beta) \to (1-p_A)^2 \sum_{\nu=1}^{\infty} p_A^{\nu} \sum_{n=1}^{\infty} e^{-2\beta h \cos\{[n/(\nu+1)]\pi\}} . \quad (31)$$

For large ν the summation can be replaced by integration, hence Eq. (31) can be reduced as

$$z(\beta) \to (1-p_A)^2 \sum_{\nu=1}^{\infty} \nu p_A^{\nu} I_0(2\beta h) = I_0(2\beta h) .$$

The averaged variational partition function given by the CSRV method is

$$z_v(\beta) \sim I_0\left(2\beta h \cos\left(\frac{\pi}{n+1}\right)\right)$$

and the best choice of n is $n \to \infty$. Thus the agreement between the CSRV method and the exact solution in the high-density limit is obtained.

(3) The very-low-temperature or $\beta \to \infty$ limit. The Lifshitz tail spectrum can be obtained very naturally by the CSRV method which is superior to any perturbation theory[14,15] and other mean-field theory or CPA (coherent-potential approximation) and ATA (average-T-matrix approximation).[16,17] But it should be noticed that as $\beta \to \infty$, although the relative error produced by the CSRV method approximation gets smaller as β becomes larger,

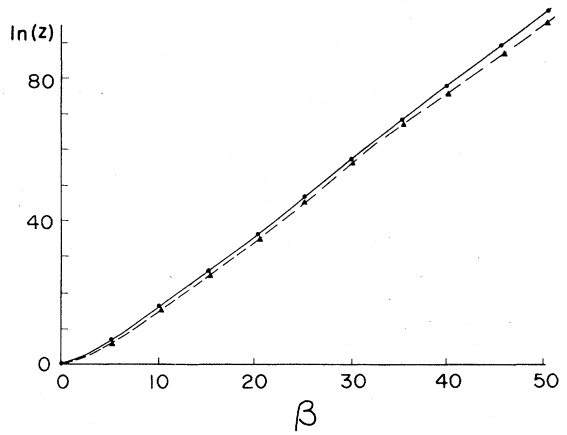

FIG. 1. The logarithm of the exact partition function (solid curve) and that of the CSRV method (broken curve); the magnitude of h is taken to be 1.0, and the density is 0.8.

the absolute error is still large. In fact, it is increasing as $\ln\beta$ compared to the correct $\beta^{1/3}$ leading term in the one-dimensional case. That is, the pre-exponent β-dependence factor is not correct but the exponent leading term is correct.

(4) By using an electronic computer, we can maximize the $z_v(\beta)$ numerically and also compute the exact formula (30). Figures 1 and 2 present the comparisons between these two results. It can be seen, for small β or large density, that the CSRV method gives good agreement.

The theory of an electron moving in random binary alloy is a simple example of a set of problems covering a wide range of phenomena. I have calculated the average partition function in a tight-binding, single-band model Hamiltonian and the Anderson's model with $\epsilon_B \to \infty$ and checked for accuracy by comparing with the exact one-dimensional results. The satisfactory agreement between them is quite encouraging and gives me some confidence in the CSRV method for some

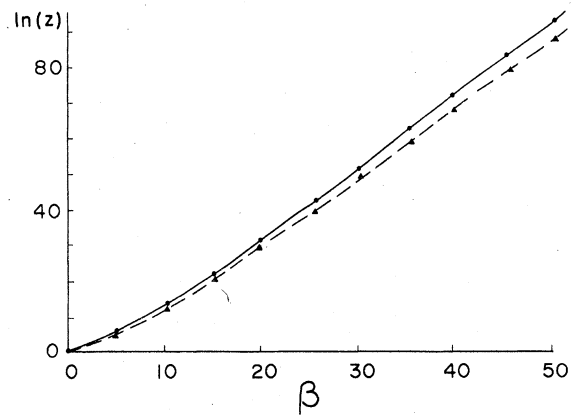

FIG. 2. The logarithm of the exact partition function (solid curve) and that of the CSRV method (broken curve); $h=1.0$ and density = 0.5.

more complicated cases which include the behavior of an electron interacting with randomly placed scatterers or with lattice vibrations and certain polymer configuration problems, or even a more realistic model Hamiltonian.

APPENDIX

In this appendix, I will prove T is the trace of any reasonable operator $\hat{B}$ in the lattice coordinate representation:

$$T=\frac{1}{N}\sum_{P,Q}[\Psi(P,Q),\hat{B}\Psi(P,Q)]$$

$$=\frac{1}{N}\sum_{P,Q}\sum_{l,l'}[\Psi^*(P,Q;l)\langle l|\hat{B}|l'\rangle\Psi(P,Q;l')]$$

$$=\frac{1}{N}\sum_{P,Q}\sum_{l,l'}e^{iP(l-l')}\chi^*(l-Q)\chi(l'-Q)\langle l|\hat{B}|l'\rangle\ .$$

First, sum over P by using the identity

$$\sum_P e^{iP(l-l')}=N\delta_{l,l'}$$

and shift Q by l, then carry out the Q summation. By the normalization requirement, we have, therefore,

$$T=\sum_l\langle l|\hat{B}|l\rangle\sum_Q|\chi(Q)|^2=\sum_l\langle l|\hat{B}|l\rangle\ ,$$

which is just the trace of $\hat{B}$ in the lattice coordinate representation.

[1]E. P. Gross, J. Stat. Phys. 17, 265 (1977).
[2]J. M. Luttinger, Phys. Rev. Lett. 37, 609 (1976).
[3]J. M. Luttinger, Phys. Rev. Lett. 37, 1221 (1976).
[4]Chih-Yuan Lu, Chin. J. Phys. (Taiwan) 17, 155 (1979).
[5]Chih-Yuan Lu, J. Non-Cryst. Solids. 40, 61 (1980).
[6]H. L. Frisch and S. P. Lloyd, Phys. Rev. 120, 1175 (1960).
[7]See the Appendix.
[8]R. H. Parmenter, Phys. Rev. 104, 22 (1956).
[9]I. M. Lifshitz, Usp. Fiz. Nauk. 83, 617 (1964).
[10]S. Kirkpatrick and T. P. Eggarter, Phys. Rev. B 6, 3598 (1972).
[11]W. Kohn and J. Olson, J. Phys. (Paris) C3, 135 (1972).
[12]V. Srivastava and D. Weaire, Phys. Rev. B 18, 6635 (1978).
[13]R. Friedberg and J. M. Luttinger, Phys. Rev. B 12, 4460 (1975).
[14]P. A. Wolff, Phys. Rev. 126, 405 (1962).
[15]E. O. Kane, Phys. Rev. 131, 1532 (1963).
[16]B. Velicky, S. Kirkpatrick, and H. Ehrenreich, Phys. Rev. 175, 747 (1968).
[17]R. Alben, M. Blume, H. Krakauer, and L. Schwartz, Phys. Rev. B 12, 4090 (1975).