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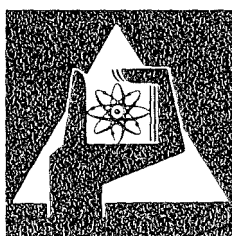
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Institut für Neutronenphysik und Reaktortechnik

**Application of a Modified Collocation Method  
to the One Dimensional,  
One Group Neutron Transport Equation**

W. Maschek



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Application of a Modified Collocation  
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## Abstract

A modified collocation method is used for solving the one group criticality problem for a uniform multiplying slab. The critical parameters and the angular fluxes for a number of slabs are displayed and compared with previously published values.

Anwendung einer modifizierten Kollokationsmethode auf die  
eindimensionale Eingruppen-Neutronentransportgleichung

## Zusammenfassung

Eine modifizierte Kollokationsmethode wird zur Lösung der monoenergetischen Neutronentransportgleichung für die Platten-geometrie herangezogen. Die Ergebnisse für die kritischen Parameter und für den Vektorfluß werden mit Resultaten anderer Autoren verglichen.

## 1. INTRODUCTION

The neutron transport equation is an integrodifferential equation in seven independent variables, which in problems of any generality can be solved only approximately. Since these numerical solutions are extremely expensive a variety of methods, e. g. the method of weighted residuals (MWR) /1-3/, has been developed with the goal to reduce the costs of computation.

The MWR unifies a number of approximate methods, one of which is the collocation technique /4-6/. The collocation method is applicable to differential- integral- and integrodifferential equations. It can be used for solving nonlinear problems too /7,8/. The collocation method usually considered to be a relatively crude approximation, gives very often surprisingly good results. Because of its simplicity and significantly reduced computational costs the collocation method is particularly suited for a first order approximation of a more complicated problem. Thus the global representation of the solution may be of great advantage. In reactor physics the collocation method has been rarely used. Applications can be found mainly in diffusion theory /9,10/ or in solving the space independent reactor kinetics equations /11-14/.

In the present work the collocation method is applied to the neutron transport equation. For that purpose a modification of the collocation technique is introduced.

The Boltzmann equation is used in the form of the constant cross-section approximation /15/ and the slab criticality problem is solved. The reason for treating such an idealized geometry was because of its simplicity, the possibility of finding a variety of results for comparison purposes and that benchmark values /16/ obtained by the method of singular eigenfunctions /17/ exist.

## 2. THE MODIFIED COLLOCATION TECHNIQUE

To derive the method of weighted residuals (MWR) one can start with a linear boundary value problem:

$$A(x_1, \dots, x_n) \psi(x_1, \dots, x_n) - f(x_1, \dots, x_n) = 0 \quad (1)$$

$A(x_1, \dots, x_n)$  denotes a differential (-integral) operator, the  $x_i$ 's are the independent variables,  $\psi(x_1, \dots, x_n)$  the dependent variable and  $f(x_1, \dots, x_n)$  is an inhomogeneous source term. The solution of Eq. (1) is approximated by a combination of linearly independent known base trial functions  $\phi_i(x_1, \dots, x_n)$  and unknown coefficients  $c_i$ , which do not depend on the  $x_i$ 's. The functions  $\phi_i(x_1, \dots, x_n)$  should satisfy given boundary conditions associated with Eq. (1).

The ansatz

$$\psi_N(x_1, \dots, x_n) = \sum_{i=1}^N c_i \phi_i(x_1, \dots, x_n) \quad (2)$$

is inserted into Eq. (1), thus giving a residual  $R$  dependent on the  $x_i$ 's and the coefficients  $c_i$ .

$$\begin{aligned} \sum_{i=1}^N c_i A(x_1, \dots, x_n) \phi_i(x_1, \dots, x_n) - f(x_1, \dots, x_n) &= \\ = R(x_1, \dots, x_n, c_1 \dots c_N) & \quad (3) \end{aligned}$$



To compute the  $c_i$ 's one multiplies Eq. (3) by suited weighting functions  $G_k$  and integrates the result over the domain  $\Omega$  under consideration.

$$\sum_i^N c_i \left\langle G_k, A\phi_i \right\rangle_{\Omega} - \left\langle G_k, f \right\rangle_{\Omega} = \left\langle G_k, R \right\rangle_{\Omega} \quad (4)$$

where

$$k = 1 \dots N$$

$$\left\langle r, s \right\rangle_{\Omega} = \int_{\Omega} r \cdot s \, d\Omega$$

As an approximation for an overall vanishing residual the weighted integral of the residual is set equal to zero:

$$\left\langle G_k, R \right\rangle_{\Omega} = 0 \quad (5)$$

$$k = 1 \dots N$$

These equations define the general MWR for the linear boundary problem (1).

Now the collocation method will be explained. For this case one chooses the Dirac delta functions for weighting /9,19,20/.

$$G_k(x_1, \dots, x_n) = \delta(x_1 - x_1^k) \dots \delta(x_n - x_n^k) \quad (6)$$

Inserting (6) into (5) makes the residual  $R$  vanish at the collocation points  $x_1^k \dots x_n^k$ .

Increasing the number  $N$  of linear independent functions  $\phi_i$  and of points  $x_k$ , the residual is forced to vanish at more and more points and in the limit presumably it approaches zero throughout  $\Omega$ .

After carrying out the integration in Eq. 5 the coefficients are determined by a system of linear algebraic equations:

$$\sum_i^N c_i A(x_1^k, \dots, x_n^k) \phi_i(x_1^k, \dots, x_n^k) - f(x_1^k, \dots, x_n^k) = 0 \quad (7)$$

$k = 1 \dots N$

Obviously, the number of collocation points is identical with the number of trial functions.

Now, by a slight modification of the weighting function  $G_k$  one can introduce additional points  $x$  without increasing the number of test functions /18/. Restricting for simplicity on two variables ( $x_1 = x$ ,  $x_2 = y$  and  $x_1^k = x_k$ ,  $x_2^j = y_j$ ) the modified weighting function is defined as:

$$G_{kj} = \sum_{j=1}^M \delta(x-x_k) \delta(y-y_j) \quad (8)$$

$G_{kj}$  is now a linear combination of delta functions.

With this weighting Eq. 5 and 7 become:

$$\left\langle \sum_{j=1}^M \delta(x-x_k) \delta(y-y_j), R(x, y, c_1 \dots c_N) \right\rangle = 0 \quad (9)$$

$$\sum_{i=1}^N \sum_{j=1}^M c_i A \phi_i(x_k, y_j) - f(x_k, y_j) = 0 \quad (10)$$
$$k = 1 \dots N$$

For a rectangular mesh  $(x_k, y_j)$  in the x-y plane, this means that one simultaneously sets a sum of M residuals equal to zero at points with the abscissa values  $x_k$ . For the tested cases, which will be discussed later the method worked satisfactorily. Nevertheless one must watch for cancelation effects within the linear combination of the residuals.

Naturally no restriction exists in applying this modified collocation technique to eigenvalue- or initial value problems. For solving the one dimensional transport equation the coordinate x is identified with the space variable and the coordinate y with the angle coordinate  $\mu = \cos \theta$ . As one is mainly interested in the angular distribution of the neutron flux, the additional points are placed in the direction of  $\mu$ .

A critical question for the collocation method is how to distribute the collocation points in the available space. In the literature it is usually proposed to distribute them on an equidistant mesh /5,6/. Basically the concept of the collocation technique is nothing more than an interpolation procedure. One knows from interpolation theory /21/ that

working with equidistant nodes can lead to defects and errors in the approximate solution.

Also the proofs of convergence and stability for specific problems /22-31/ depend essentially on the choice of the collocation points. Usually the use of either the Chebyshev- /24,29/ the Gauss base points /24,27,29/ or the zero's of other orthogonal polynomials is recommended. For details we refer to the literature. The position of collocation points can also be derived from the discrete method of least squares. The collocation points then coincide with the mesh for integration. Higher order integration formulas /32/ will again lead to a nonequidistant distribution of points. Utilizing trigonometric trial functions /24/ a good distribution seems to be

$$\xi_j = \frac{2j - 1}{2N + 1} \pi \quad j = 1 \dots N \quad (11)$$

The position of the points will often be strongly influenced by the physical structure of the problem. For example the case of a control rod /9/ in a reactor. This requires a placing of at least one point in the control rod channel, otherwise no information about the rod position would be available.

### 3. APPLICATION OF THE MODIFIED COLLOCATION METHOD TO THE CRITICAL SLAB PROBLEM

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The modified collocation method is applied to the one-dimensional homogeneous slab with finite thickness  $D$ . The thickness  $D = 2a$  is given in units of the mean free path. Working with the constant cross-section approximation /15/ and assuming isotropic scattering the angular neutron density  $\psi(x, \mu)$  satisfies the equation

$$\mu \frac{\partial \psi(x, \mu)}{\partial x} + \psi(x, \mu) = \frac{c}{2} \int_{-1}^{+1} \psi(x, \mu') d\mu' \quad (12)$$

$$\mu = \cos \theta$$

with the boundary and symmetry conditions (the origin is at the center of the slab):

$$\begin{aligned} \psi(a, \mu) &= 0 & \mu < 0 \\ \psi(-a, \mu) &= 0 & \mu > 0 \\ \psi(x, \mu) &= \psi(-x, -\mu) \end{aligned} \quad (13)$$

$c$  denotes the mean number of secondaries per collision and is regarded as the criticality factor of the multiplying medium.

With the procedure outlined in Chap. 2 equation 12 takes on the form:

$$\sum_{j=1}^M \sum_{i=1}^N c_i \left[ \mu_j \frac{\partial \phi_i(x_k, \mu_j)}{\partial x_k} + \phi_i(x_k, \mu_j) - \frac{c}{2} \int_{-1}^{+1} \phi_i(x_k, \mu') d\mu' \right] = 0 \quad k = 1 \dots N \quad (14)$$

The linear combination of the testfunctions  $\phi_i(x, \mu)$  is synthesized multiplicatively of space-dependent- and of specifically tailored angular-dependent functions. From symmetry considerations it follows that  $\psi_N(x, \mu)$  must be an even function.

To obtain a relation between the critical quantities  $c$  and  $D$ , the slabthickness or a related parameter has to be incorporated in the testfunction. This can be achieved by using a relationship between  $D$  and the diffusion length  $L$  /33,34/.

For the space dependence a product of trigonometric trial functions and exponential expressions has been chosen to satisfy the boundary conditions. The adequate angular functions are constructed by following the ideas of Kaplan and Natelson /35-37/.

To define the angular dependent part of the  $\phi_i$ 's, at first functions  $r = r(\theta)$  are derived which have the form of circles and ellipses when represented in polar coordinates  $(r, \theta = \cos^{-1} \mu)$ . The radius vector  $r$  also depends on some other parameters  $a, b, \epsilon$  by which the shape of the ellipses can be influenced.

These parameters a and b are the axes and the factor  $\epsilon$  takes into account the degree of "off-centeredness" when the center of the ellipse is shifted on the axis a to the right.

For the calculations a is set equal to one. Then the dependence of the radius vector r on  $\mu = \cos \theta$  is given by an odd and an even function.

$$r = \frac{\mu \epsilon b^2}{1 + \mu^2 (b^2 - 1)} + \frac{b \left[ 1 - \epsilon^2 + \mu^2 (b^2 - 1 + \epsilon^2) \right]^{\frac{1}{2}}}{1 + \mu^2 (b^2 - 1)} \quad (15)$$

$$r = \hat{U}(\mu, b, \epsilon) \epsilon b^2 + \hat{G}(\mu, b, \epsilon) b$$

Using the functions  $\hat{G}(\mu, b, \epsilon)$  and  $\hat{U}(\mu, b, \epsilon)$  as the angular functions for the approximation one must specify the parameters b and  $\epsilon$  and thus one can control the shape of the angular trial function.

A parameter study revealed that the approximation with these functions was not satisfactory, because one is forced to make an exact separate choice of axis b for each specific slab thickness. It would be much more desirable to cover a wider range of slab thicknesses with one value for parameter b. Therefore the respective angular trial functions have been modified by implicitly incorporating the slab thickness, to achieve a more "insensitive" approximation.

The denominator of  $\hat{G}(\mu, b, \epsilon)$  and  $\hat{U}(\mu, b, \epsilon)$  is modified by a correction factor depending on the diffusion length L

$$\mu^{2n} \left(\frac{1}{L}\right)^{2n} \quad n = 1, 2, \dots \quad (16)$$

yielding new functions  $G(\mu, b, \epsilon, \frac{1}{L}, n)$  and  $U(\mu, b, \epsilon, \frac{1}{L}, n)$ .

For constructing the trial functions  $\{\phi_1 \dots \phi_N\}$  which depend on space and angle the following notation is used. The set of trial functions  $\{\phi_1 \dots \phi_N\}$  is denoted as a vector  $\vec{\phi}$ . The diagonal elements of a matrix S (N\*N) contain the space-dependent functions (All other elements are zero.). This matrix S is multiplied by a vector  $\vec{\chi}$  representing the angular functions.

$$\vec{\phi} = S \cdot \vec{\chi} \quad (17)$$

Choosing e.g. N = 4 the matrix S has the following elements:

$$\begin{aligned} s_{i\ell} &= 0 \quad \text{for } i \neq \ell \\ s_{11} &= \cos \frac{x}{L} (e^{\gamma a} - e^{-\gamma x}) & s_{22} &= \sin \frac{x}{L} \cdot \frac{1}{L} \cdot (e^{\gamma a} - e^{-\gamma x}) \\ s_{33} &= \cos \frac{x}{L} (e^{\gamma a} - e^{\gamma x}) & s_{44} &= \sin \frac{x}{L} \cdot \frac{1}{L} \cdot (e^{\gamma a} - e^{\gamma x}) \end{aligned} \quad (18)$$



Vektor  $\vec{\chi}$  can be written as:

$$\vec{\chi}^T = (G^+(\mu, b, \epsilon, \frac{1}{L}, n) \ U^+(\mu, b, \epsilon, \frac{1}{L}, n) \ G^-(\mu, b, \epsilon, \frac{1}{L}, n) \ U^-(\mu, b, \epsilon, \frac{1}{L}, n))$$

with

$$G^+(\mu, b, \epsilon, \frac{1}{L}, n) = \begin{cases} \left[ \frac{1 - \epsilon^2 + \mu^2 (b^2 - 1 + \epsilon^2)}{1 + \mu^2 (b^2 - 1) + \mu^{2n} (\frac{1}{L})^{2n}} \right]^{\frac{1}{2}} & u > 0 \\ 0 & u < 0 \end{cases} \quad (19)$$

$$U^+(\mu, b, \epsilon, \frac{1}{L}, n) = \begin{cases} \frac{\mu}{1 + \mu^2 (b^2 - 1) + \mu^{2n} (\frac{1}{L})^{2n}} & u > 0 \\ 0 & u < 0 \end{cases}$$

The functions  $G^-(\mu, b, \epsilon, \frac{1}{L}, n)$  and  $U^-(\mu, b, \epsilon, \frac{1}{L}, n)$  have the same form as  $G^+$  and  $U^+$  but vanish for  $\mu > 0$ .

The parameters  $\gamma$  in Eq. 18 and  $n$  in Eq. 19 have been set equal to one. For the base calculations  $\epsilon$  is equal zero.

#### 4. NUMERICAL RESULTS AND COMPARISON WITH OTHER METHODS

In this section the numerical results for the critical slab problem with isotropic scattering will be presented. They have been obtained on the basis of equation (14). These data are compared with the results of the benchmark problem (BENCHMARK) /16/ and those obtained by other approximate methods. Each method is denoted by an abbreviation given in curved parentheses. The index N will denote the order of the corresponding method.

The critical values  $c$  as a function of the various slab-thicknesses  $D$  for the collocation method are given in the column COLL-1.

For comparison special attention has been given the values obtained from standard methods such as  $P_N$ -( $P_N$ ),  $DP_N$ -( $DP_N$ ) /15, 34,38/ and  $S_N$ -( $S_N$ ) /38/ approximations. Carlvik /39/ starts from the integral form of the transport equation expanding the flux in a series of Legendre polynomials (CARL), Kiesewetter /40/ uses a Wiener Hopf-type technique denoting it as the FT-method (FT). This Fourier transformation technique leads as Case's (CASE) /41/ and Bowden's method (BOW-) /42/ to a singular integral equation. The angular flux can also be obtained by solution of a regular homogeneous Fredholm integral equation of second kind by applying the finite Laplace transformation (FLT) to the Boltzmann equation /34/. Good results can also be obtained from Asaoka's multiple

collision method /43/ using a statistical approach. This analytical method is denoted as  $j_N$ -method ( $j_N$ ). A variational point of view (VARI) can be found in reference /33/. Values from a variational principle are given also in /34/. An angular synthesis approximation used on thin critical slabs is reported by Zwibel /44/. R.W. Albrecht /45/ expands the angular variable in the transport equation in the orthogonal, complete, binary valued set of Walsh functions,  $wal(n, \mu)$ , called  $W_N$  approximation ( $W_N$ ). The slab problem is also attacked by more recent methods such as invariant imbedding /46-48/, (IMBED), and the finite element method /49,50/, ( $E_N$ ). Further comparison may be made with the  $C_N$ -method ( $C_N$ ) /57/ and the degenerate kernel technique (DKT) /52/. Finally the results of Mitis (MITIS) /53/ and the analytical approaches by Kschwendt /54/ and Certainé /55/ are mentioned. For more details refer to the authors.

In Table I, II, III and IV a synopsis of the various results is presented either by giving the critical value  $c$  and computing  $D$  or vice versa. Of course for the criticality problem of a finite slab  $c$  is always  $> 1.0$ , and for  $D \rightarrow \infty$ ,  $c$  asymptotically approaches 1.0. In Fig. 1 the results of Tab. I and III, IV are displayed. The value  $c = 2.00$  is given and the corresponding critical slab thickness is approximated by different methods. The deviation from the benchmark value  $D = 0.62204$  can readily be seen.

Comparing the results one recognizes that for the slab criticality problem the  $P_N$  approximation gives the strongest deviation from the exact value. The  $S_N$ -method appears to be superior. For the  $P_N$  approximation one can also see the influence of the employed boundary condition and that the Marshak condition is better for small  $N$ . Under this conditions also the improvement of the results with Yvon's method ( $DP_N$ ) can be seen. Excellent results can also be obtained with Asaoka's multiple collision method, with invariant imbedding and finally with the  $C_N$ - and degenerate kernel technique. If one analyzes the values obtained from collocation one can find good agreement with the benchmark values. Additionally to the COLL-1 value a value COLL-2 is given where only circles are used for the approximation. Of course the result of COLL-2 is worse, as one expects the angular trial function to be more pronounced in direction parallel to the slab surface.

Finally the angular neutron distribution  $\psi(x,\mu)$  is presented in Figs. 2 - 4. For a qualitative comparison of the angular fluxes one can use the results given by Mitis /53/, Kiesewetter /40/, Bowden /42/, Asaoka /43/ and Kaper /16/.

D	c			
	BENCHMARK	COLL-1	DKT	Diffusion
6.600527	1.05	1.050003	1.050019	1.052663
4.226619	1.10	1.099999	1.100001	1.108725
2.578759	1.20	1.200027	1.200026	1.228184
1.473207	1.40	1.400058	1.400024	1.488541
1.023926	1.60	1.600071	1.599984	1.770796
0.777563	1.80	1.800104	1.800190	2.071105
0.622042	2.00	2.000346	2.000755	2.387177

Table I: The Critical Multiplication Factor  $c$  as a Function of the Critical Slab Thickness  $D$  ( $D$  is the Corresponding Critical Slab Thickness for the  $c$  Values of the Benchmark Problem)

D	c							
	BENCHMARK	COLL-1	CARL	$j_4$	$j_6$	N=5	IMBED N=7	FT
2.0000	1.27710182	1.277126	1.22710	1.2771086	1.2771033			1.277
1.0000	1.61537852	1.615391	1.61538	1.6153850	1.6153800	1.6155	1.6154	1.615
0.9000		1.688472	1.68788			1.6880	1.6879	
0.8000		1.776814	1.77707			1.7772	1.7771	
0.7000		1.885921	1.88955			1.8897	1.8895	
0.6000		2.037943	2.03598			2.0360	2.0360	
0.5000		2.235212	2.23501	2.2350160	2.2350120	2.2344	2.2351	
0.4000		2.521888	2.52253			2.5202	2.5228	
0.3000		2.978997	2.97868			2.9716	2.9788	
0.2000		3.832976	3.83031					
0.1000		6.103402	6.11704					

Table II: The Critical Multiplication Factor  $c$  as a Function of the Critical Slab Thickness  $D$

c	D												
	BENCHMARK	P <sub>1</sub> MARSHAK		P <sub>3</sub> MARSHAK		P <sub>5</sub>	P <sub>7</sub>	DP <sub>1</sub>	DP <sub>3</sub>	S <sub>2</sub>	S <sub>4</sub>	S <sub>8</sub>	S <sub>16</sub>
1.01	16.659027123												
1.02	11.331010912			11.3660		11.3446	11.338	11.330	11.330	11.4524	11.3494	11.3404	11.3388
1.05	6.600527544	6.976	6.807	6.6383	6.6131	6.6146	6.608	6.594	6.600	6.7436	6.6156	6.6064	6.6046
1.10	4.226619332	4.617	4.457	4.2707	4.2427	4.2420	4.234	4.212	4.226	4.3968	4.2396	4.2310	4.2292
1.20	2.578758857	2.970	2.825	2.6371	2.6040	2.5970	2.5378	2.554	2.5786	2.7792	2.5898	2.5824	2.5804
1.30	1.875451120												
1.40	1.473207100	1.838	1.716	1.5546	1.5153	1.5002	1.4854	1.4458	1.4734	1.6910	1.4870	1.4766	1.4744
1.60	1.023925960	1.359	1.254	1.1118	1.0767	1.0598	1.0404	1.0054	1.0238	1.2394	1.0446	1.0276	1.0250
1.80		1.086	0.993	0.8775	0.8364	0.8202	0.7984	0.7696	0.7768	0.9848	0.8048	0.7818	0.7786
2.00	0.622041960	0.907	0.824	0.7240	0.6841	0.6696	0.6468	0.6232	0.6204	0.8194	0.6524	0.6274	0.6232

Table III: The Critical Slab Thickness D as a Function of c, the Critical Multiplication Factor

c	D												
	CASE		VARI	C <sub>o</sub>	E <sub>8</sub>	W <sub>2</sub>	W <sub>4</sub>	W <sub>8</sub>	W <sub>16</sub>	MITIS	FLT	BOW	
	0-Iterat.	1.Iterat.										N=10	N=40
1.01	16.6590	16.6590								16.690		16.65908	16.65904
1.02					11.3368	10.1138	10.0310	11.2562	11.3124				
1.05			6.6069			6.0410	6.4526	6.5632	6.5912		6.6069	6.60058	6.60054
1.10	4.2266	4.2265	4.2329	4.22483		3.9988	4.1528	4.2074	4.2218	4.240	4.2328	4.22668	4.22662
1.20	2.5796	2.5786	2.5850	2.57821		2.5780	2.5534	2.5712	2.5768		2.5850	2.57888	2.57876
1.30	1.8776	1.8749		1.87535						1.780		1.87564	1.87546
1.40	1.4568	1.4723	1.4810	1.47321		1.4920	1.4838	1.4728	1.4730		1.4810	1.47344	1.47322
1.60	1.0303	1.0228	1.0335	1.02383		1.0770	1.0508	1.0266	1.0244	1.022	1.0335	1.02424	1.02394
1.80	0.7963	0.7853	0.7885	0.77736		0.8404	0.8154	0.7826	0.7784		0.7885	0.77788	0.77756
2.00	0.7527	0.6397	0.6340	0.62188		0.7854	0.6668	0.6294	0.6232	0.621	0.6340	0.62238	0.62206

Table IV: The Critical Slab Thickness D as a Function of c, the Critical Multiplication Factor



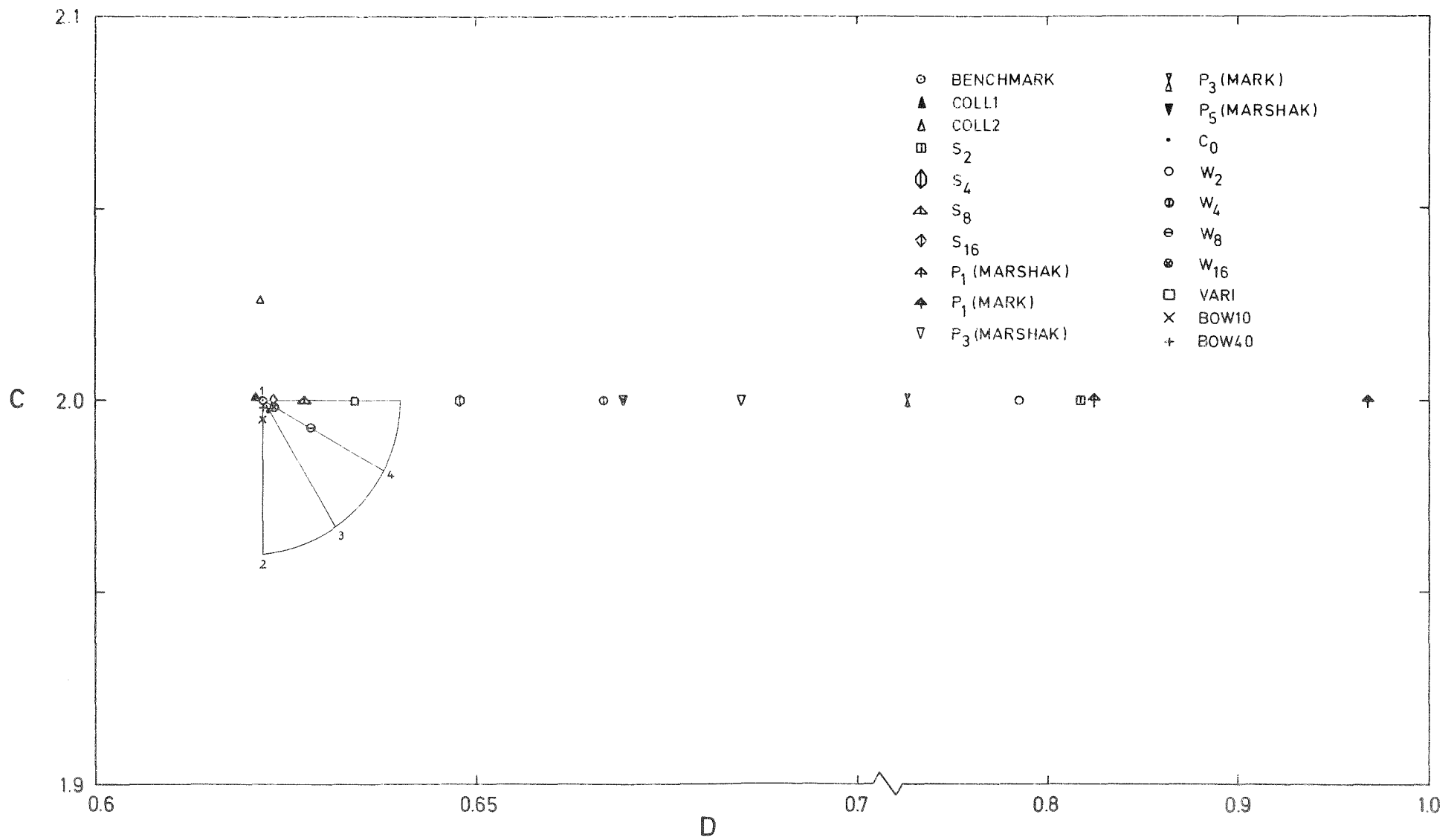


FIG.1 : APPROXIMATION OF C=2.00 BY VARIOUS METHODS  
 (THE RAYS:  $\bar{12}, \bar{13}, \bar{14}$  CORRESPOND TO C = 2.00 )

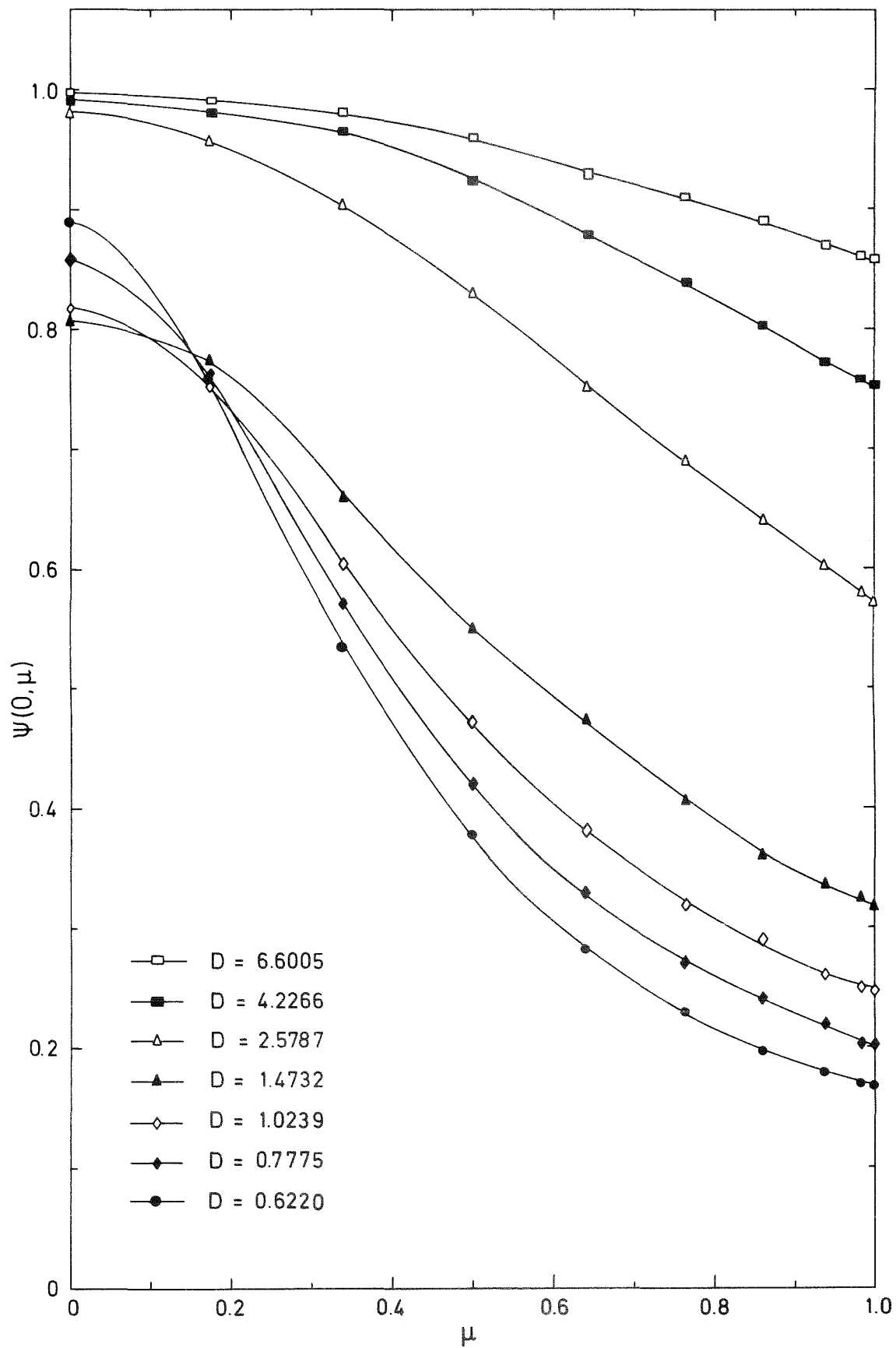


FIG. 2 : ANGULAR DISTRIBUTION AT THE CENTER

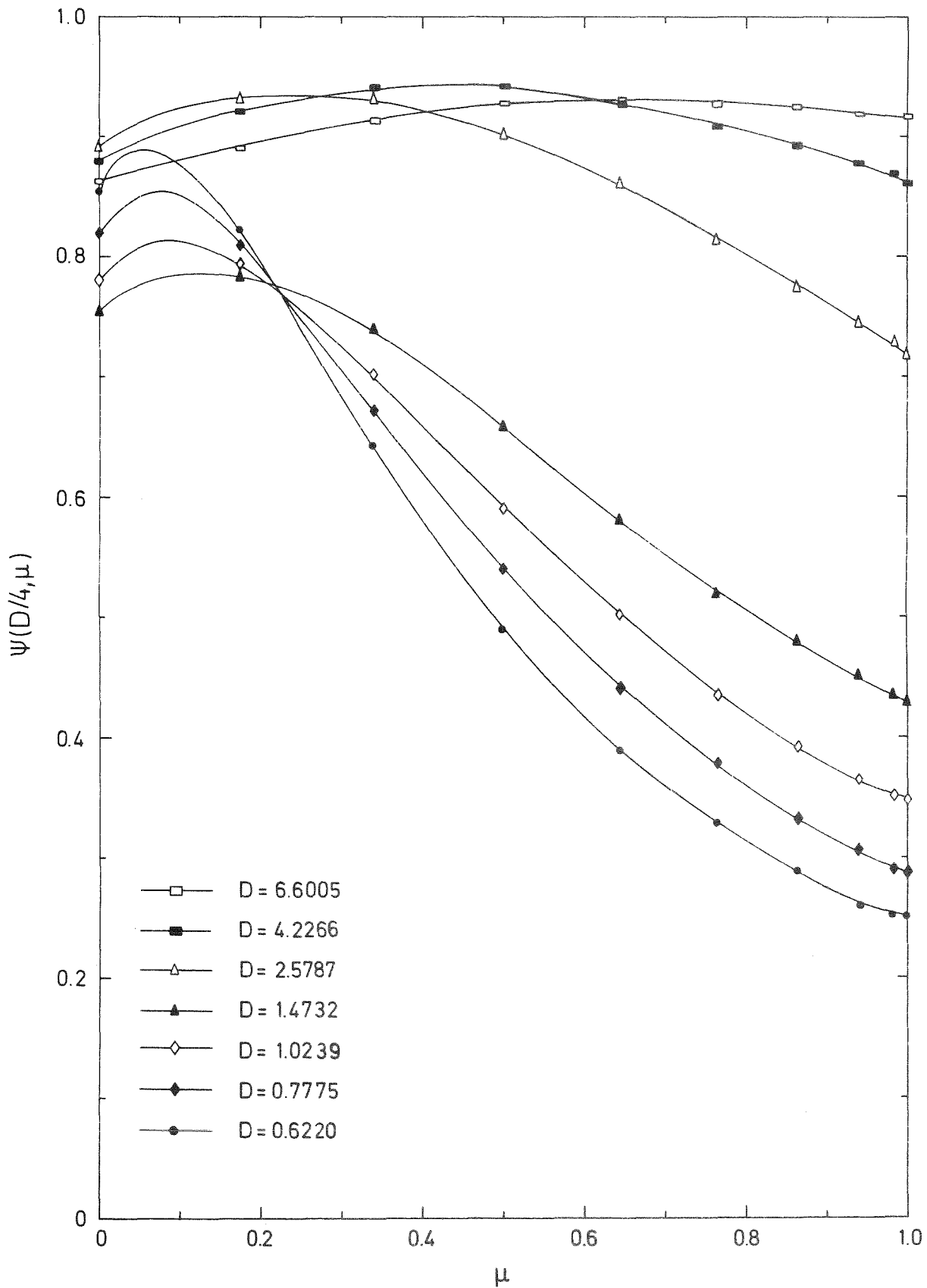


FIG. 3: ANGULAR DISTRIBUTION AT POSITION  $X = D/4$

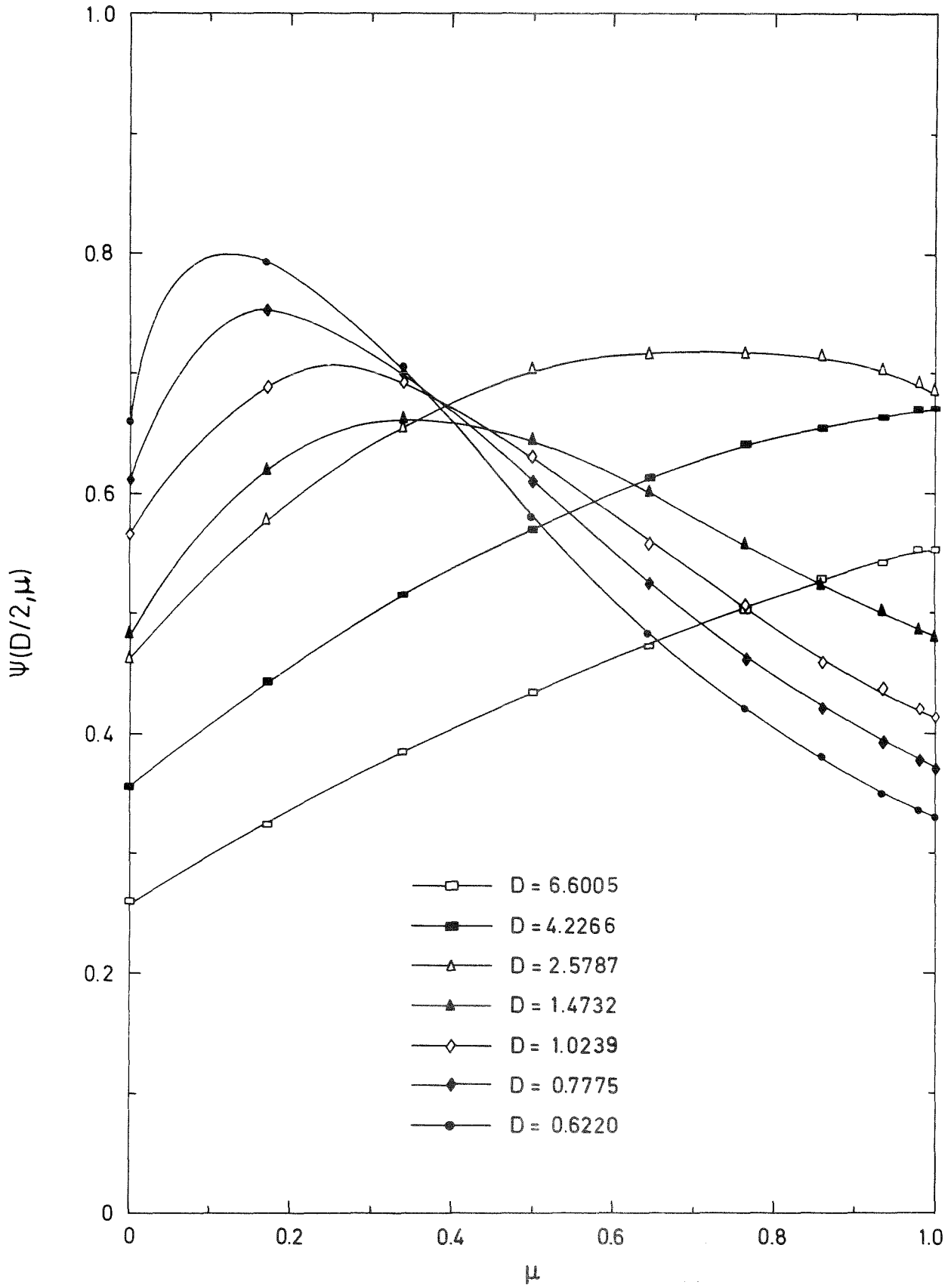


FIG.4: ANGULAR DISTRIBUTION AT THE BOUNDARY

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