# A PATH INTEGRAL FOR NUMERICAL COMPUTATIONS OF THE ENERGY LEVEL DENSITY OF A PARTICLE IN A GAUSSIAN RANDOM POTENTIAL

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Using the Bromwich integral to express the energy level density as the inverse Laplace transform of the statistical sum and writing the latter in the path integral form we propose a path integral for the energy level density of a particle moving in a Gaussian random potential. A simple method to transform this path integral into the conditional Wiener integral is presented. This enables us to utilize a Monte Carlo method to perform the path integration numerically assuming the autocorrelation function of the potential to be a Gaussian "bell", which seems to be physically acceptable. The results of the numerical procedure are compared to those obtained from the quadratic approximation of the autocorrelation function due to Bezák (1970).

## ИСПОЛЬЗОВАНИЕ ИНТЕГРАЛОВ ПО ТРАЕКТОРИЯМ ДЛЯ ЧИСЛЕННОГО РАСЧЕТА ПЛОТНОСТИ СОСТОЯНИЙ ЧАСТИЦЫ, ДВИЖУЩЕЙСЯ В ГАУССОВСКОМ СЛУЧАЙНОМ ПОТЕНЦИАЛЕ

Используя выражение для плотности состояний в виде обратного преобразования Лапласа от статистической суммы и записав последнюю в виде интеграла по траекториям, можно полушить интеграл по траекториям для плотности состояний частицы, движущейся в гауссовском случайном потенциале. Приводится простой метод для преобразования этого интеграла по траекториям в условный интеграл Винера. Для численного расчета этого интеграла используется метод Монте-Карло в предположении, что автокорреляционная функция гауссовского случайного потенциала имеет гауссовский вид, который с физической точки зрения считается вполне приемлемым. Приводится также сравнение с результатами, полученными на основе аппроксимации автокорреляционной функции при помоши полинома второй степени (Безак, 1970 г.)

## I. INTRODUCTION

Path integrals are frequently used in quantum physics, especially if fundamental problems are treated. On the other hand, the Schrödinger equation seems to be

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a more appropriate tool for "practical" problems like calculations of the energy levels of a given quantum mechanical system. However, the problem of the energy levels turns out to be very difficult if we replace the potential by a random function of the coordinates. The random potential is a natural concept to describe disordered solids. In such a model [1, 2] we are interested in average values (or higher statistical moments) of physical functionals (e.g. energy level density) where averaging is meant with respect to the randomness of the potential. Although significant progress has been achieved in the study of the properties of Schrödinger operators with random potentials [3, 4], the problem of the energy level density calculations remains still to a great extent open. Concerning this problem path integrals seem to be an appropriate formalism not only for analytical treatment but also for numerical computations.

In the present paper, a conditional Wiener path integral expressing the energy level density of a particle moving in a scalar Gaussian random potential $V(\boldsymbol{r})$ is derived (Sec. III). The formulation of the problem by means of the conditional Wiener path integral enables us to use a numerical Monte Carlo procedure for its evaluation (Sec. IV). A numerical example is given and the results are compared to those derived from the approximation introduced in [1].

## II. FORMULATION OF THE PROBLEM

We will consider a gas of particles moving in a Gaussian random potential. The random potential is assumed to be statistically homogeneous and isotropic. Thus, its mean value is a constant which may be set to zero. Interactions between particles of the gas are neglected. Therefore, throughout this paper the non-particle problem is considered whenever the statistical sum or the density matrix are mentioned.

The energy level density can be obtained from the statistical sum (partition function) by means of the inverse Laplace transformation. The statistical sum can be calculated as the trace of the canonical density matrix, which can be expressed in the path integral form. Thus, to obtain the energy level density, we should be able to evaluate the path integral expressing the diagonal elements of the canonical density matrix for complex "inverse temperatures" $\beta$, corresponding to the Bromwich integration path in the inverse Laplace transformation formula. While the canonical density matrix for real "inverse temperatures" $\beta$ can be expressed as a conditional Wiener path integral which can be computed numerically by standard methods, the situation is more complicated for imaginary $\beta$.

After averaging with respect to the randomness of the potential and taking into account its statistical homogeneity, the relevant canonical density matrix is given [1] by the path integral

$$\langle C(\boldsymbol{r}_b, \boldsymbol{r}_a, \beta)\rangle = \int_{\boldsymbol{r}(0)=\boldsymbol{r}_a}^{\boldsymbol{r}(\hbar\beta)=\boldsymbol{r}_b} \mathcal{D}[\boldsymbol{r}(u)] \exp\left( -\frac{1}{\hbar}\int_0^{\hbar\beta} \frac{m}{2}\dot{\boldsymbol{r}}^2(u)\,\mathrm{d}u + \right. \tag{1}$$



$$\left. + \frac{1}{2\hbar^2}\int_0^{\hbar\beta}\mathrm{d}u'\int_0^{\hbar\beta}\mathrm{d}u'' B_v[\boldsymbol{r}(u'), \boldsymbol{r}(u'')]\right),$$

where $B_v$ is the autocorrelation function of the random potential $V(\boldsymbol{r})$, $\mathcal{D}[\boldsymbol{r}(u)]$ represents the integration over all paths going from the point $\boldsymbol{r}=\boldsymbol{r}_a$ at the time $u=0$ to the point $\boldsymbol{r}=\boldsymbol{r}_b$ at the time $u=\hbar\beta$, $\beta=1/k_BT$; where $k_B$ is the Boltzmann constant, $m$ is the mass of the particle and $\hbar$ is the Planck constant, divided by $2\pi$; the brackets $\langle\ \rangle$ denote the averaging with respect to the randomness of the potential $V$.

Let us consider the usual approximation to the path integral (1)

$$\langle C_n(\boldsymbol{r}_b, \boldsymbol{r}_a, \beta)\rangle = \int_\infty \mathrm{d}\boldsymbol{r}_1 \ldots \int_\infty \mathrm{d}\boldsymbol{r}_n (2\pi\hbar(u_1-u_0)/m)^{-3/2} \tag{2}$$

$$\exp\left(-\frac{(\boldsymbol{r}_1-\boldsymbol{r}_0)^2}{2\hbar(u_1-u_0)/m}\right)(2\pi\hbar(u_2-u_1)/m)^{-3/2}\exp\left(-\frac{(\boldsymbol{r}_2-\boldsymbol{r}_1)^2}{2\hbar(u_2-u_1)/m}\right)\ldots$$

$$\ldots(2\pi\hbar(u_{n+1}-u_n)/m)^{-3/2}\exp\left(-\frac{(\boldsymbol{r}_{n+1}-\boldsymbol{r}_n)^2}{2\hbar(u_{n+1}-u_n)/m}\right)$$

$$\exp\left(\frac{1}{2\hbar^2}\sum_{i=0}^{n}\sum_{j=0}^{n}(u_{i+1}-u_i)(u_{j+1}-u_j)B_v(\boldsymbol{r}_i, \boldsymbol{r}_j)\right)$$

where $u_i=\hbar\beta_i$, $(i=1, 2, \ldots, n)$, $u_0=0$, $u_{n+1}=\hbar\beta$,
$\boldsymbol{r}_i=\boldsymbol{r}(u_i)$, $(i=1, 2, \ldots, n)$, $\boldsymbol{r}_0=\boldsymbol{r}_a$, $\boldsymbol{r}_{n+1}=\boldsymbol{r}_b$.
This integral converges to $\langle C(\boldsymbol{r}_b, \boldsymbol{r}_a, \beta)\rangle$ as $n$ goes to infinity. If $\beta$ is real, then the terms

$$(2\pi\hbar^2(\beta_{i+1}-\beta_i)/m)^{-3/2}\exp\left(-\frac{(\boldsymbol{r}_{i+1}-\boldsymbol{r}_i)^2}{2\hbar^2(\beta_{i+1}-\beta_i)/m}\right) \tag{3}$$

can be interpreted as the probability densities corresponding to Brownian random walks from the points $\boldsymbol{r}_i$ at the times $u_i=\hbar\beta_i$ to the points $\boldsymbol{r}_{i+1}$ at the times $u_{i+1}=\hbar\beta_{i+1}$ and with the diffusion coefficient $D=\frac{1}{2}\frac{\hbar}{m}$. Thus, the trajectory $\boldsymbol{r}$ can be considered as a Brownian-bridge trajectory with the starting point $\boldsymbol{r}_a$ at the time $u=0$, the ending point $\boldsymbol{r}_b$ at the time $u=\hbar\beta$ and with the diffusion coefficient $D=\frac{1}{2}\frac{\hbar}{m}$. Clearly, such an interpretation is not possible for imaginary $\beta$.

It should be emphasized that the formulae (1), (2) contain a "two-time" action so that we cannot utilize the well-known property

$$C(\boldsymbol{r}_2, \boldsymbol{r}_1, \beta_2+\beta_1) = \int_{(\infty)} \mathrm{d}^3\boldsymbol{r}\, C(\boldsymbol{r}_2, \boldsymbol{r}, \beta)C(\boldsymbol{r}, \boldsymbol{r}_1, \beta_1)$$

neither for the computation nor for the definition of the path integral (1). To overcome this difficulty in some special cases we can proceed as in Sec. III.

## III. THE PATH INTEGRAL FOR THE ENERGY LEVEL DENSITY COMPUTATIONS

Let us define a dimensionless "time" variable

$$\tau = \frac{u}{\hbar\beta}$$

and a dimensionless quantity

$$\varrho(\tau) = \sqrt{\frac{m}{\hbar^2\beta}}\,(r(\hbar\beta\tau) - \tau r_b - (1-\tau)r_a)\,. \tag{4}$$

From the mathematical point of view, the quantity $\varrho(\tau)$ corresponds to a three-dimensional Brownian bridge random walk with the "diffusion coefficient" $D = 1/2$ ($D$ is now dimensionless). Clearly, $\varrho(0) = \varrho(1) = \mathbf{0}$. Such a Brownian bridge is sometimes called a standard one. It can be seen after some calculations that the $3n$-fold integral (2) can be written in the form

$$\langle C_n(r_b, r_a, \beta)\rangle = \left(\frac{m}{2\pi\hbar^2\beta}\right)^{3/2} \exp\left(-\frac{(r_b - r_a)^2}{2\hbar^2\beta/m}\right) \int \frac{\mathrm{d}\varrho_1}{(2\pi)^{3/2}} \cdots \tag{5}$$

$$\cdots \int \frac{\mathrm{d}\varrho_n}{(2\pi)^{3/2}} \exp\left(-\frac{(\varrho_1 - \varrho_0)^2}{2(\tau_1 - \tau_0)}\right) \exp\left(-\frac{(\varrho_2 - \varrho_1)^2}{2(\tau_2 - \tau_1)}\right) \cdots \exp\left(-\frac{\varrho_n - \varrho_{n-1})^2}{2(\tau_n - \tau_{n-1})}\right)$$

$$\exp\left(-\frac{(\varrho_{n+1} - \varrho_n)^2}{2\tau_{n+1} - \tau_n)}\right) \exp\left(\frac{\beta^2}{2} \sum_{i=0}^{n} (\tau_{i+1} - \tau_i) \sum_{j=0}^{n} (\tau_{j+1} - \tau_j)\right.$$

$$\left. B_v\left(\tau_i r_b + (1-\tau_i)r_a + \sqrt{\frac{\hbar^2\beta}{m}}\,\varrho_i,\ \tau_j r_b + (1-\tau_j)r_a + \sqrt{\frac{\hbar^2\beta}{m}}\,\varrho_j\right)\right)$$

where $\varrho_i = \varrho(\tau_i)$, $(i = 1, 2, \ldots, n)$, $\varrho_0 = \varrho_{n+1} = \mathbf{0}$, $\tau_0 = 0$, $\tau_{n+1} = 1$. The exponential terms $\exp\left(-\frac{(\varrho_{i+1} - \varrho_i)^2}{2(\tau_{i+1} - \tau_i)}\right)$ do not depend on $\beta$. Thus, the product $\exp\left(-\frac{(\varrho_1 - \varrho_0)^2}{2(\tau_1 - \tau_0)}\right) \exp\left(-\frac{(\varrho_2 - \varrho_1)^2}{2(\tau_2 - \tau_1)}\right) \cdots \exp\left(-\frac{(\varrho_n - \varrho_{n-1})^2}{2(\tau_n - \tau_{n-1})}\right) \exp\left(-\frac{(\varrho_{n+1} - \varrho_n)^2}{2(\tau_{n+1} - \tau_n)}\right)$ can be interpreted as the probability density due to the "piecewise" approximation of the Brownian bridge, no matter what value the "inverse temperature" $\beta$ may acquire. The $\beta$-dependence of the $3n$-fold integral in (5) is included completely in the last exponential term with the autocorrelation function $B_v$. If $n \to \infty$, then the relation (5) gives the limit

$$\langle C(r_b, r_a, \beta)\rangle = \left(\frac{m}{2\pi\hbar^2\beta}\right)^{3/2} \exp\left(-\frac{(r_b - r_a)^2}{2\hbar^2\beta/m}\right) \tag{6}$$



$$\int \mathrm{d}\nu \exp\left(\frac{\beta^2}{2} \int_0^1 \mathrm{d}\tau' \int_0^1 \mathrm{d}\tau'' B_v(\tau' r_b + (1-\tau')r_a + \sqrt{\frac{\hbar^2\beta}{m}}\,\varrho(\tau'),\right.$$

$$\left.\tau'' r_b + (1-\tau'')r_a + \sqrt{\frac{\hbar^2\beta}{m}}\,\varrho(\tau'')\right)\right)$$

where $\mathrm{d}\nu$ denotes the probability measure corresponding to the three-dimensional standard Brownian bridge introduced above. The complex square root $\sqrt{\hbar^2\beta/m}$ can have two possible values differing by the sign. However, this causes no ambiguity since the probability densities corresponding to the Brownian bridge random walks $\varrho(\tau)$ and $-\varrho(\tau)$ are equal.

The density matrix for complex "inverse temperatures" $\beta$ can be obtained as an analytic continuation of $C(r_b, r_a, \beta)$ for $\beta$ real. Clearly, the applicability of this method depends on the form of $B_v$. If we choose $B_v$ in the form

$$B_v(r', r'') = \eta^2 \exp\left(-\frac{(r' - r'')^2}{L^2}\right), \tag{7}$$

where $\eta$ is a constant with the physical dimension of energy and $L$ is the correlation length, then the second exponent in (6) is a regular function of $\beta$ in the complex $\beta$ plane. It can be shown that if (7) holds, then the r.h.s. of (6) is a regular function of $\beta$ too, provided that $\mathrm{Re}\,\beta > 0$. We may conclude that the method is usable for the autocorrelation function (7). Such an expression seems to be a reasonable approximation to a physically acceptable autocorrelation function [5].

Obviously, this method of analytic continuation of the path integral representing the density matrix can be applied also to the path integral

$$\int_{r(0)=r_a}^{r(\hbar\beta)=r_b} \mathscr{D}[r_{(u)}] \exp\left(-\frac{1}{\hbar}\int_0^{\hbar\beta} \frac{m}{2}\,\dot{r}^2(u)\,\mathrm{d}u - \frac{1}{\hbar}\int_0^{\hbar\beta} V[r(u)]\,\mathrm{d}u\right)$$

which corresponds to the canonical density matric of a particle in any "non-random" potential $V$. The formula obtained in this way is identical with that derived in [6] by a different method. However, the conditions under which such a formula holds are formulated in a different way. In our approach, regularity of the functional integral

$$\int \mathrm{d}\nu \exp\left(-\beta \int_0^1 V\left[\tau r_b + (1-\tau)r_a + \sqrt{\frac{\hbar^2\beta}{m}}\,\varrho(\tau)\right]\mathrm{d}\tau\right)$$

with respect to the parameter $\beta$ is required rather than the conditions concerning the potential function $V$ directly as in [6]. It should be stressed that these requirements are in both methods rather severe. For example, neither of the methods is applicable to the case of the linear harmonic oscillator because of the

quadratic growth of its potential which is too fast to satisfy these restrictions. The traditional approach based on the Schrödinger equation seems to be a more appropriate tool for numeric computations whenever a "non-random" potential is concerned.

Since we assume that the random potential is statistically homogeneous we write

$$Z(\beta)=\langle C(\boldsymbol{r}, \boldsymbol{r}, \beta)\rangle=\langle C(\boldsymbol{0}, \boldsymbol{0}, \beta)\rangle\,. \tag{8}$$

Assuming that the statistical sum $Z(\beta)$ is not singular for Re $\beta>0$, we can obtain the energy level density $g(E)$ by means of the inverse Laplace transform which can be written in the form of the Bromwich integral

$$g(E)=\frac{1}{2\pi i}\int_{\beta_0-i\infty}^{\beta_0+i\infty} Z(\beta)\exp(E\beta)\,\mathrm{d}\beta \tag{9}$$

where $\beta_0>0$ so that $Z(\beta)$ is regular for Re $\beta\geqq\beta_0$. Using the relations (6), (8), (9), we can write the energy level density per unit volume in the form of an integral relation

$$g(E)=\frac{1}{2\pi i}\int_{\beta_0-i\infty}^{\beta_0+i\infty}\mathrm{d}\beta\left(\frac{m}{2\pi\hbar^2\beta}\right)^{3/2}\exp(E\beta)\int\mathrm{d}\nu\exp\left(\frac{\beta^2}{2}\int_0^1\mathrm{d}\tau'\right.$$
$$\left.\int_0^1\mathrm{d}\tau'' B_v\left(\sqrt{\frac{\hbar^2\beta}{m}}\,\varrho(\tau'),\sqrt{\frac{\hbar^2\beta}{m}}\,\varrho(\tau'')\right)\right). \tag{10}$$

As mentioned above, the symbol $\int\mathrm{d}\nu$ means the integration with respect to the probabilistic measure corresponding to the Brownian bridge.

Although formula (10) can be in principle used for the energy level density calculations, its direct application to numerical computations is not possible. The reason is that the numerical inverse Laplace transformation is a notoriously ill-conditioned procedure. If the functional integration in (10) is performed numerically by a Monte Carlo integration, then the result is too inaccurate to be transformed by the Bromwich integral (9) in (10). This can be overcome by reversing the order of integrations in (10). Thus we arrive at the final result in the form

$$g(E)=\frac{1}{2\pi i}\int\mathrm{d}\nu\int_{\beta_0-i\infty}^{\beta_0+i\infty}\left(\frac{m}{2\pi\hbar^2\beta}\right)^{3/2}\exp\left(E\beta+\right. \tag{11}$$
$$\left.+\frac{\beta^2}{2}\int_0^1\mathrm{d}\tau'\int_0^1\mathrm{d}\tau'' B_v\left(\sqrt{\frac{\hbar^2\beta}{m}}\,\varrho(\tau',\sqrt{\frac{\hbar^2\beta}{m}}\,\varrho(\tau'')\right)\right)\mathrm{d}\beta\,.$$



Considering that $B_v$ is given by formula (7), the step from formula (10) to (11) can be based on the Fubini theorem since the integral

$$\int\mathrm{d}\nu\int_{\beta_0-i\infty}^{\beta_0+i\infty}\mathrm{d}\beta\left|\exp\left(E\beta+\frac{\eta^2\beta^2}{2}\int_0^1\mathrm{d}\tau'\int_0^1\mathrm{d}\tau''\exp\left(-\frac{\hbar^2\beta}{mL^2}\right.\right.\right.$$
$$\left.\left.\left.(\varrho(\tau')-\varrho(\tau''))^2\right)\right)\right|$$

turns out to be finite.

An application of formula (11) is presented in the next Section.

## IV. THE IMPLEMENTATION OF THE METHOD AND THE NUMERICAL RESULTS

To investigate the applicability of the formula (11) to numerical computations, the function (7) was chosen to represent an autocorrelation function of the random Gaussian potential. The energy level density $g$ depends not only on the energy $E$, but also on the physical quantities $m$, $\eta$, $L$. Thus, numerical computations of $g(E)$ based on the relation (11) would give a three-parametric system of curves $g=g_{m,\eta,L}(E)$. To reduce the number of the parameters involved we define dimensionless quantities $\alpha=\hbar^2/m\eta L^2$, $s=\eta\beta$ and $\gamma=\eta L^3 g(E)$. Clearly, $\gamma\,\mathrm{d}(E/\eta)=L^3 g(E)\,\mathrm{d}E$. The functional integral (11) can be rewritten in the form

$$\gamma\left(\frac{E}{\eta}\right)=\int\mathrm{d}\nu\frac{1}{2\pi i}\int_{s_0-i\infty}^{s_0+i\infty}\mathrm{d}s(2\pi\alpha s)^{-3/2}\exp\left\{\frac{E}{\eta}s+\right. \tag{12}$$
$$\left.+\frac{s^2}{2}\int_0^1\mathrm{d}\tau'\int_0^1\mathrm{d}\tau''\exp\left(-\alpha s(\varrho(\tau')-\varrho(\tau''))^2\right)\right\}$$

so that the dependence on $m$, $\eta$, $L$ is reduced to the dependence on the parameter $\alpha$ only.

The Brownian bridge random walk can be approximated by means of an optimal orthonormal expansion [7—8] choosing the set of functions $\{\sin(k\pi\tau)\}_{k=1}^{\infty}$ as the base. Each of the $x$, $y$ and $z$ components of the Brownian bridge random walk can be approximated by the finite sum $\sum_{k=1}^{n}(\xi_k/k\pi)\sqrt{2}\sin(k\pi\tau)$, where $\xi_k$ are independent normally distributed random variables with the mean value 0 and the dispersion 1 and the factor $\sqrt{2}$ arises from the normalization of the sine functions on the interval [0, 1]. The "integration over all paths" can be approximated [7] by an appropriate generation of the random variables $\xi_k$. In our case, the normally distributed random numbers are approximated by sums of 12 uniformly distributed random numbers obtained by a linear congruence generator.

Having generated the random walk $\varrho$ we can evaluate the integral $\int_0^1 d\tau' \int_0^1 d\tau'' \exp(-\alpha s(\varrho(\tau')-\varrho(\tau''))^2)$, for a given value of $s$ by a numerical method. The Gaussian quadrature rule using Legendre polynomials of high order turns out to be suitable for this purpose. The order of the rule is set up by hand (usually to 40). The algorithm must be, of course, efficient. For this reason we cannot afford an automatic integrator (i.e. a program which sets the order of the quadrature rule automatically).

The integration with respect to $ds$ in relation (12) can be performed by a Gaussian quadrature with Hermite polynomials. The Hermite polynomials are chosen because of the factor $s^2/2$ in the exponent of (12) which tends to $-(\mathrm{Im}s)^2/2$ for $s \to \infty$, $\mathrm{Re}s = s_0$. Since the use of an automatic integrator would be non-economic, the order of the quadrature rule is set up empirically together with the parameter $s_0$. The quadrature rule of the 48th order[1]) and the parameter $s_0$ equal to 1 seem to be suitable for these purposes.

It is worth mentioning that the implementation of Gaussian quadrature rules of high order is not a trivial task. About $10^3$ coefficients are needed to make the numerical experiments with various orders of the Gauss-Legendre and the Gauss-Hermite quadrature rules possible. Obviously, these coefficients should be computed rather than entered by hand. Such a computation requires evaluation of zeros of the appropriate classical orthogonal polynomials, i.e. the Legendre and Hermite polynomials. The most straighforward way is to evaluate the coefficients of the polynomial of the $n$-th order by well-known formulae and then use any standard method to find its roots. However, such an algorithm turns out to be unusable for high $n$ because of rounding errors. This can be overcome if the polynomial coefficients are altogether avoided using well-known recurrence relations to compute directly the values of the polynomial function $P_n(x)$ for given $x$. As far as the Legendre and Hermite polynomials are concerned, this improved algorithm seem to be numerically stable at least for $n \leqslant 100$ provided that a standard 64 bit double precision arithmetic is used. Mathematical explanation of the numerical stability of this algorithm is given in [9].

To verify our method, a comparison was made between our results and the results of two approximations which give the statistical sum analytically. First, the statistical sum due to the approximation

$$B_v(\boldsymbol{r}', \boldsymbol{r}'') = \eta^2 \left(1 - \frac{(\boldsymbol{r}' - \boldsymbol{r}'')^2}{L^2}\right) \tag{13}$$

introduced in [1] was used to compute the inverse Laplace transform (9) by

Poznámka[1]) (with the values of $\alpha$ equal to 0.5 and 0.3)



a numerical integration. Secondly, the same procedure was also executed for a trivial approximation

$$B_v(\boldsymbol{r}', \boldsymbol{r}'') = \mathrm{const} = \eta^2 \tag{14}$$

The numerical results for $\alpha = 0.5$ and 0.3 are presented in Fig. 1 and Fig. 2, respectively, where the logarithm of the dimensionless quantity $\gamma$ against the ratio $E/\eta$ is plotted. The results of the Monte Carlo method are depicted by vertical line segments representing the statistical error estimates ("$3\sigma$ rule") of the method. About 800 trajectories were gnerated during the Monte Carlo simulation. The results obtained from the approximation (13) are represented by the full line. The results due to the trivial approximation (14) are depicted by the dashed line.

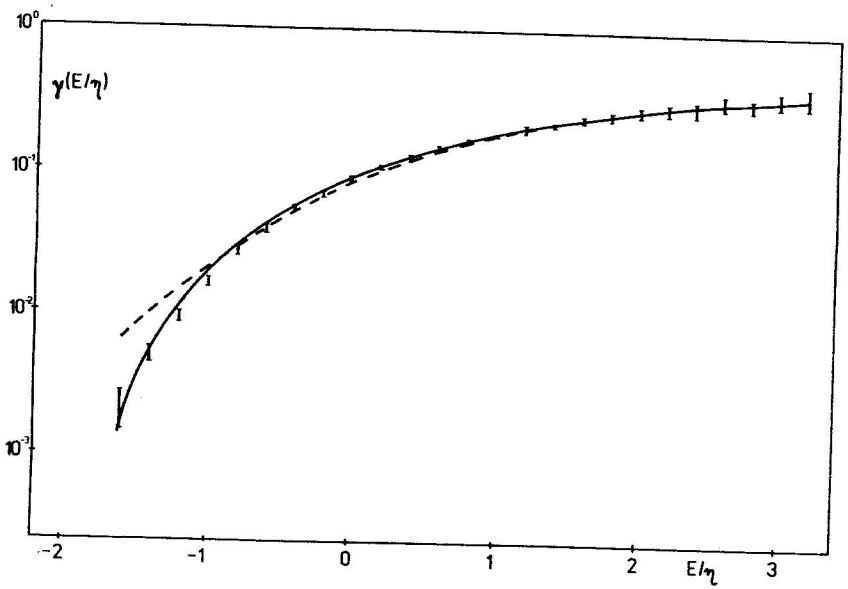


Fig. 1. The dependence of the dimensionless quantity $\gamma$ given by the path integral (12) on the ratio $E/\eta$. The dimensionless parameter $\hbar^2/m\eta L^2$ has the value 0.5. The full line represents the results due to the approximation (13) of Bezák, the dashed line represents the results obtained from the trivial approximation (14). The results of our computations are depicted by the vertical line segments representing the errors due to the statistical nature of the Monte Carlo method ($\pm 3$ standard deviations are taken as the error estimate).

As can be seen from Fig. 1 and Fig. 2, our method is usable provided that the ratio $E/\eta$ is above a certain limit, which is about $-1.6$ for $\alpha = 0.5$ and about $-2.0$ for $\alpha = 0.3$. The approximation (13) works well for a similar range of the ratio $E/\eta$ as mentioned above. This is a remarkable fact because the canonical statistical sum

corresponding to the approximation (13) has singularities even for Re $\beta > \beta_0$ ($\beta_0$ is an arbitrary real number) and the application of the Bromwich integral (9) is mathematically incorrect. Moreover, the statistical sum of any reasonable physical system should not have singularities for Re $\beta > 0$ provided that it is finite for $\beta$ real and positive. This can easily be seen from the definition of the statistical sum.

If $E/\eta > 0$, then the energy level density seems to be almost independent of the shape of the autocorrelation function. In Fig. 1 a slight difference between the two curves for $E/\eta$ close to 0 is observed. This is (in the author's opinion) caused by the analytical properties of the statistical sum corresponding to the approximation (13).

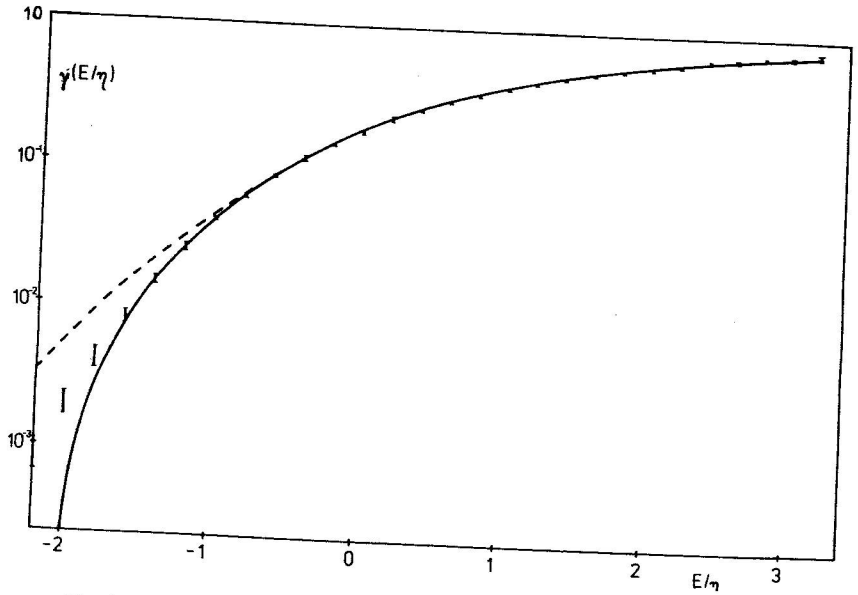


Fig. 2. The curve $\gamma = \gamma(E/\eta)$ for $\hbar^2/m\eta L^2 = 0.3$. See the comments to Fig. 1.

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