

# Short-range repulsion and symmetry of two-body wave functions

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## Abstract

We calculate the stationary wave functions for two identical particles moving in a common one-dimensional potential well and interacting through a repulsive delta-potential. We show how a *symmetric* noninteracting state  $\psi_{m,n}^{(+)}$ , where the particles occupy the single-particle orbitals  $m$  and  $n$ , evolves as a function of the interaction strength. In the limit of very strong repulsion, the energy levels coincide with those for the adjacent *antisymmetric* states  $\psi_{m,n+1}^{(-)}$ . The spatial probability distributions also coincide revealing the apparent change of statistics. However, the relative momentum wave functions are different keeping memory of original statistics.

## I. INTRODUCTION

In many instructive quantum-mechanical problems, an actual short-range potential interaction can be replaced by the zero-range forces. In the one-dimensional case, this is equivalent to the use of the  $\delta$ -function potential [1]. In practice, the problem is reduced to the matching condition for the derivative of the wave function on different sides of the potential. In the three-dimensional problems with central symmetry, the presence of the short-range potential at the origin also can be taken into account by a boundary condition for the external wave function which was used in theory of the deuteron in the early age of nuclear physics [2]. Recently, a similar approach was suggested [3] for the three-body wave function in hyperspherical coordinates which describes “Borromean” nuclei like  ${}^6\text{He}$  and  ${}^{11}\text{Li}$ . The delta-function three-dimensional “pseudopotential” was widely used for low-energy neutron scattering by protons, nuclei and crystals [4]. A similar approach works as well in meson physics [5] and atomic physics [6].

The one-dimensional potential  $\delta(x)$  actually can mimic even long-range interactions. The ground state wave function and binding energy for this potential are the same as for the three-dimensional Coulomb problem, mainly due to the fact that the virial theorem takes the same form for both cases [7]. In this way one can treat [7–9] two-electron problems of He-like ion and  $\text{H}_2$  molecule with infinitely heavy nuclei substituting both nucleus-electron and electron-electron electrostatic potentials by the corresponding  $\delta$ -functions. The one-dimensional many-body problems with  $\delta$ -potentials between identical bosons or fermions can be solved exactly with the aid of the Bethe ansatz [10] being a testing ground of many approximate methods in statistical physics. In many realistic cases one has to deal with the combination of the short-range and long-range potentials. One of typical examples is given by the nuclear pairing problem. Two fermions moving in a common nuclear potential of radius  $R$ , interact through the residual forces which have a range of the order of an average internucleon distance  $r_0 \approx RA^{-1/3}$  where  $A \gg 1$  is the mass number of a nucleus.

As an illustration of phenomena emerging in such situations, we consider a simple one-

dimensional two-body model (or rather three-body problem with the infinitely heavy third body) where the external field is approximated by an infinite box while the residual interaction is modeled by the  $\delta$ -potential. The symmetry requirements for identical particles select the allowed two-body states even with no dynamic interaction. The repulsive  $\delta$ -interaction suppresses the relative wave function at short distances. This is seen already in perturbation theory [11]. We solve the problem exactly and show that the quenching of the wave function becomes complete in the strong repulsion limit so that the symmetric wave function has the same energy and spatial structure as the corresponding antisymmetric wave function without interaction. In some sense, the  $\delta$ -interaction mimics the change of the particle statistics.

## II. THE MODEL

The hamiltonian for two interacting identical particles can be written as

$$H = K_1 + K_2 + U_{12} + U_1 + U_2 \tag{1}$$

$$= \frac{p_1^2}{2m} + \frac{p_2^2}{2m} + V_0\delta(x_1 - x_2) + U(x_1) + U(x_2) \tag{2}$$

where the potential  $U(x)$  represents a well with the bottom value  $U(x) = 0$  for  $0 < x < a$  and infinitely high walls at  $x = 0$  and  $x = a$ . The boundary conditions imply the disappearance of the wave function for any of coordinates  $x_1$  or  $x_2$  on the walls and discontinuity of the derivative of the wave function along the line  $x_1 = x_2$ . Because of the presence of the single-particle field  $U(x)$ , the center-of-mass coordinate cannot be separated (a harmonic oscillator field is known [12] to be an exception) and we have to solve a genuine two-dimensional problem.

The unperturbed (no interaction,  $V_0 \rightarrow 0$ ) single-particle wave functions are ( $n = 1, 2, \dots$ )

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin(k_n x), \quad k_n = \frac{n\pi}{a}. \tag{3}$$

The normalized two-particle unperturbed wave functions with a certain spatial symmetry are

$$\Psi_{nn'}^{(\pm)}(x_1, x_2) = \frac{1}{\sqrt{2}} \left[ \psi_n(x_1)\psi_{n'}(x_2) \pm \psi_{n'}(x_1)\psi_n(x_2) \right] \quad (4)$$

if two different orbits are occupied,  $n \neq n'$ ; for the two particles occupying the same orbit  $n$ , only the symmetric function is possible,

$$\Psi_{nn}(x_1, x_2) = \psi_n(x_1)\psi_n(x_2). \quad (5)$$

Only symmetric functions  $\Psi_{nn}$  and  $\Psi_{nn'}^{(+)}$  are allowed for identical spinless particles or for fermions of spin  $1/2$  with total spin  $S = 0$  whereas the antisymmetric functions  $\Psi_{nn'}^{(-)}$  are the only permitted for fermion pairs with  $S = 1$ . For antisymmetric functions, the probability of the particle collision ( $x_1 = x_2$ ) vanishes because  $\Psi_{nn'}^{(-)}(x, x) = 0$ . Therefore the  $\delta$ -interaction is active in symmetric states only and we will limit our consideration by those states omitting below the superscript (+) if it does not lead to a confusion. The symmetry arguments stay valid for interacting identical particles as well, as long as they are indistinguishable in the hamiltonian (2).

The eigenfunctions  $\Psi(x, y)$  of the total hamiltonian satisfy the two-dimensional Schrödinger equation

$$(\nabla^2 + \epsilon)\Psi(x, y) = v\delta(x - y)\Psi(x, y) \quad (6)$$

where  $\nabla^2 = (\partial^2/\partial x^2) + (\partial^2/\partial y^2)$  is the two-dimensional Laplace operator,  $\epsilon = 2mE$  and  $v = 2mV_0$ , with the zero boundary conditions with respect to both coordinates on the square boundary,

$$\Psi(0, y) = \Psi(a, y) = \Psi(x, 0) = \Psi(x, a) = 0. \quad (7)$$

The difficulties arise because the natural variables separating the equation (6) correspond to the center of mass,  $(x + y)/2$ , and to relative motion,  $x - y$ , while the boundary conditions are simple in the original coordinates  $x$  and  $y$ . Since there is no exact analytical solution of the problem, we first reduce it to the form which is adapted in the best way to the numerical solution. This aim can be reached with the help of the Green's function method.

### III. GREEN'S FUNCTION

We define the Green's function  $G_0(x, y; x', y')$  of the unperturbed problem,  $v = 0$ , as the solution of the equation

$$(\nabla^2 + \epsilon)G_0(x, y, x', y') = \delta(x - x')\delta(y - y') \quad (8)$$

with zero boundary conditions with respect to both coordinates. Here the dependence of the Green's function on running energy  $\epsilon$  is not indicated explicitly.

Any stationary eigenfunction of the full problem with a potential  $v(x, y)$  satisfies the integral equation

$$\Psi(x, y) = \int dx' dy' G_0(x, y; x', y') v(x', y') \Psi(x', y') \quad (9)$$

along with the correct boundary conditions. For our case of the delta-potential, we obtain

$$\Psi(x, y) = v \int dx' G_0(x, y; x', x') \Psi(x', x'), \quad (10)$$

or, introducing the wave function on the diagonal line  $x = y$ ,

$$F(x) = \Psi(x, x), \quad (11)$$

we come to the one-dimensional Fredholm integral equation

$$F(x) = v \int_0^a dx' K(x, x') F(x') \quad (12)$$

with the symmetric integral kernel

$$K(x, x') = G_0(x, x; x', x'). \quad (13)$$

The nontrivial solutions of eq.(12) exist if the Fredholm determinant of the kernel  $K(x, x')$  vanishes which determines the eigenvalues  $\epsilon$ .

The standard procedure of calculating the Green's function uses its expansion into a double series of unperturbed solutions (3),

$$G_0(x, y; x', y') = \sum_{nn'} G^{(nn')}(x', y') \psi_n(x) \psi_{n'}(y). \quad (14)$$

Such a series of oscillating functions is not convenient for numerical calculations because of poor convergence. We prefer here another method which leads to a single series with much better convergence properties. First we seemingly violate the  $x \leftrightarrow y$  symmetry looking for the Green's function in the form

$$G_0(x, y; x', y') = \sum_n g_n(y; x', y') \psi_n(x) \quad (15)$$

where the coefficient functions  $g_n(y; x', y')$  also depend on  $\epsilon$ .

Due to the completeness of the set  $\{\psi_n(x)\}$ ,

$$\delta(x - x') = \sum_n \psi_n(x) \psi_n(x'), \quad (16)$$

we see that the  $x'$ -dependence of  $g_n(y; x', y')$  can be factorized,

$$g_n(y; x', y') = h_n(y; y') \psi_n(x'), \quad (17)$$

and the remaining function  $h_n(y; y')$  is Green's function of the one-dimensional equation

$$\left( \frac{\partial^2}{\partial y^2} - q_n^2 \right) h_n(y; y') = \delta(y - y'). \quad (18)$$

Here the notation

$$\epsilon - k_n^2 = -q_n^2 \quad (19)$$

is introduced for “energy” remaining for the  $y$  degree of freedom in eq.(18). For large  $n$ , the wave vector  $q_n$  is real, and instead of oscillating expressions we will deal with hyperbolic functions.

The solution of (18) is straightforward. All functions  $h_n$ ,  $g_n$  and  $G_0$  are continuous at coinciding arguments but their first derivatives have discontinuities. The solution satisfying the boundary conditions as well as the matching condition at  $y = y'$  can be written with the use of the step functions as

$$h_n(y; y') = -\frac{1}{q_n \sinh(q_n a)} \left[ \sinh(q_n y) \sinh(q_n(a - y')) \theta(y' - y) \right. \\ \left. + \sinh(q_n y') \sinh(q_n(a - y)) \theta(y - y') \right]. \quad (20)$$

This determines the coefficient functions  $g_n(y; x', y')$ , the full Green's function  $G_0(x, y; x', y')$  and the kernel (13) of the integral equation (12),

$$K(x, x') = \sum_n \psi_n(x) \psi_n(x') h_n(x, x'). \quad (21)$$

The result can be transformed to the regular form (14) of the double series,

$$K(x, x') = \sum_{mn} \frac{\psi_n(x) \psi_n(x') \psi_m(x) \psi_m(x')}{\epsilon - k_n^2 - k_m^2}, \quad (22)$$

with the aid of identities which can be found, for example, in [13].

For the numerical analysis, we will need the following integral,

$$I(x) = \int_0^a dx' K(x, x'). \quad (23)$$

The direct calculation using eqs. (21) and (21) gives

$$I(x) = \sum_n \frac{\psi_n^2(x)}{2(p^2 - k_n^2)} \quad (24)$$

where  $p = \sqrt{\epsilon/2}$ . The sum can be easily calculated comparing two equivalent representations of one-dimensional Green's function with the same zero boundary conditions, one as an expansion in terms of the wave functions  $\psi_n$ , and another one from the direct solution of the wave equation. The result, analogously to (21), is

$$\sum_n \frac{\psi_n(x) \psi_n(x')}{k_n^2 - p^2} = \frac{1}{p \sin(pa)} \left[ \sin(px) \sin(p(a - x')) \theta(x' - x) \right. \\ \left. + \sin(px') \sin(p(a - x)) \theta(x - x') \right]. \quad (25)$$

From here we find

$$I(x) = -\frac{\sin(px) \sin(p(a - x))}{2p \sin(pa)}. \quad (26)$$

#### IV. RESULTS AND DISCUSSION

By direct discretization we convert the integral eigenvalue problem (12), with the kernel defined by eqs. (21) and (21), into a finite ( $N \gg 1$ ) set of homogeneous linear algebraic equations. First, we rewrite the integral equation subtracting from the two sides the quantity  $vI(x)F(x)$  where the integral of the kernel  $I(x)$  was calculated in (26). This gives

$$F(x)[1 - vI(x)] - v \int_0^a K(x, x')[F(x') - F(x)] = 0 \quad (27)$$

where now there is no diagonal singularity at  $x = x'$  in the integral term.

The decomposition of the physical domain  $0 \leq x \leq a$  into  $N$  small intervals  $\Delta_j = x_j - x_{j-1}$  gives the discretized set of equations for  $F_i \equiv F(x_i)$ ,  $i = 1, \dots, N$ ,

$$(1 - vI_i)F_i - v \sum_{j=1}^N \Delta_j K_{ij}(F_j - F_i) = 0, \quad (28)$$

where  $I_i \equiv I(x_i)$  and  $K_{ij} \equiv K(x_i, x_j)$ . Practically, the integration with Gaussian weights [14] ensures better convergence. Here we do not go into details of the numerical procedure.

The eigenvalues  $\epsilon_{nn'}(v)$  of the system are the roots of the determinant of the set (28). They can be found as functions of the interaction strength  $v$  starting with the independent particle case of  $v = 0$ . The eigenvalues are labeled by pairs of integers  $(n, n')$  which are identified by the continuous evolution of energy as a function of  $v$ , with

$$\epsilon_{nm}(v = 0) = k_n^2 + k_m^2 \quad (29)$$

as an initial value. The solution of the set (28) for a given eigenvalue  $\epsilon_{nn'}$  determines the wave functions  $F_i$  at coincided arguments, and then, via eq.(10), the total wave function. The wave functions start from the unperturbed symmetric solutions  $\Psi_{nn'}$ , eq.(4), for  $n \neq n'$ , and from  $\Psi_{nn}$ , eq.(5), at  $n' = n$ .

We consider here only the repulsive case,  $v \geq 0$ , and the symmetric solutions  $\Psi(x, y) = \Psi(y, x)$  because the antisymmetric solutions do not feel the presence of the interaction. The evolution of the lowest eigenvalues corresponding to the symmetric solutions is shown in



Fig. 1. All eigenvalues behave qualitatively the same changing between two values which belong to the unperturbed spectrum. We consider the energy terms  $\epsilon_{nn'}(v)$ , assuming, with no restriction of generality,  $n' \geq n$ . The terms start at the unperturbed values (29), monotonically increase and saturate at the closest unperturbed values  $\epsilon_{n,n'+1}$ . The ending point always corresponds to a level which is still unoccupied by the previous ascending levels so that there is no level crossings. The higher  $n$  and  $n'$  the larger is the value of the interaction strength which corresponds to the saturation of the energy term.

The regularity of the pattern can be understood as follows. Consider for example the ground state  $n = 1, n' = 1$ . Its wave function

$$\Psi_{11} = \frac{2}{a} \sin \frac{\pi x}{a} \sin \frac{\pi y}{a} \quad (30)$$

has no nodes inside the box  $0 < x, y < a$ . The repulsive short range force suppresses the probability for the particles to be found at small  $r = x - y$ . The corresponding wave function for the interacting system is still continuous and positive everywhere. But this function acquires the discontinuity of the derivative being proportional to  $|r|$  near the diagonal line  $r = 0$ . In the limit of very strong repulsion  $v$ , the suppression becomes absolute, and the wave function goes to zero on the diagonal (from above). Fig. 2 shows the spatial image and the contour map of the probabilities  $|\Psi|^2$  for the ground state with no interaction, part (a), at the intermediate interaction strength, part (b), and in the limit of strong repulsion, part (c).

It is easy to realize that the limiting function at very strong repulsion should coincide, up to mirror reflection, with the lowest *antisymmetric* solution

$$\Psi_{12}^{(-)} = \frac{\sqrt{2}}{a} \left( \sin \frac{\pi x}{a} \sin \frac{2\pi y}{a} - \sin \frac{2\pi x}{a} \sin \frac{\pi y}{a} \right). \quad (31)$$

Indeed, this function vanishes, apart from the boundaries of the box, on the diagonal  $r = 0$  where it remains continuous and changes its sign from negative in the triangle  $-a \leq r < 0$  to positive in the triangle  $0 < r \leq a$ . Therefore this function, being nodeless inside each triangle, represents the lowest energy solution of the equation with zero conditions on the

triangle boundaries. But the same is valid for the *symmetric* function of the preceding paragraph. The only difference is related to the fact that the continuation of the symmetric function from the first triangle to the second one proceeds here with mirror reflection which makes the function positive in both disconnected parts. Since, in the strong repulsion limit, the symmetric wave function vanishes on the diagonal, the energy eigenvalue and the probability distribution should be identical with those for the lowest unperturbed antisymmetric solution.

Similar consideration holds for higher states. There is a one-to-one correspondence between the starting symmetric solutions at  $v = 0$ ,  $\Psi_{nn'}^{(+)}(0)$ ,  $n' \geq n$ , and their descendants at  $v = \infty$ ,  $\Psi_{n,n'}^{(+)}(\infty)$ , which have the same energy and the same probability distribution as the antisymmetric solutions  $\Psi_{n,n'+1}^{(-)}(0)$  for  $v = 0$ . Fig. 3 shows the generic behavior at the diagonal  $r = 0$  of an initial symmetric function as compared to its antisymmetric counterpart in the vicinity of  $r = 0$ . Fig. 4 shows several contour maps for such pairs.

We came to an interesting conclusion. A strong repulsion at short distances makes the two-particle spatially symmetric wave function look as belonging to the opposite symmetry, i.e. mimics the change of the particle statistics. This is seen both in the spectrum of allowed energy levels and in the relative coordinate probability distribution. The idea to include the Pauli antisymmetrization effects via short-range repulsion in a trial many-body wave function is quite natural and it was used repeatedly in nuclear physics. Our simple delta-function model partially justifies this procedure. However it is necessary to have in mind that the wave function, in contrast to the spatial probability distribution, remembers its exact symmetry. Therefore the relative motion momentum distribution for the exact symmetric solution is different from that for the corresponding antisymmetric noninteracting solution.

The relative momentum wave function for the zero center-of-mass momentum ( $p_x = -p_y = p$ ) is given by the Fourier transform of the coordinate wave function  $\Psi(x, y)$ ,

$$\phi(p) = \int dx dy e^{ip(x-y)\pi/L} \Psi(x, y). \quad (32)$$

This function is real for symmetric states and pure imaginary for antisymmetric states. The

relative momentum wave functions for the symmetric state (1,1) in the limit of  $v \rightarrow \infty$  and for the corresponding antisymmetric state (1,2) at  $v = 0$  are shown in Fig. 5, (a) and (b), respectively. Their analytical expressions are

$$\phi^{(+)}(p) = \text{const} \frac{(2p^2 - 5)/3 - \cos(\pi p)}{(p^2 - 4)(p^2 - 1)} \quad (33)$$

and

$$-i\phi^{(-)}(p) = \text{const} \frac{\sin(\pi p)}{(p^2 - 4)(p^2 - 1)}. \quad (34)$$

The kink at the coinciding values of the coordinates is responsible for the appearance of the nonoscillating power law tail,  $\propto p^{-2}$ , in the symmetric wave function (33) at large relative momenta. The symmetric solution has also a nonzero limit at zero relative momentum while the zero Fourier component of the antisymmetric function vanishes.

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## Figure captions

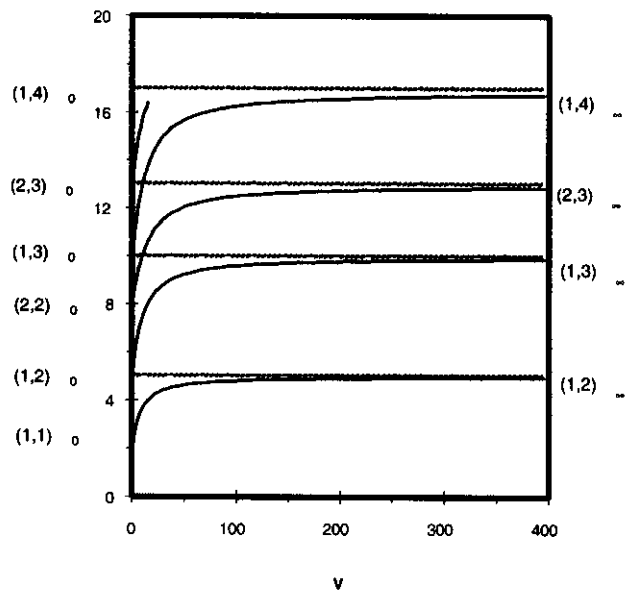
**Figure 1.** Energy spectrum of symmetric states of the two-particle system in a box with the delta-function repulsion as a function of the interaction strength  $v$ . The levels are labeled by the quantum numbers  $(n, n')$ ,  $n' \geq n$ , of the occupied orbitals in the case of no interaction,  $v = 0$ . In the limit of  $v \rightarrow \infty$ , the terms come to the energies of unperturbed antisymmetric states  $(n, n' + 1)$ .

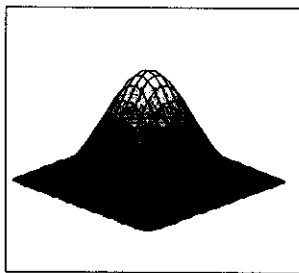
**Figure 2.** The spatial probability distribution, left column, and the corresponding contour maps, right column, for the lowest symmetric state ( $n = n' = 1$  at  $v = 0$ ) and for different values of the interaction strength,  $v = 0$ , part (a);  $v = 5$ , part (b), and  $v \rightarrow \infty$ , part (c). The development of a deep valley at  $r = x - y = 0$  is clearly seen.

**Figure 3.** Comparison of the behavior of the symmetric wave function  $\Psi_{nn'}^{(+)}$  along the diagonal  $x = y$ , solid line, and the antisymmetric function  $\Psi_{n,n'+1}^{(-)}$  in the vicinity of  $x = y$ , dashed line.

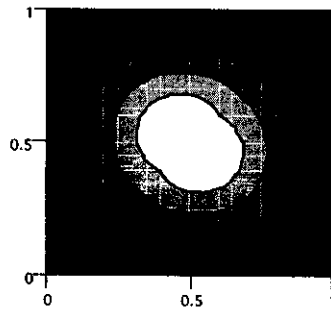
**Figure 4.** Contour maps of the spatial probability distribution for the unperturbed states  $(n, n')_0 = \Psi_{nn'}^{(+)}$  at  $v = 0$ , left column, and for their counterparts  $(n, n')_\infty = \Psi_{n,n'+1}^{(-)}$  at  $v \rightarrow \infty$  in the strong repulsion limit, right column. The states shown are  $(2, 2)_0 \rightarrow (2, 3)_\infty$ , part (a),  $(2, 3)_0 \rightarrow (2, 4)_\infty$ , part (b), and  $(2, 6)_0 \rightarrow (2, 7)_\infty$ , part (c).

**Figure 5.** The wave functions  $\phi(p)$  in the relative momentum representation, for the symmetric state  $\Psi_{11}^{(+)}(v \rightarrow \infty)$ , part (a), and for the antisymmetric state  $\Psi_{12}^{(-)}(v = 0)$  of the same energy, part (b).



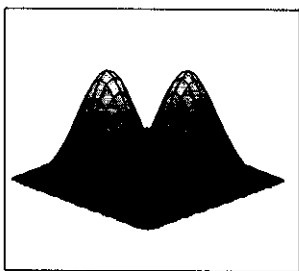


M0

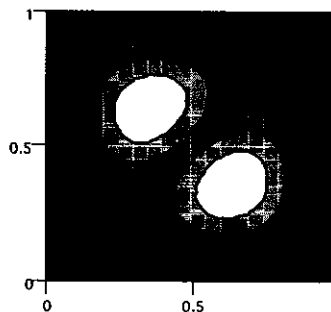


M1

(a)  $v = 0$

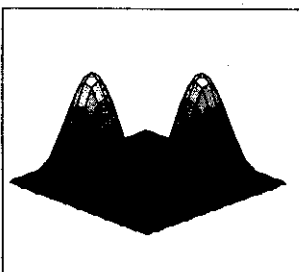


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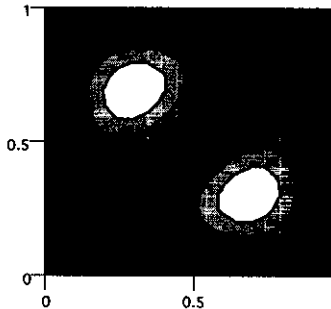


M5

(b)  $v = 5$

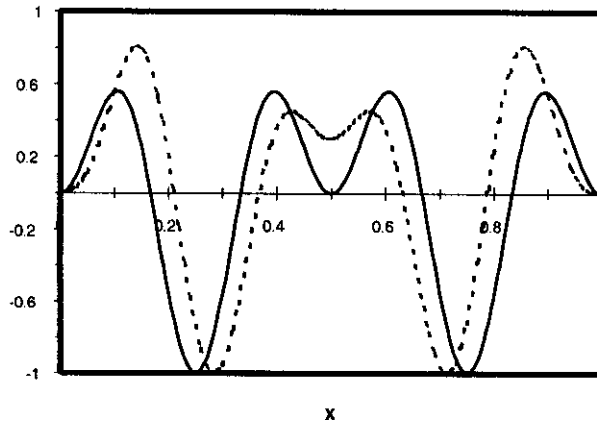


M1

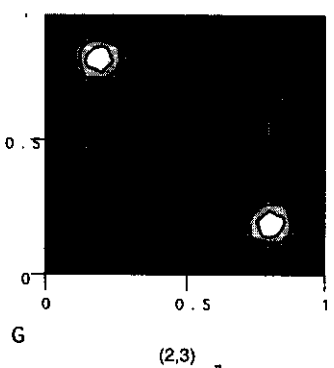
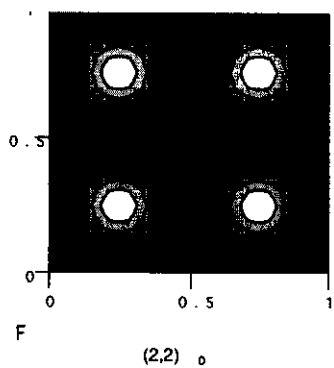


M1

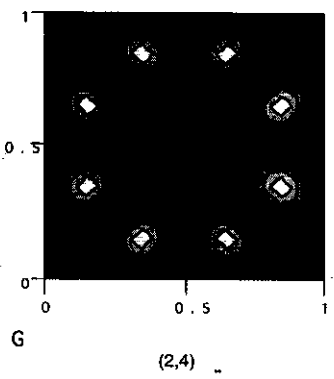
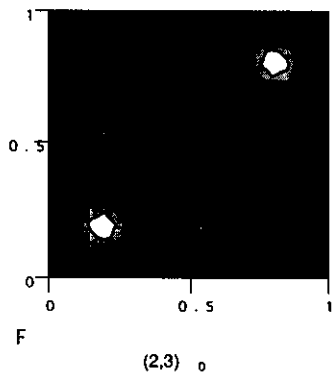
(c)  $v \rightarrow \infty$



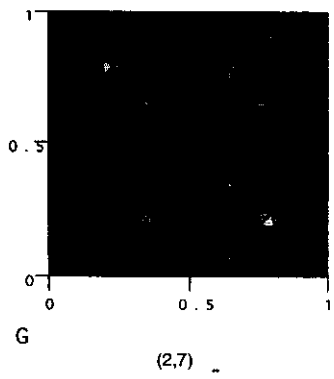
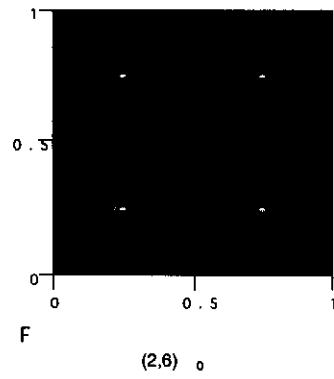




(a)



(b)



(c)