Debye-Huckel theory on random fractals

1986 J. Phys. A: Math. Gen. 19 L785

(http://iopscience.iop.org/0305-4470/19/13/006)

J. Phys. A: Math. Gen. 19 (1986) L785-L790. Printed in Great Britain

LETTER TO THE EDITOR

Debye–Hückel theory on random fractals

R Blender and W Dieterich

Fakultät für Physik, Universität Konstanz, D-775 Konstanz, West Germany

Received 5 June 1986

Abstract. We investigate the screened Coulomb potential in a weakly coupled charged fluid bound to a random fractal geometry. An approximate solution of the corresponding Debye-Hückel equation suggests that the screened potential decays asymptotically according to an exponential of a fractional power of distance. This form is tested numerically for different types of percolation clusters with fractal dimensionalities $d_f = 2.5$ and $d_f = 2$.

Studies of fractal models for disordered systems (Bunde 1986) frequently face the problem of many-particle interactions present in real materials. To investigate many-particle effects in fractal geometries therefore seems to be an important theoretical task. Of particular interest is the role of Coulomb interactions among charged particles (Gefen and Halley 1984, Laibowitz and Gefen 1984). It is well known that the properties of charged fluids in Euclidean geometries strongly depend on the dimensionality d of the system. As a simple but important example we consider the screened Coulomb potential $\phi(r)$ due to a point charge e in a weakly coupled classical one-component plasma. According to Debye-Hückel theory

$$\phi(r) = (e^2/r)\exp(-\kappa_D r) \tag{1}$$

for $d = 3$. Here $\kappa_D = (4\pi n e^2/k_B T)^{1/2}$ denotes the inverse Debye-Hückel screening length, which is determined by the average particle density n and the temperature T. On the other hand, if the fluid particles are bound to a two-dimensional plane, the screened potential inside the plane (obtained from the three-dimensional Poisson equation) decays algebraically as r^{-3}, in contrast to the exponential decay in (1) for the case $d = 3$ (Baus and Hansen 1980). This sensitivity to geometrical constraints suggests that screening will be modified in a characteristic way when the fluid particles are bound to fractal geometries.

In order to investigate this we consider random fractals embedded in ordinary three-dimensional space. Their average structure is characterised by the mass correlation function (Mandelbrot 1983)

$$\langle \theta(\boldsymbol{r})\theta(0)\rangle \simeq \gamma |\boldsymbol{r}|^{d_f - 3} \tag{2}$$

where $\theta(\boldsymbol{r})$ is the characteristic function which is unity if the point $\boldsymbol{r}$ belongs to a particular realisation of the fractal and zero otherwise and d_f denotes the fractal dimensionality. In the presence of a fixed charge e at the origin $\boldsymbol{r} = 0$, the potential $\phi(\boldsymbol{r})$ satisfies the three-dimensional Poisson equation

$$\nabla^2 \phi(\boldsymbol{r}) = -4\pi e^2[\delta(\boldsymbol{r}) + n_0 \theta(\boldsymbol{r})(g(\boldsymbol{r}) - 1)] \tag{3}$$

0305-4470/86/130785+06$02.50

where n_0 is the average density of fluid particles on the fractal and $g(r)$ is their pair correlation function with respect to the origin. The last term in equation (3) ensures overall charge neutrality. By using the linearised Debye-Hückel approximation, we write

$$g(r) - 1 \simeq -\beta\phi(r) \tag{4}$$

where $\beta = (k_B T)^{-1}$. Our problem is now to solve (3) together with (4) for $\phi(r)$ and then to average over configurations $\{\theta(r)\}$ with $\theta(0) = 1$.

Before we present detailed numerical results, let us first discuss a simple mean-field-type approach, which is based on the assumption that the equilibrium charge distribution is mainly determined by the average structure described by (2). Therefore, on averaging (3), we substitute (4) and factorise $\langle\theta(r)\phi(r)\rangle \simeq \langle\theta(r)\rangle\langle\phi(r)\rangle$. Since averages are taken under the condition $\theta(0) = 1$, we can use (2) to obtain

$$\nabla^2\langle\phi(r)\rangle = -4\pi e^2\delta(r) + \kappa^2 r^{d_f-3}\langle\theta(r)\rangle \tag{5}$$

where $\kappa^2 = \gamma\kappa_0^2$ and $\kappa_0^2 = 4\pi e^2 n_0\beta$. At this stage it is convenient to write $\langle\phi(r)\rangle = (e^2/r)\psi(r)$ with a screening function $\psi(r)$ which describes deviations from the bare Coulomb potential e^2/r. From (5) we obtain

$$\psi''(r) = \kappa^2 r^{d_f-3}\psi(r) \tag{6}$$

for $r \neq 0$. Next we introduce the scaled variable

$$x = \kappa r^{1/2\nu} \qquad \nu = (d_f - 1)^{-1} \tag{7}$$

and set $\psi = x^\nu f$. Then, by using (6), the function f satisfies the differential equation for modified Bessel functions I_ν, K_ν of order ν (Abramowitz and Stegun 1970, Kamke 1964). Employing boundary conditions $\psi(r) \to 1$ as $r \to 0$ and $\psi(r) \to 0$ as $r \to \infty$ we find the solution

$$\psi(r) = \frac{2\nu^\nu}{\Gamma(\nu)} x^\nu K_\nu(2\nu x). \tag{8}$$

For $d_f = 3$ or $\nu = \frac{1}{2}$, equation (8) reduces to $\psi(r) = e^{-\kappa r}$, which agrees with (1) after setting $n = \gamma n_0$. In the general case $1 < d_f \leqslant 3$ we obtain the asymptotic behaviour (Abramowitz and Stegun 1970)

$$\psi(r) \sim \text{constant} \times x^{\nu-1/2} e^{-2\nu x} \qquad x \to \infty. \tag{9}$$

According to this expression, the decay of the screened Coulomb interaction with distance r is governed by a fractional power $(d_f - 1)/2 < 1$ in the exponential. Obviously, as d_f is decreased, screening becomes less and less effective. For $d_f = 2$ we have verified numerically that (8) agrees with the spherical average of the screened potential in the Euclidean case $d = 2$ (Baus and Hansen 1980).

To test the above results we have performed detailed numerical studies. As our fractal structures we have chosen percolation clusters on a three-dimensional simple cubic lattice of sites l. Clusters are grown within a box of length $2L + 1 = 93$, starting at the centre $l = 0$ and following the procedure of Leath (1976). Two types of clusters are considered. One corresponds to the infinite cluster at the threshold concentration $p_c \simeq 0.31$, characterised by a fractal dimension $d_f \simeq 2.5$. Second, we have chosen a concentration $p = 0.25$ generating objects with $d_f \simeq 2.0$, the so-called 'lattice animals'. To obtain sufficiently large clusters we employed the enrichment method successfully used by Djordjevic *et al* (1984) in connection with percolation.

A particular cluster grown in this way is represented by the discrete characteristic function θ_l. The discrete analogue of the Poisson equation (3) in connection with (4) now takes the form ($e=1$)

$$\sum_{\delta}(\phi_{l+\delta}-\phi_l)=-4\pi\delta_{l,0}+\kappa_0^2\theta_l\phi_l \tag{10}$$

where the summation is over nearest neighbours of site l. This set of difference equations is solved by iteration (Ames 1977). Since our procedure is confined to a finite domain $|l|\leq L$, we replace the condition of a vanishing potential at infinity by the boundary condition $\phi_l=\phi$ for sites l in the shell $L\leq|l|<L+1$. The constant ϕ is taken to be the average potential at a distance $|r|=L$ as obtained from the approximate expression (8). The iteration is started with a constant zero-order potential $\phi_l^{(0)}=\phi$. To accelerate convergence we apply the method of successive over-relaxation, where $\phi_l^{(n)}$ is replaced by $(r+1)\phi_l^{(n)}-r\phi_l^{(n-1)}$ at each step n. During the iteration process the parameter r is controlled by the relative change $(\phi_l^{(n)}-\phi_l^{(n-1)})/\phi_l^{(n-1)}$ and increases from zero to, typically, 0.3. The iteration is stopped once the potential at sites along the cubic axes becomes stable to within 10^{-5}. To achieve this we need about 200–500 steps. In the subsequent average over configurations $\{\theta_l\}$ we were limited to five clusters. For that purpose we selected clusters with small fluctuations in the mass correlation function.

Results for the spherically averaged potential in the case of percolation clusters with $d_f=2.5$ are presented in figure 1 for three different κ_0. To compare the data with

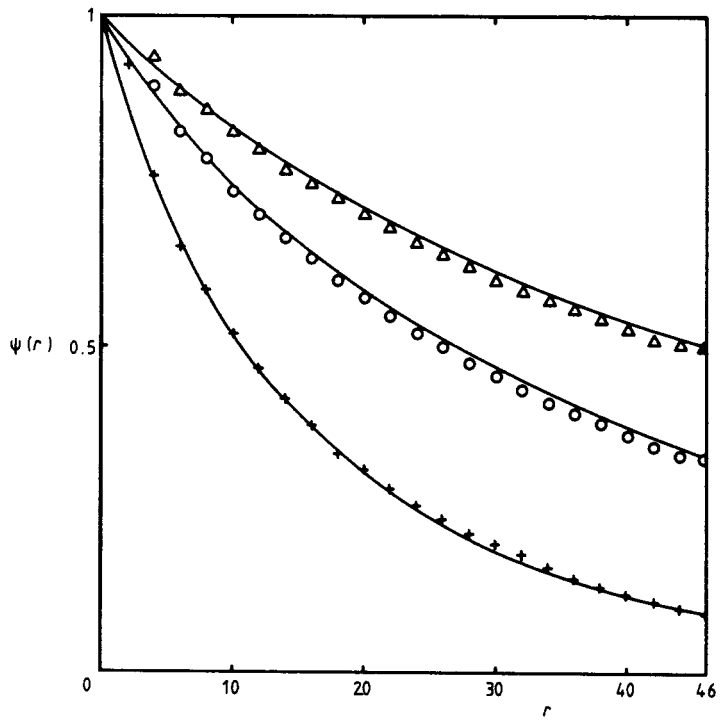

Figure 1. Screening function $\psi(r)$ against r for percolation clusters with $p_c=0.311$ and $d_f=2.5$. Data points are from numerical solutions of equation (10) for three values of κ_0^{-1}: +, 5; ○, 10; △; 15. The mean-field approximation, equation (8), is represented by the full curve.

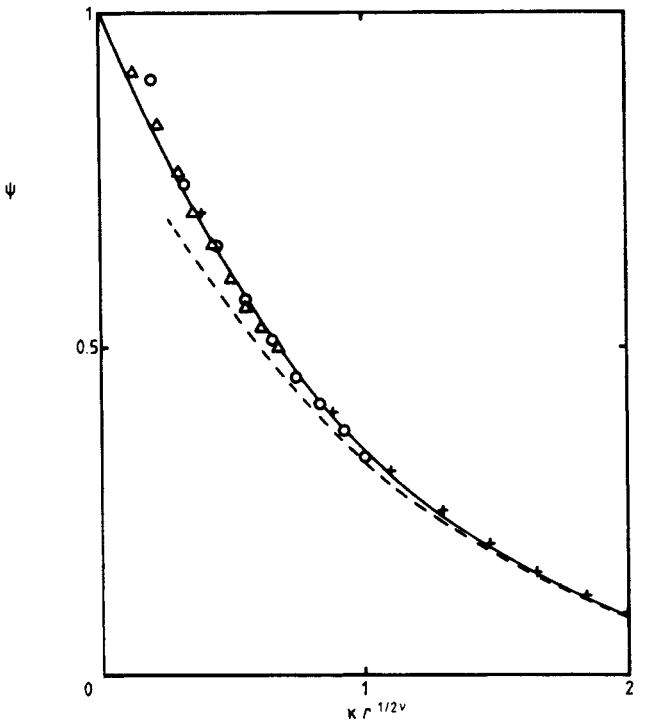

Figure 2. Screening function $\psi(r)$ against the scaled variable $\kappa r^{1/2\nu}$. The numerical data are those of figure 1. The full curve follows equation (8) and the broken curve represents the asymptotic behaviour, equation (9).

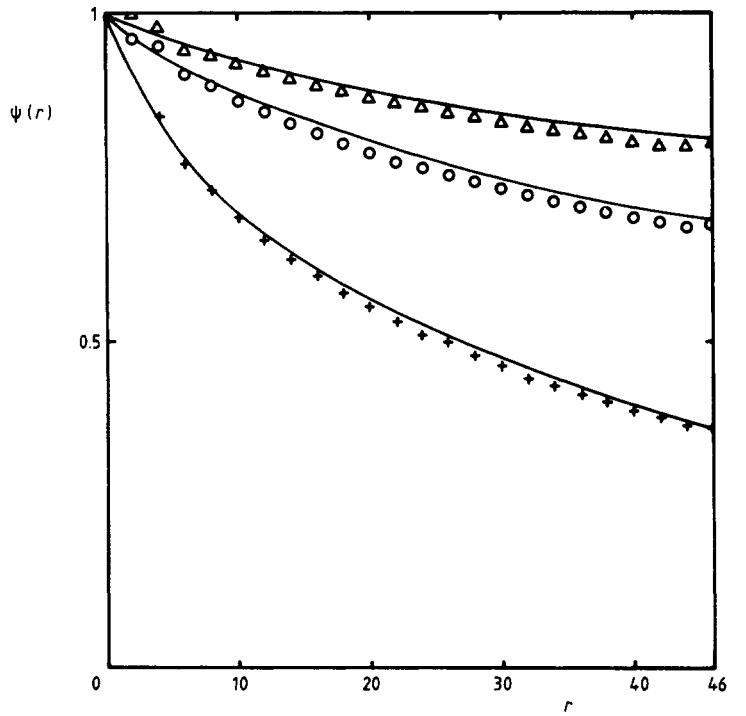

Figure 3. Same as figure 1 for the lattice animals with $p = 0.25$ and dimension $d_f = 2$.

(8) we first determine the prefactor $\gamma \simeq 0.334$ (± 0.005) in the mass correlation function (2) for our simulated clusters. Expression (8) with $d_f = 2.5$ and the screening parameter $\kappa = \gamma^{1/2}\kappa_0$ is shown by the full curves in figure 1. The agreement with the numerical data is excellent. Calculations for a smaller box with $L = 23$ performed under the boundary condition as described above gave very similar results, the change being of the order of the difference between data points and the full curves (figure 1).

As suggested by (8), data for different screening parameters should fall on a single curve when plotted against the scaled variable x, equation (7). This is confirmed in figure 2, which also shows the asymptotic expression (9).

As a further test of (8) for more dilute fractal structures we repeat the above analysis using our 'lattice animals' with $d_f = 2$. A comparison with numerical data is shown in figure 3. The quality of the data collapse is similar to that of figure 2.

We conclude that our findings support the analytic form (8) for the screening function $\psi(r)$ for random fractals. We also note that the good agreement between analytic and numerical results provides an *a posteriori* justification of the boundary condition which we have imposed on our solutions of (10). To illustrate the validity of our analytic approach under more general boundary conditions, we have artificially fixed the potential at the boundary such that $\psi(L) = 1$. In that case (6) is solved by

$$\psi(r) = \frac{2\nu^{\nu}}{\Gamma(\nu)} x^{\nu}(K_{\nu}(2\nu x) + aI_{\nu}(2\nu x)) \tag{11}$$

with a suitably chosen constant a. This expression, for $d_f = 2.5$, is plotted in figure 4 which shows the screening of the surface potential towards the interior of the box. Again, (11) agees well with the corresponding numerical solution, also shown in figure 4.

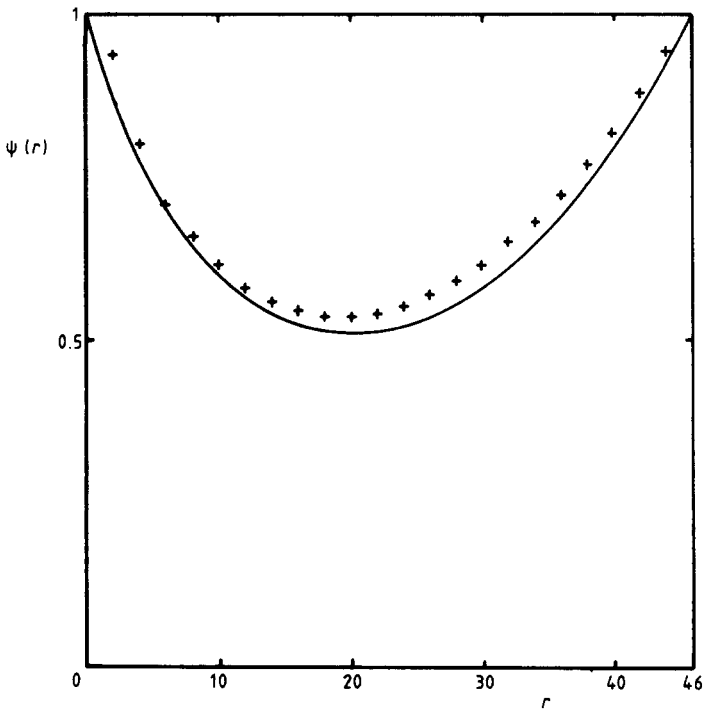

Figure 4. Comparison between numerical and analytic screening function for a boundary value problem with $\psi(L) = \psi(0) = 1$.

We thank A Bunde and H Harder for interesting conversations. In particular we have benefited from discussions with S Havlin on the method of cluster growth.

References

Abramowitz M and Stegun I A 1970 *Handbook of Mathematical Functions* (New York: Dover)
Ames W F 1977 *Numerical Methods for Partial Differential Equations* (New York: Academic)
Baus M and Hansen J P 1980 *Phys. Rep.* **59** 2
Bunde A 1986 *Festkörperprobleme, Advances in Solid State Physics* **26** (Braunschweig: Vieweg-Verlag) in press
Djordjevic Z V, Havlin S, Stanley H E and Weiss G H 1984 *Phys. Rev.* B **30** 478
Gefen Y and Halley J W 1984 *Kinetics of Aggregation and Gelation* (Amsterdam: Elsevier) p 161
Kamke E 1964 *Gewöhnliche Differentialgleichungen* (Leipzig: Akademische Verlagsgesellschaft)
Laibowitz R B and Gefen Y 1984 *Phys. Rev. Lett.* **53** 380
Leath P L 1976 *Phys. Rev.* B **14** 5046
Mandelbrot B B 1983 *The Fractal Geometry of Nature* (San Francisco: Freeman)