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LOWER BOUND FOR THE VALUE OF A WIENER PATH INTEGRAL WITH A NON-LOCAL POTENTIAL

M. KOLIBIAR[1]), Bratislava

The lower bound for the value of the path integral expressing the averaged canonical density matrix of a non-interacting electron gas in a Gaussian random potential is estimated. The idea of the paper is to apply the convexity theorem (Jensen's inequality) to the double-integral (non-local) potential-energy term of the "*action*" in the exponent of the path integral. Under the assumption that the potential energy autocorrelation function is of the type $\exp(-(r_1 - r_2)^2/L^2)$, the lower bound of the path integral is derived in the form of a sum of exactly solvable path integrals with quadratic non-local potentials. Comparison with numerical Monte Carlo results is given.

НИЖНИЙ ПРЕДЕЛ ДЛЯ ИНТЕГРАЛА ПО ТРАЕКТОРИЯМ ВИНЕРА С НЕЛОКАЛЬНЫМ ПОТЕНЦИАЛОМ

В работе приведена оценка нижнего предела интеграла по траекториям, выражающего усредненную матрицу плотности для невзаимодействующего электронного газа в поле гауссовского случайного потенциала. Основная идея метода состоит в использовании неравенства Йенсена для подынтегрального выражения двухкратного интеграла, которое формально соответствует нелокальному потенциалу в выражении для «действия», входящего в показатель интеграла по траекториям. Предполагая автокорреляционную функцию гауссовского случайного поля в виде $\exp[-(r_1 - r_2)^2 . L^{-2}]$, нижний предел интеграла по траекториям получается как сумма точно решаемых интегралов по траекториям с нелокальными квадратичными потенциалами. Приводится сравнение полученного выражения с численными значениями, вычисленными при помощи метода Монте-Карло.

I. INTRODUCTION

We shall consider a non-interacting gas of particles moving in a time-independent random potential $V(\mathbf{r})$. The randomness of the potential is assumed to be Gaussian. As the mutual interactions of the particles are neglected, we may restrict ourselves to the "*one-particle*" statistical sum and "*one-particle*" density matrix

[1]) Katedra všeobecnej fyziky MFF UK, Mlynská dolina, 842 15 BRATISLAVA, Czechoslovakia.

(i.e. the statistical operator). Such a model is used in the quantum theory of disordered solids [1—7].

Let the brackets $\langle\ \rangle$ denote averaging with respect to the potential $V(\mathbf{r})$. The, assuming that $\langle V(\mathbf{r})\rangle=0$, we define the dispersion $\eta^2=\langle(V(\mathbf{r})-\langle V(\mathbf{r})\rangle)^2\rangle=\langle V^2(\mathbf{r})\rangle$ and the autocorrelation function $W(\mathbf{r}',\mathbf{r}'')=\eta^{-2}\langle V(\mathbf{r}')\,V(\mathbf{r}'')\rangle$. As usually, we define the parameter β by the relation $\beta=1/k_BT(k_B=k_{\mathrm{Boltzmann}}$ and T is the absolute temperature).

As shown in [1], the averaged canonical "*one-particle*" density matrix can be written as the path integralover the Wiener measure:

$$\langle C(\beta,\mathbf{r}_b,\mathbf{r}_a)\rangle=\int_{\mathbf{r}_a}^{\mathbf{r}_b}\mathscr{D}[\mathbf{r}(u)]\exp\left\{-\frac{1}{\hbar}\int_0^{\hbar\beta}\frac{m}{2}\dot{\mathbf{r}}^2(u)\,du+\right.\tag{1}$$
$$\left.+\frac{\eta^2}{2\hbar^2}\int_0^{\hbar\beta}du'\int_0^{\hbar\beta}du''\,W[\mathbf{r}(u')\mathbf{r}(u'')]\right\},$$

where $\mathbf{r}_a=\mathbf{r}(0)$ and $\mathbf{r}_b=\mathbf{r}(\hbar\beta)$ are the "*starting*" and the "*ending*" points of the path integration, respectively. Obviously, the autocorrelation function W plays the role of a non-local potential here.

The basic problem is to elaborate an effective way for computing the path integral (1). This problem was shown to be solvable analytically only when the autocorrelation function (i.e. the non-local potential in (1)) was replaced by a quadratic function:

$$W_q(\mathbf{r}',\mathbf{r}'')=1-(\mathbf{r}'-\mathbf{r}'')^2/L^2.\tag{2}$$

Here L denotes the correlation length. The approximation (2) was introduced by Bezák [1]. The evaluation of the path integral (1) for $W=W_q$ was carried out by various methods [1—6], which gave the formula

$$\langle C_q(\beta,\mathbf{r}_b,\mathbf{r}_a)\rangle=\left(\frac{m}{2\pi\hbar^2\beta}\right)^{3/2}\left(\frac{\gamma_G}{\sinh\gamma_G}\right)^3\times\tag{3}$$
$$\times e^{\frac{1}{2}\eta^2\beta^2}\exp\left\{-\frac{m\omega_G(\beta)}{4\hbar}\frac{(\mathbf{r}_b-\mathbf{r}_a)^2}{\tanh\gamma_G(\beta)}\right\},$$

where $\omega_G(\beta)=\frac{\eta}{L}\left(\frac{2\beta}{m}\right)^{1/2}$, $\gamma_G(\beta)=\frac{1}{2}\beta\hbar\omega_G(\beta)$.

Provided that $(\mathbf{r}'-\mathbf{r}'')^2\ll L^2$, the function (2) can be considered as a reasonable approximation of some more realistic autocorrelation functions, say

$$W_e(\mathbf{r}',\mathbf{r}'')=\exp\left(-\frac{(\mathbf{r}'-\mathbf{r}'')^2}{L^2}\right).\tag{4}$$

We assume that the random potential $V(\mathbf{r})$ is statistically uniform and isotropic. Then the autocorrelation function W depends only on the distance $|\mathbf{r}'-\mathbf{r}''|$. It

should be pointed out that the linear term in the Taylor expansion of a general autocorrelation function with respect to $|\mathbf{r}'-\mathbf{r}''|$ vanishes for physical reasons [7].

It can easily be seen that under the assumptions

$$L^2\gg\hbar^2\beta/m$$

and

$$L^2\gg(\mathbf{r}_b-\mathbf{r}_a)^2$$

the value of the path integral (1) is not much influenced by the approximation (2). The inequality $L^2\gg\hbar\beta/m$ corresponds to high temperatures or large correlation lengths. Nevertheless, there are some intuitive arguments that the function (3) is a good approximation of the integral (1) with a general functtion W(like W_e) also in the range of extremely low temperatures. This is of crucial importance for any perturbation expansion of expression (1) using expression (3) as the zeroth-order approximation [7].

For simplicity we confine ourselves to the diagonal elements of the averaged density matrix (1) when $\mathbf{r}_b=\mathbf{r}_a$, although the methods presented here are valid for the more general case when $\mathbf{r}_a$, $\mathbf{r}_b$ are arbitrary. Since the system is statistically invariant with respect to the translations, the statistical sum per unit volume $Z(\beta)$ given simply by $\langle C(\beta,\mathbf{r},\mathbf{r})\rangle$ is independent of $\mathbf{r}$.

Let $\langle C_q(\beta,\mathbf{r}_b,\mathbf{r}_a)\rangle$ and $\langle C_e(\beta,\mathbf{r}_b,\mathbf{r}_a)\rangle$ denote, respectively, the path-integral (1) corresponding to the cases $W=W_q$ and $W=W_e$.

In Sect. II the inequality

$$\langle C_e(\beta,\mathbf{r},\mathbf{r})\rangle>\exp\left(\frac{5}{8}\frac{\hbar^2\beta}{mL^2}\right)\langle C_q(\beta,\mathbf{r},\mathbf{r})\rangle\quad\text{for }\beta\to\infty\tag{5}$$

is proved. Thus $\langle C_q\rangle$ differs greatly from $\langle C_e\rangle$ for sufficiently low temperatures. Nevertheless, if we are interested in the free energy (and other thermodynamic quantities) of gas, this difference does only lead to a small correction because of the logarithmic relation $F=-k_BT\ln Z$. However, path integrals like (1) frequently occur also "*non-logarithmically*" in some problems concerning disordered structures and random processes [7]. In case of random processes β corresponds to the time variable. Then inequalities like (5) are undoubtedly important.

In Sect. III we present our results obtained by a Monte Carlo procedure for the evaluation of the path integral (1) for $W=W_e$. These results are compared with formula (3), which is exact for $W=W_q$, and with the r.h.s. of inequality (5). As such calculations require some considerable amount of computer time, we have restricted ourselves to one-dimensional problems.

II. THE RELATION BETWEEN $\langle C_q(\beta,\mathbf{r},\mathbf{r})\rangle$ AND $\langle C_e(\beta,\mathbf{r},\mathbf{r})\rangle$

Obviously, $W_q(\mathbf{r}',\mathbf{r}'')\leq W_e(\mathbf{r}',\mathbf{r}'')$. Therefore $\langle C_q(\beta,\mathbf{r}_b,\mathbf{r}_a)\rangle\leq\langle C_e(\beta,\mathbf{r}_b,\mathbf{r}_a)\rangle$. Thus $\langle C_q\rangle$ given by (3) is a lower bound for $\langle C_e\rangle$. The aim of this section is to find a better lower bound.

Introducing the dimensionless quantities

$$a=a(\beta)=\sqrt{\frac{\hbar^2\beta}{mL^2}},\quad b=b(\beta)=\frac{1}{\sqrt{2}}\eta\beta$$

and substituting

$$u=\hbar\beta t,\quad \mathbf{r}=\sqrt{\frac{\hbar^2\beta}{m}}\boldsymbol{\varrho}$$

in (1), we obtain for $W=W_e$ the integral

$$\langle C_e(\beta,\boldsymbol{\varrho}_b,\boldsymbol{\varrho}_a)\rangle=\left(\frac{m}{\hbar^2\beta}\right)^{3/2}\int_{\boldsymbol{\varrho}(0)=\boldsymbol{\varrho}_a}^{\boldsymbol{\varrho}(1)=\boldsymbol{\varrho}_b}\mathcal{D}[\boldsymbol{\varrho}(t)]\exp\Big\{-\frac{1}{2}\int_0^1\dot{\boldsymbol{\varrho}}^2(t)\,\mathrm{d}t+ \tag{6}$$
$$+b^2\int_0^1\mathrm{d}t_1\int_0^1\mathrm{d}t_2\exp[-a^2(\boldsymbol{\varrho}(t_1)-\boldsymbol{\varrho}(t_2))^2]\Big\}.$$

The approximation (2) means the replacing of the integral

$$I_e=\int_0^1\mathrm{d}t_1\int_0^1\mathrm{d}t_2\exp[-a^2(\boldsymbol{\varrho}(t_1)-\boldsymbol{\varrho}(t_2))^2]$$

in the exponent of the path integral (6) by the integral

$$I_q=\int_0^1\mathrm{d}t_1\int_0^1\mathrm{d}t_2[1-a^2(\boldsymbol{\varrho}(t_1)-\boldsymbol{\varrho}(t_2))^2].$$

Obviously $I_e\geq I_q$ and $I_e>0$ for any function (path) $\boldsymbol{\varrho}(t)$, while I_q may also be negative. The idea of the following calculations is based on replacing I_q by a functional of $\boldsymbol{\varrho}(t)$ which is less than I_e but positive for any $\boldsymbol{\varrho}(t)$.

We shall use Jensen's inequality[1]) (well-known also as "*the convexity theorem*") for the "*potential energy*" term in the exponent of path integral (6):

$$\int_0^1\mathrm{d}t_1\int_0^1\mathrm{d}t_2\exp[-a^2(\boldsymbol{\varrho}(t_1)-\boldsymbol{\varrho}(t_2))^2]\geq\exp\Big[-a^2\int_0^1\mathrm{d}t_1\int_0^1\mathrm{d}t_2(\boldsymbol{\varrho}(t_1)-\boldsymbol{\varrho}(t_2))^2\Big].$$

[1]) An exact and general formulation of this theorem is given e.g. in [12].

Using this inequality we obtain the following relation:

$$\langle C_e(\beta,\mathbf{r},\mathbf{r})\rangle\geq$$
$$\geq\left(\frac{m}{\hbar^2\beta}\right)^{3/2}\int_{\boldsymbol{\varrho}(0)=0}^{\boldsymbol{\varrho}(1)=0}\mathcal{D}[\boldsymbol{\varrho}(t)]\exp\Big\{-\frac{1}{2}\int_0^1\dot{\boldsymbol{\varrho}}^2(t)\,\mathrm{d}t+b^2\exp\Big[-a^2\int_0^1\mathrm{d}t_1\times$$
$$\times\int_0^1\mathrm{d}t_2(\boldsymbol{\varrho}(t_1)-\boldsymbol{\varrho}(t_2))^2\Big]\Big\}=\left(\frac{m}{\hbar^2\beta}\right)^{3/2}\int_{\boldsymbol{\varrho}(0)=0}^{\boldsymbol{\varrho}(1)=0}\mathcal{D}[\boldsymbol{\varrho}(t)]\times$$
$$\times\exp\Big\{-\frac{1}{2}\int_0^1\dot{\boldsymbol{\varrho}}^2(t)\,\mathrm{d}t\Big\}\sum_{n=0}^{\infty}\frac{b^{2n}}{n!}\exp\Big[-na^2\int_0^1\mathrm{d}t_1\int_0^1\mathrm{d}t_2(\boldsymbol{\varrho}(t_1)-\boldsymbol{\varrho}(t_2))^2\Big]=$$
$$=\sum_{n=0}^{\infty}\frac{b^{2n}}{n!}\left(\frac{m}{\hbar^2\beta}\right)^{3/2}\int_{\boldsymbol{\varrho}(0)=0}^{\boldsymbol{\varrho}(1)=0}\mathcal{D}[\boldsymbol{\varrho}(t)]\exp\Big\{-\frac{1}{2}\int_0^1\dot{\boldsymbol{\varrho}}^2(t)\,\mathrm{d}t-$$
$$-na^2\int_0^1\mathrm{d}t_1\int_0^1\mathrm{d}t_2(\boldsymbol{\varrho}(t_1)-\boldsymbol{\varrho}(t_2))^2\Big\}.$$

The last path integrals are of the same type as (1) for $W=W_q$. Thus, formula (3) can be applied and the inequality

$$\langle C_e(\beta,\mathbf{r},\mathbf{r})\rangle\geq\left(\frac{m}{2\pi\hbar^2\beta}\right)^{3/2}\sum_{n=0}^{\infty}\frac{b^{2n}}{n!}\left(\frac{a\sqrt{n}}{\sinh(a\sqrt{n})}\right)^3 \tag{7}$$

is obtained. For the one-dimensional problem we have the result

$$\langle C_e(\beta,x,x)\rangle\geq\left(\frac{m}{2\pi\hbar^2\beta}\right)^{1/2}\sum_{n=0}^{\infty}\frac{b^{2n}}{n!}\frac{a\sqrt{n}}{\sinh(a\sqrt{n})}. \tag{7'}$$

(We remind that $a=a(\beta)$, $b=b(\beta)$.)

Obviously, this procedure can be applied without difficulties to the more general case when $\mathbf{r}_a\neq\mathbf{r}_b$.

To compare the estimate (7) or (7') for large values of β with $\langle C_q\rangle$ given by formula (3) we rewrite function (3) for $\mathbf{r}_a=\mathbf{r}_b$ in the form

$$\langle C_q(\beta,\mathbf{r},\mathbf{r})\rangle=\left(\frac{m}{2\pi\hbar^2\beta}\right)^{3/2}\left(\frac{ab}{\sinh(ab)}\right)^3 e^{b^2}\ \text{(the three dimensional case)}$$

$$\langle C_q(\beta,x,x)\rangle=\left(\frac{m}{2\pi\hbar^2\beta}\right)^{1/2}\frac{ab}{\sinh(ab)}e^{b^2}\ \text{(the one dimensional case)}$$

The sum of the series in (7), (7') can be estimated by the values of their largest terms since all the terms are nonnegative. Using the Stirling's formula

$$n!=\sqrt{2\pi n}\left(\frac{n}{e}\right)^n E(n)\ \text{where}\ \lim_{n\to\infty}E(n)=1$$

and the expansion

$$\ln(1-t) = -\left(t + \frac{t^2}{2} + \frac{t^3}{3} + \dots\right) \qquad |t|<1$$

it can easily be seen that for large β the most important terms of the series in (7), (7′) correspond to

$$n \approx b^2 - \frac{3}{2}ab \quad \text{and} \quad n \approx b^2 - \frac{1}{2}ab, \text{ respectively.}$$

This means that n may be very large for large values of β.

We shall not present the estimation of the values of these terms here because it is a tedious exercise in calculus. The result is formula (5) and its one-dimensional analogon

$$\langle C_e(\beta,x,x)\rangle > \exp\left(\frac{1}{8}\frac{\hbar^2\beta}{mL^2}\right)\langle C_q(\beta,x,x)\rangle \quad \text{for } \beta\to\infty\,. \qquad (5')$$

It is worth mentioning that this result cannot be further improved essentially by considering more (or eventually all) the non-negligible terms of the series (7), (7′). The reason is that the "*width*" of the maximum (on the "*n-scale*") is of the order of ab. Any multiplicative factor of such an order of magnitude does not seem to be important enough in the r.h.s. of relations (5) and (5′), since the estimates based on Jensen's inequality may give values which are still too far from the exact ones. Indeed, the values of the r.h.s. of inequalities (7), (7′) obtained by performing numerically the summation are much smaller than those for $\langle C_e\rangle$ obtained by a Monte Carlo integration in Sect. III (Fig. 1). That is why we have refrained from

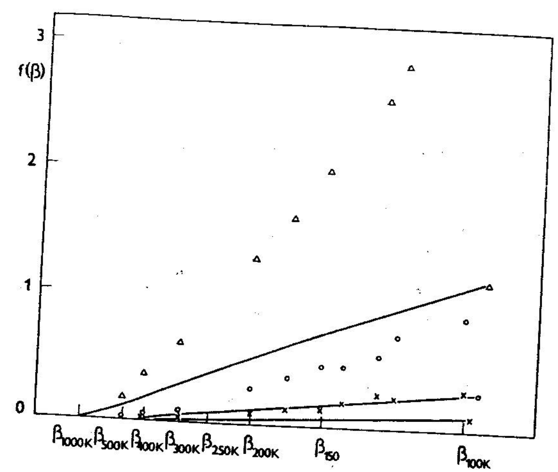

Fig. 1.

seeking such a refinement as, e.g., the use of a better asymptotic formula for the series in (7), (7′) in the low temperature limit ($\beta\to\infty$).

III. RESULTS OF NUMERICAL INTEGRATING

This section refers to a Monte Carlo integration procedure for the path integral (1) in the one-dimensional case:

$$\langle C(\beta,x_b,x_a)\rangle = \qquad (1')$$

$$= \int_{x(0)=x_a}^{x(\hbar\beta)=x_b} \mathcal{D}[x(u)] \exp\left\{-\frac{1}{\hbar}\int_0^{\hbar\beta}\frac{m}{2}\dot{x}^2(u)\,du + \frac{\eta^2}{2\hbar^2}\int_0^{\hbar\beta}du_1\int_0^{\hbar\beta}du_2\,W[x(u_1),x(u_2)]\right\}.$$

The term, written symbolically as $\dot{x}^2(u)$ corresponds to the conditional Wiener measure. From the mathematical point of view expression (1′) is the functional integral with respect to the conditional Wiener measure over the space of all the functions continuous on the interval $[0,\hbar\beta]$. Integral (1′) can be computed numerically by several methods [8—10].

For our purposes the following procedure was chosen:

1. With the fixed starting point x_a and the ending point x_b the path $x(u)$ can be generated as a random walk of a Brownian particle. Let x', x'' be the positions of the Brownian particle at the times t', t'', respectively (The quantity $\hbar\beta$ has the dimension of a time variable.) Then the position of the particle at the time $\tau\in[t',t'']$ (we assume $t'<t''$) is a normally distributed random variable with the mean value

$$\bar{x}(\tau) = \frac{1}{t''-t'}\left[(t''-\tau)x' + (\tau-t')x''\right]$$

and the variance

$$\sigma^2(\tau) = \frac{(t''-\tau)(\tau-t')}{t''-t'}\frac{\hbar}{m}.$$

Therefore the value $\hbar/2m$ plays the role of a diffusion coefficient of the Brownian motion. To generate the normally distributed random numbers, an algorithm based on the central limit theorem was used. Having this algorithm at hand we can subsequently divide the "*time*" interval $[0,\hbar\beta]$ to 2, 4, 8, 16, …, 2^k subintervals and generate the positions of the particle at the end points of these subintervals so that a discretization of the random path of the particle is obtained.

It should be emphasized that this analogy with the Brownian motion is purely mathematical. It has nothing to do with the real physical motion of the particle.

2. Having generated such an approximation of the path with straightline sections, we can evaluate the functional

$$F[x(u)] = \exp\left\{\frac{\eta^2}{2\hbar^2}\int_0^{\hbar\beta} du_1 \int_0^{\hbar\beta} du_2\, W[x(u_1), x(u_2)]\right\}. \tag{8'}$$

This can be done using a suitable numerical quadrature. In our case the two-dimensional trapezium rule turned out to operate well. The calculations were made for $W = W_e \equiv W_e(|x_1 - x_2|)$. A table of values of the function e^{-x^2} was used instead of evaluating e^{-x^2} repeatedly. The procedure was speeded up by about 2.5 times by this simple trick.

3. The steps 1 and 2 are repeated N-times. The arithmetical mean of the N values of the functional (8′) multiplied by the quantity $\left(\frac{m}{2\pi\hbar^2\beta}\right)\times \exp\left(-\frac{m}{2\hbar^2\beta}(x_b - x_a)^2\right)$ is the approximation of the integral (1′) with the standard deviation $\left(\frac{D(F)}{N}\right)^{1/2}$, where $D(F)$ is the variance of the functional (8′). $D(F)$ can be estimated empirically during the computations so that the procedure can be stopped when the desired value of the standard deviation is achieved.

In addition to the error arising from the statistical nature of the Monte Carlo method, there is an error due to the approximation of the path by the table of the positions of the Brownian particle at a finite number of times and to the subsequent numerical quadrature to obtain the values (8′). This error can be reduced by increasing the number of the subintervals. However, the number of the arithmetic operations per path is determined mainly by the requirements of the quadrature in exponential (8′), which are obviously proportional to the square of the number of the time subintervals. Thus, to achieve the maximum accuracy a compromise must be found between the number of the subintervals and the number of paths generated in a time unit. The generating of one path and evaluating exponential (8′) requires about 0.11 s for 32 subintervals and about 0.5 s for 64 subintervals using the Siemens 4004/150 computer system.

Obviously, the variance of the functional (8′) increases rapidly with the increase of the quantity $\eta\beta$. As was found empirically, the method is practically of no use for $\eta\beta \gtrsim 10$.

The results for $m = m_{\text{electron}}$, $\eta = 0.1$ eV, $L = 1$ nm, 2 nm and 3 nm are presented in Fig. 1 where the functions

$$f_1(\beta) = \ln\frac{\langle C_e(\beta, x, x)\rangle}{\langle C_q(\beta, x, x)\rangle} \qquad f_2(\beta) = \ln\frac{S(\beta)}{\langle C_q(\beta, x, x)\rangle}$$

(with $S(\beta)$ denoting the r.h.s. of (7′)) are plotted. The function $f_1(\beta)$ is represented by the symbols ×, O, △ corresponding to the correlation lengths $L = 3$ nm, 2 nm, 1 nm, respectively. The function $f_2(\beta)$ is represented by continuous lines. To reduce the influence of the statistical errors due to the Monte Carlo method, all the computations were carried out several times with various starting numbers for the random number generator.

The numerical results for $\langle C_e\rangle$ are in a very good agreement with (3), i.e. $f_1 \approx 0$ provided that $L^2 > \hbar^2\beta/m$. As can be seen in Fig. 1, both functions $f_1(\beta)$, $f_2(\beta)$ seem to be almost linear even for $\beta > \beta_0 > L^2 m/\hbar^2$ (with suitable β_0), although the formula (3) fails in this case. As to the function $f_2(\beta)$ this linearity was verified by the "*exercise in calculus*" mentioned in Sect. II. Unfortunately we are not able to verify the linear shape of the function $f_1(\beta)$ for $\beta \to \infty$, since the Monte Carlo method is inapplicable in the low-temperature limit. The linear asymptotics of $f_1(\beta)$ is consistent with the results of E. Haluška [11] obtained in a different way.

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