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1971 J. Phys. A: Gen. Phys. 4 L82

(http://iopscience.iop.org/0022-3689/4/5/017)

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and (3) becomes

$$B' = b \exp(i\beta) + 4\omega \Psi \left[\exp(-i\eta) + \exp\left\{ i\left(\eta - \theta + \frac{\pi}{2}\right) \right\} \right]$$

= $b \exp(i\beta) + 4\omega \Psi \left[\exp(-i\eta) + \exp\{i(\eta + 2\beta)\} \right]$
= $\exp(i\beta) \left\{ b + 4\omega \Psi \cos(\eta + \beta) \right\}.$

It can be seen from this equation that it is always possible to choose a ψ such that B' = 0. For example, we make take

$$\psi = -\frac{b}{8\omega}\exp(-\mathrm{i}\beta).$$

This reduces (2) to the form (1) for which $\omega = \frac{1}{2}|\sigma|$.

It has thus been established that the energy momentum tensor for neutrino fields with positive energy density may always be written in the form (1). This is in agreement with results established by Wainwright (1971).

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AUDRETSCH, J., 1971, Commun. math. Phys., 21, 303-13. Collinson, C. D., 1971, Preprint, University of Hull. GRIFFITHS, J. B., and NEWING, R. A., 1971, J. Phys. A: Gen. Phys., 4, 208-13. WAINWRIGHT, J., 1971, J. math. Phys., 12, 828-35.

Shape of a self-avoiding walk or polymer chain

Abstract. If $p_n(r)$ is the probability that a self-avoiding walk of *n* steps reaches a distance *r* from the origin, then it is shown, for large *n* and $r \gg R_n$, that

$$p_n(\mathbf{r}) \sim R_n^{-d} (r/R_n)^t \exp\{-(r/R_n)^{1/(1-\nu)}\}$$

where R_n is a scaling length which varies as n^{ν} , and d is the dimensionality. Furthermore, the index t is related to d, ν , and a further index γ which describes the asymptotic behaviour of the total number of self-avoiding walks.

We have also shown, on the assumption that $p_n(r) \sim R_n^{-d}(r/R_n)^r$ for large *n* and $r \ll R_n$ that the index *g* can be related to *d*, ν , γ , and an index *a* which describes the asymptotic behaviour of the total number of self-avoiding walks which return to the origin.

A self-avoiding walk on a lattice is a random walk such that no lattice site is visited more than once in the walk. Such walks are of interest as models of polymer chains in which 'excluded volume' effects are important. Furthermore such walks are connected with certain properties of the Ising model (Domb 1969, Fisher 1966) so that a study of their properties may have application in the more general problem of second-order phase transitions. In this note, we use the analogy between the probability distribution, $p_n(r)$ of self-avoiding walks of *n* steps which reach the point *r* on starting from the origin, and the high-temperature series expansion of the spin-spin correlation function of the Ising model.

For a random walk on a *d*-dimensional lattice without the self-avoiding condition, it is known that $p_n(\mathbf{r})$ behaves for large n as

$$p_n(\mathbf{r}) \sim R_n^{-d} \exp\{-(\mathbf{r}/R_n)^{\delta}\}$$
(1)

where $R_n = R_0 n^{\nu}$, $\delta = 1/(1-\nu)$, and $\nu = \frac{1}{2}$ (Domb 1969). R_0 is a constant of the order of a lattice spacing. R_n can be thought of as a 'scaling length', which measures the mean end-to-end distance. However, the analytical behaviour of $p_n(r)$ for the self-avoiding walk is not completely known, although Fisher (Fisher 1966), has advanced a powerful argument which suggests that for $r \gg R_n$,

$$p_n(\mathbf{r}) \sim R_n^{-d} A(r/R_n) \exp\{-(r/R_n)^{\delta}\}$$
(2)

where A(y) does not vary exponentially fast for large y. R_0 and ν are both changed from their random walk values. There is a large body of numerical and heuristic evidence (Domb 1969) to indicate that

$$\nu = \frac{3}{2+d} \qquad d \leq 3. \tag{3}$$

Consequently, in two dimensions $\nu = \frac{3}{4}$ and $\delta = 4$, and in three dimensions, $\nu = \frac{3}{5}$ and $\delta = \frac{5}{2}$. In this paper, we shall derive two new results concerning the behaviour of the function A(y).

Our first new result is to demonstrate that

$$A(y) \sim y^t \qquad y \to \infty$$
 (4)

with

$$t = (1 - d/2 - \gamma + d\nu)/(1 - \nu).$$
(5)

The index γ is defined by the statement that, asymptotically for large *n*, the total number of walks of *n* steps C_n behaves as

$$C_n \sim C_0 n^{\gamma - 1} \mu^n \tag{6}$$

where μ is the so called 'connective constant' (Hammersley 1957). For the random walk C_n is just q^n , where q is the coordination number of the lattice, so that $\gamma = 1$ and $\mu = q$. For the self-avoiding walk, numerical studies (Martin *et al.* 1967) show that $\gamma = \frac{4}{3}$ in two dimensions and $\frac{7}{6}$ in three dimensions. The connective constant μ must clearly be smaller than (q-1). The connective constant is sometimes referred to as the 'effective coordination number of the lattice'. Substituting for γ in (5) gives $t = \frac{2}{3}$ in two dimensions and $t = \frac{1}{3}$ in three dimensions.

We derive the relation (5) from a consideration of the generating function

$$\Gamma(\boldsymbol{r},\theta) = \sum_{n=1}^{\infty} C_n p_n(\boldsymbol{r}) \mu^{-n} \mathrm{e}^{-n\theta}$$
(7)

which is analogous to the spin-spin correlation function of the Ising model. The limit $\theta \to 0$ in (7) corresponds to the limit $T \to T_{\rm o}+$ in the Ising model, where $T_{\rm o}$ is the transition temperature. Our argument will be readily comprehended by those

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familiar with the papers of Ornstein and Zernike (1914), Fisher (1964), and Fisher and Burford (1967). That is, the Fourier transform of $\Gamma(\mathbf{r}, \theta)$, $\hat{\Gamma}(\mathbf{k}, \theta)$, is assumed to behave as

$$\hat{\Gamma}(\boldsymbol{k},\theta) \sim \frac{A\kappa^{\eta}}{\kappa^2 + k^2} \tag{8}$$

as $k \to 0$, where $\kappa = \kappa(\theta)$ and A is a constant. Furthermore κ , the inverse coherence length, is assumed to behave as

$$\kappa \sim \kappa_0 \theta^{\nu} \tag{9}$$

as $\theta \to 0$, with $\frac{1}{2} < \nu < 1$. The reasons for assuming (8) are: first, following Ornstein and Zernike, the inverse of $\hat{\Gamma}(\mathbf{k}, \theta)$, which is equivalent to the direct correlation function defined by Ornstein and Zernike, can be expanded in a power series in k^2 , and the series can be truncated when k is small; and second, exploiting the analogy with the Ising model, the exact solution of the two-dimensional Ising model due to Onsager suggests the inclusion of the term κ^n in (8) so that the behaviour of $\hat{\Gamma}(\boldsymbol{\theta}, \theta)$ agrees with the known solution. The addition of this factor is also supported by numerical studies. The assumption (9) is supported by results for the completely random walk and the walks consisting only of completely straight configurations. It is readily deduced that in the former case $\kappa \sim \theta^{1/2}$, and in the latter case $\kappa \sim \theta$. The self-avoiding walks are assumed to behave somewhere between these extremes. Finally, to maintain agreement between $\hat{\Gamma}(\boldsymbol{\theta}, \theta)$ and the expression (6) we must have

$$\eta = 2 - \gamma/\nu. \tag{10}$$

If we now take the inverse Fourier transform of (10) we obtain

$$\Gamma(\mathbf{r},\theta) \sim \kappa^{\eta - (3-d)/2} r^{-(d-1)/2} \mathrm{e}^{-\kappa r}$$
(11)

for $\kappa r \gg 1$ and $\theta \rightarrow 0$.

Given the expression (11) one can find $p_n(r)$ by inverting (7) with the aid of Cauchy's theorem. Thus with $z = e^{-\theta}$ we obtain

$$q_{n}(\mathbf{r}) = C_{n}p_{n}(\mathbf{r})\mu^{-n} = \frac{1}{2\pi i} \oint \frac{dz}{z} z^{-n} \Gamma(\mathbf{r}, z)$$
$$= \frac{1}{2\pi i} \int_{c-i\pi}^{c+i\pi} d\theta \exp(n\theta) \Gamma(\mathbf{r}, \theta)$$
(12)

where c is larger than the real part of any singularity of $\Gamma(\mathbf{r}, \theta)$. We now introduce the variables $X = (\kappa_0 r/n^{\nu})^{\delta}$, with $\delta = 1/(1-\nu)$, and $\rho = n\theta/X$, so that, substituting (11) into (12) we obtain for large n

$$q_n(\mathbf{r}) = n^{\gamma - 1 - d\nu} G(X) \tag{13}$$

where

$$G(X) = \kappa_0^{d-2+\eta} X^{1-(d-2+\eta)(1-\nu)} \\ \times \frac{1}{2\pi i} \int_{c'-i\infty}^{c'+i\infty} d\rho (X\rho^{\nu})^{\eta+(d-3)/2} \exp\{X(\rho-\rho^{\nu})\}.$$
(14)

For large X, the integral in (14) can be performed by steepest descents, provided $\nu < 1$. The argument of the exponential in (14) has a stationary point at $\rho = \rho_s = \nu^{\delta}$.

Expanding the argument about the stationary point so that

$$X(\rho - \rho^{\nu}) = -X\nu^{\nu\delta}(1 - \nu) + X\nu^{-\delta}(1 - \nu)(\rho - \rho_s)^2/2 + \dots$$
(15)

one sees that the 'range' of the saddle, that is the region from which the bulk of the integral arises, is given by

$$|\rho - \rho_{\rm s}| \sim X^{-1/2}$$
 (16)

Consequently when X is large, which implies that κr is large, the saddle point technique is consistent with our use of the Ornstein-Zernike form (10). If we define R_n by

$$R_{n} = (1 - \nu)^{-1/\delta} \nu^{\nu} \kappa_{0}^{-1} n^{\nu}$$

= $R_{0} n^{\nu}$ (17)

we find for $r \ge R_n$

$$G(r/R_n) \sim (r/R_n)^t \exp\{-(r/R_n)^\delta\}$$
(18)

with t given by (5). Hence follows our first result.

Our second result concerns the behaviour of $p_n(r)$ in the opposite limit, this time for end-to-end distances much less than the scaling length R_n . This result depends among other things on the assumption that $p_n(r)$ attains a limiting shape in the limit $n \ge 1$ in the sense that

$$p_n(\mathbf{r}) = R_n^{-d} F(r/R_n) \tag{19}$$

for arbitrary values of the ratio (r/R_n) . This assumption is known, in the context of the Ising model, as 'strong scaling'. The 'strong scaling' assumption is valid for the two-dimensional Ising model for which an exact solution is available but it appears to fail for the three-dimensional Ising model (Ferer *et al.* 1969).

In addition we make the assumption that $C_n(r)$, the number of self-avoiding walks of *n* steps which reach the point *r* from the origin, behaves as

$$C_n(\mathbf{r}) \sim f(\mathbf{r}) n^{\alpha - 2} \mu^n \tag{20}$$

for fixed r and large n. The index α is defined by the statement that, asymptotically for large n, U_n the number of returns to the origin of n steps (polygons) behaves as

$$U_n \sim U_0 n^{\alpha - 2} \mu^n. \tag{21}$$

Numerical studies show that $\alpha = \frac{1}{2}$ in two dimensions and $\alpha = \frac{1}{4}$ in three dimensions (Martin *et al.* 1967). The μ occurring in (20) and (21) has been proved by Hammersley (1961) to be identical with the μ occuring in (6). The term $n^{\alpha-2}$ in (21), and the term $n^{\gamma-1}$ in (6) are conjectures. The expression (20) though plausible and substantiated by numerical studies, has not been established rigorously. A proof of the weaker statement that the limit as $n \to \infty$, of $C_n(r_1)/C_n(r_2)$ is finite and greater than zero, would be useful.

Using (20) and (6) we obtain

$$p_n(\mathbf{r}) = C_n(\mathbf{r})/C_n \sim C_0^{-1} f(\mathbf{r}) n^{\alpha - 1 - \gamma}$$
(22)

for fixed r as $n \to \infty$. For (22) to be consistent with (19) we require that

$$F(y) \sim y^g \quad \text{as } y \to 0$$
 (23)

with

$$g = (\gamma + 1 - d\nu - \alpha)/\nu.$$
(24)

AB*

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Hence (24) predicts that in two dimensions $g = \frac{4}{9}$ while in three dimensions $g = \frac{7}{36}$.

The validity of results (5) and (24) can be tested using numerical data. The numerical data support the relation (5) and support the assumptions made in its derivation. On the other hand, relation (24) is not supported by the numerical data for self-avoiding walks in three dimensions. The numerical work will be published at a later date.

One of us (DSM) has been supported by a Science Research Council Fellowship.

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DOMB, C., 1969, Adv. chem. Phys., 15, 229-59.
DOMB, C., GILLIS, J., and WILMERS, G., 1965, Proc. Phys. Soc., 85, 625-45.
FERER, M., MOORE, M. A., and WORTIS, M., 1969, Phys. Rev. Lett., 22, 1382-5.
FISHER, M. E., 1964, J. math. Phys., 5, 944-62.
— 1966, J. chem. Phys., 44, 616-22.
FISHER, M. E., and BURFORD, R. J., 1967, Phys. Rev., 156, 583-622.
HAMMERSLEY, J. M., 1957, Proc. Camb. Phil. Soc., 53, 642-5.
— 1961, Proc. Camb. Phil. Soc., 57, 516-23.
MARTIN, J. L., SYKES, M. F., and HIOE, F. T., 1967, J. chem. Phys., 46, 3478-81.

ORNSTEIN, L. S., and ZERNIKE, F., 1914, Proc. Acad. Sci. Amsterdam, 17, 793.

On the exact propagator

Abstract. We evaluate the propagator for an electron subject to a harmonic force, a constant magnetic field and a time prescribed electric field, exactly. However, our primary concern is to draw attention to important works in the literature that have been overlooked, a result of which has brought some duplication without always corresponding methodological improvement.

We employ functional integration and a result due to Pauli (1952), who evaluated the propagator for a harmonically bound particle under the influence of a time varying force. Pauli's method is based on Van Vleck's work (1928) in connection with the correspondence principle. Extensions of these works appear in a beautiful paper of De Witt (1957) dealing with quantization in curvilinear spaces.

The functional integration methods are mainly Lagrangian based, and the derivation that follows demonstrates the power of Lagrangian quantum mechanics in that an exact propagator can be obtained in cases in which neither energy levels nor eigenfunctions in the configuration representation exist. However, one should not preclude the existence of eigenfunctions, for example, in the momentum representation. An example of this nature is provided in ter Haar (1964) for the propagator of a particle in a constant field of force.