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# Magic angular momenta of a quantum dot under a strong magnetic field: the effect of a Coulomb impurity

K S Chan<sup>1</sup> and W Y Ruan<sup>2</sup>

<sup>1</sup> Department of Physics and Materials Science, City University of Hong Kong, Hong Kong, People's Republic of China

<sup>2</sup> Department of Applied Physics, South China University of Technology, Guangzhou 510641, People's Republic of China

E-mail: phwyruan@scut.edu.cn (W Y Ruan)

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## Abstract

The ground-state energies of several interacting electrons ( $N \leq 12$ ) confined in a parabolic quantum dot with an impurity ion at the centre are obtained by numerical diagonalizations. Series of magic values of angular momentum are determined. The rules for identifying the magic numbers are established.

One of the most fascinating phenomena in the study of few-electron quantum dots is the existence of magic values of the total angular momentum associated with particularly stable ground states [1]. As regards the interpretation of the origin of magic numbers and their rules, three radically different theoretical models have been proposed: the composite-fermion model [2], the geometrical configuration model based on symmetry [3–7], and the  $\ell$ -configuration model [8]. In the composite-fermion approach, an even number of magnetic flux quanta are attached to an electron. The interacting electrons occupying the lowest Landau level are then transformed into non-interacting composite fermions occupying several Landau levels. Jain *et al* argued that all possible magic numbers are states where the composite fermions can compactly fill each Landau level from the lowest possible angular momentum [2]. One principal advantage of the composite-fermion approach is that it enables one, in the majority of cases, to directly construct the ground-state wavefunctions with good accuracy, but it does reject some well-known magic numbers (e.g.,  $L = 40$  and  $L = 50$  for  $N = 6$ ) [9]. In the geometrical configuration model, it is assumed that the pairwise Coulomb repulsion compels  $N$  electrons in a parabolic potential to form a Wigner molecular polygon with  $N$ -fold symmetry for  $N \leq 5$  or  $(N - 1)$ -fold symmetry for  $N = 6, 7$  (i.e., there is one electron at the centre of the polygon). From a consideration of rotational and permutation symmetries, the polygon configurations are prohibited unless the total angular momentum takes the magic values. It turns out that the magic numbers predicted by the geometrical configuration model are in full agreement with those obtained by exact numerical diagonalizations when  $N \leq 6$ . But the model is only partly successful when  $N = 7$  since it does not predict the magic number

series  $L = 36, 41, 46, \dots$  [2, 5]. The geometrical configuration model does not apply to systems with  $N > 7$  since the lowest-energy configuration of the system is then a multi-shell structure  $(n_1, n_2, n_3, \dots, n_k)$ , where  $n_1$  is the number of electrons in the innermost shell,  $n_2$  is the number of electrons in the second shell, etc. Note that

$$\sum_j n_j = N.$$

A multi-shell Wigner molecule does not have any rotational symmetry as a regular polygon, unless, as on some rare occasions,  $n_1, n_2, n_3, \dots$ , and  $n_k$  happen to be commensurable. However, numerical calculations show that magic numbers continue to exist in systems with any number of particles.

The  $\ell$ -configuration model proposed in reference [8] is based on the observation of a short-range attraction among electrons rotating in different orbits in the lowest Landau level. The short-range attraction results from the antisymmetrization and is thus a many-body force in nature. Due to this short-range attraction, electrons tend to fill some adjacent orbits to form several compact bunches. The numbers of electrons in the bunches are determined by the saturation of the short-range attraction. Since in the large- $L$  limit the electrons tend to form a multi-shell Wigner molecule, the energetically most favourable bunch structure should coincide with the multi-shell structure having the globally minimal energy, while the energetically less favourable bunch structures should coincide with the multi-shell structures having the locally minimal energies. In addition, since the energy differences between the global minimum and the local minima decrease with the increase of  $N$ , several bunch structures become comparable in reducing the interaction energy when  $N$  is large. In this case several series of magic numbers can appear. As we have shown in reference [8], the  $\ell$ -configuration model can explain all magic numbers for both few and many electrons.

To our knowledge, all of the work on the magic numbers to date has been limited to impurity-free dots. The doping of a homogeneous host matrix with acceptor and donor impurities has been traditionally one of the central subjects in semiconductor physics, both because of its intrinsic basic interest and because of its technological implications. The consideration of impurity effects in quantum dots is not new. For example, Halonen *et al* have studied the effects of off-centre Gaussian-type repulsive impurities on the energy levels of a parabolic dot [10, 11], where the orbital angular momentum is no longer a good quantum number. In some other works [12, 13], the eigenstates of a Coulomb impurity in spherical dots have been discussed using various methods. In this paper, we study the magic numbers of quantum dots with impurities and establish the rules with the aid of the  $\ell$ -configuration model. This allows us to further test the validity of the model.

Consider the motion of electrons confined in a disc-like parabolic dot subjected to a vertical magnetic field. Here we assume that the magnetic field is so strong that only the lowest Landau level is occupied. The effect of higher Landau levels can be included simply by using the perturbation theory as in reference [8]. The single-particle eigenenergies and eigenfunctions for the lowest Landau level are [1]

$$\epsilon_l = (l+1)\hbar\omega - \frac{l}{2}\hbar\omega_c \quad (l = 0, 1, 2, \dots) \quad (1)$$

and

$$|l\rangle = [2^l l! a^{2(l+1)}]^{-1/2} r^l e^{-r^2/(4a^2)} \frac{e^{il\varphi}}{\sqrt{2\pi}} \quad (l = 0, 1, 2, \dots). \quad (2)$$

The meanings of the symbols above are as follows:  $l\hbar$  is the angular momentum,  $\omega_c$  is the magnetic cyclotron frequency,  $\omega$  is the effective oscillator frequency, and  $a$  is the effective oscillator length.

In the case of  $N$  electrons, we introduce the hyperspherical coordinates to describe the motion of electrons:

$$\begin{aligned}
 r_1 &= R \cos \alpha_1 \\
 r_2 &= R \sin \alpha_1 \cos \alpha_2 \\
 r_3 &= R \sin \alpha_1 \sin \alpha_2 \cos \alpha_3 \\
 &\vdots \\
 r_{N-1} &= R \sin \alpha_1 \sin \alpha_2 \cdots \sin \alpha_{N-2} \cos \alpha_{N-1} \\
 r_N &= R \sin \alpha_1 \sin \alpha_2 \cdots \sin \alpha_{N-2} \sin \alpha_{N-1}
 \end{aligned} \tag{3}$$

where the hyperradius  $R = (r_1^2 + r_2^2 + \cdots + r_N^2)^{1/2}$  is completely symmetric with respect to particle exchange, and measures the size of the system.  $\alpha_1, \dots, \alpha_{N-1}$  are  $(N-1)$  hyperangles. With hyperspherical coordinates, the antisymmetrized wavefunctions of  $N$  non-interacting electrons occupying the  $l_1, l_2, \dots, l_N$  orbits separate into the product of a radial and an angular function:

$$|l_1, l_2, \dots, l_N\rangle = F_L(R) Y_{l_1 \dots l_N}(\Omega) \tag{4}$$

with

$$F_L(R) = [2^{L+N-1} (L+N-1)! a^{2(L+N)}]^{-1/2} R^L e^{-R^2/(4a^2)} \tag{5}$$

$$Y_{l_1 \dots l_N}(\Omega) = \text{Det} \left\{ \frac{\tilde{r}_1^{l_1} e^{il_1 \varphi_1}}{\sqrt{2\pi(2l_1)!}}, \frac{\tilde{r}_2^{l_2} e^{il_2 \varphi_2}}{\sqrt{2\pi(2l_2)!}}, \dots, \frac{\tilde{r}_N^{l_N} e^{il_N \varphi_N}}{\sqrt{2\pi(2l_N)!}} \right\} \tag{6}$$

where  $\Omega$  denotes collectively  $(2N-1)$  angular variables  $\alpha_1, \dots, \alpha_{N-1}$ , and  $\varphi_1, \dots, \varphi_N$ ,  $\tilde{r}_j = r_j/R$ ;  $\text{Det}\{\dots\}$  represents a Slater determinant.

The Hamiltonian for  $N$  interacting electrons in the lowest Landau level of a parabolic dot with an impurity ion at the centre can be written as

$$\hat{H} = \sum_l \epsilon_l \hat{b}_l^\dagger \hat{b}_l + \frac{e^2}{4\pi\epsilon} \frac{U(\Omega)}{R} \tag{7}$$

with

$$U(\Omega) = R \left[ \eta \sum_{j=1}^N \frac{1}{r_j} + \sum_{j>k}^N \frac{1}{r_{jk}} \right] \tag{8}$$

where  $\hat{b}_l^\dagger$  ( $\hat{b}_l$ ) are the creation (annihilation) operators.  $\eta = 1$  and  $-1$  for acceptor and donor ions respectively. The single-particle angular momentum is no longer conserved due to the electron–electron interaction. But the total angular momentum  $L$  continues to be a good quantum number even in the presence of a centred impurity ion. For a prescribed  $L$ , we expand the trial wavefunction  $\Psi_L(R, \Omega)$  in terms of the basis set  $\{|l_1, l_2, \dots, l_N\rangle; L = l_1 + l_2 + \cdots + l_N\}$ :

$$\Psi_L(R, \Omega) = \sum_{l_1 \dots l_N} c_{l_1 \dots l_N} |l_1, l_2, \dots, l_N\rangle = F_L(R) \sum_{l_1 \dots l_N} c_{l_1 \dots l_N} Y_{l_1 \dots l_N}(\Omega) \tag{9}$$

where  $c_{l_1 \dots l_N}$  are the expansion coefficients. The Hamiltonian is diagonalized numerically to obtain the eigenfunctions and eigenenergies. The  $k$ th eigenfunction and the corresponding eigenenergy can be written as

$$\Psi_{kL}(R, \Omega) = F_L(R) \Phi_{kL}(\Omega) \tag{10}$$

$$E_k(L) = (L+N)\omega\hbar - \frac{L}{2}\omega_c\hbar + \frac{e^2}{4\pi\epsilon\beta(L)}\lambda_k(L) \tag{11}$$

with

$$\beta(L) = \frac{1}{\langle F_L | 1/R | F_L \rangle} = \frac{a[2(L+N-1)]!!}{[2(L+N-1)-1]!!} \left(\frac{2}{\pi}\right)^{1/2} \approx \sqrt{(L+N)a} \quad (12)$$

$$\lambda_k(L) = \int \Phi_{kL}(\Omega)^* U(\Omega) \Phi_{kL}(\Omega) d\Omega \quad (k = 1, 2, \dots) \quad (13)$$

where  $\beta(L)$  gives the average size of the system. It is easy to see from equation (12) that  $\beta(L)$  increases monotonically with  $L$ .  $\lambda_k(L)$ , called the correlation factor, is the average interaction energy on the  $R = 1$  hyperspherical surface. It contains information about electron correlations. The factorization of the wavefunction into a radial function and an angular function is a unique characteristic of the lowest Landau level. Here we would like to point out that while the eigenenergies depend on  $\omega$ ,  $\omega_c$ , and  $a$ , the  $\lambda_k(L)$  are independent of all of these dynamical parameters, exhibiting the universality of electron correlation in the lowest Landau level. With the method described above, we have computed the eigenenergies for  $N = 3-12$ . In what follows, since we are focusing our attention on the magic numbers, only the lowest states are considered.

For dots with a centred acceptor ion, the results are presented in the left columns of figure 1, where  $\lambda_1(L)$ , the correlation factors of the lowest states, are presented as functions of  $L$ . In each graph, the  $\lambda_1(L)$  curve shows a number of sharp downward cusps. The corresponding  $L$ -values are the magic numbers. Since these states have a particularly low energy in comparison with their neighbours, they can form the ground state for a wide range of  $B$ -field strengths. Comparing the results for impurity-free dots in references [5, 8] and the results here, we find that the magic numbers in the two cases are identical for  $N \leq 5$ , but are quite different for  $N \geq 6$ . As we have demonstrated in references [5, 8], the electrons in an impurity-free dot tend to form a single compact bunch if  $N \leq 5$  since the structure associated with the globally minimal energy is a  $N$ -sided polygon, but two compact bunches of  $(n_1, N - n_1)$  if  $6 \leq N \leq 15$  since the structure associated with the globally minimal energy is a two-shell structure. Here  $n_1 = 1$  for  $N = 6$  and 7,  $n_1 = 2$  for  $N = 8, 9$ , and 10,  $n_1 = 3$  for  $N = 11$  and 12, etc. The electrons in the inner bunch occupy the innermost orbits  $l = 0, 1, \dots, n_1 - 1$ . In the presence of an acceptor ion, the repulsive electron-impurity interaction makes the existence of a few electrons in the innermost orbits energetically very unfavourable. Hence it is reasonable to expect that the inner electrons will leave the inner orbits and join the outer electrons to form a bigger compact bunch, resulting in the changes of magic number for  $N \geq 6$ . The necessary condition for  $N$  electrons to form a compact bunch is

$$L = j + (j+1) + (j+2) + \dots + (j+N-1) = N(N-1)/2 + Nj \quad (j = 0, 1, 2, \dots). \quad (14)$$

It is easy to check that equation (14) gives all of the magic numbers for acceptor-doped dots shown in the left columns of figure 1, justifying the supposition above. A more direct justification is gained by comparing the weights of different  $\ell$ -configurations in an eigenstate, i.e.,  $|c_{l_1 l_2 \dots l_N}|^2$ . We find that in the lowest state for an  $L$  fulfilling equation (14) the  $|c_{l_1 l_2 \dots l_N}|^2$  associated with the compact filling is significantly larger than the other components, while in the lowest state for an  $L$  not fulfilling equation (14) the compact filling is inaccessible; there are several components that have about the same magnitudes. In both cases the components associated with a dispersive filling of the electrons in different orbits are always exceedingly small.

In the right columns of figure 1 are the results for donor-doped dots. For  $N \leq 5$ , there are no evident downward cusps in the  $\lambda_1(L)$  curves. In the case of  $N = 3$ , the attractive electron-impurity interaction is strong enough to hold the electrons in orbits  $l = 0, 1, 2$  such

that a ground state with  $L = 3$  is always maintained as the magnetic field increases. Since the magnetic length  $a$  decreases with increasing field strength [2], the system will shrink continuously. In the case of  $N = 4$ , three electrons are held in the  $l = 0, 1, 2$  orbits and the fourth electron jumps successively to orbits with higher  $l$  as the magnetic field increases. Consequently, the total angular momentum of the ground state increases successively. In the case of  $N = 5$ , the  $\ell$ -configuration in the ground state is ambiguous. The total angular momentum of the ground state also increases successively for  $N = 4$  except at some  $L$ -values where  $\lambda_1(L)$  shows an upward cusp. The downward cusps in  $\lambda_1(L)$  start to appear for  $N \geq 6$ . In the case of  $N = 6$ , the magic numbers can be classified into two sequences:  $L_{(1,5)} = 15, 20, 25, 30, 35, \dots$  and  $L_{(2,4)} = 15, (19), 23, 27, (31), (35), \dots$ . In a state in a sequence  $L_{(1,5)}$  the dominant  $\ell$ -configuration is as follows: one electron fills the  $l = 0$  orbit and the other five fill some outer orbits compactly; the total angular momentum is given by

$$L_{(1,5)} = 0 + j + (j + 1) + (j + 2) + (j + 3) + (j + 4) = 10 + 5j \quad (j = 1, 2, 3, \dots). \quad (15)$$

In a state in a sequence  $L_{(2,4)}$ , two electrons fill the inner orbits  $l = 0, 1$  and the other four fill some outer orbits compactly; the state has a total angular momentum given by

$$L_{(2,4)} = 0 + j + j + (j + 1) + (j + 2) + (j + 3) = 7 + 4j \quad (j = 2, 3, 4, \dots). \quad (16)$$

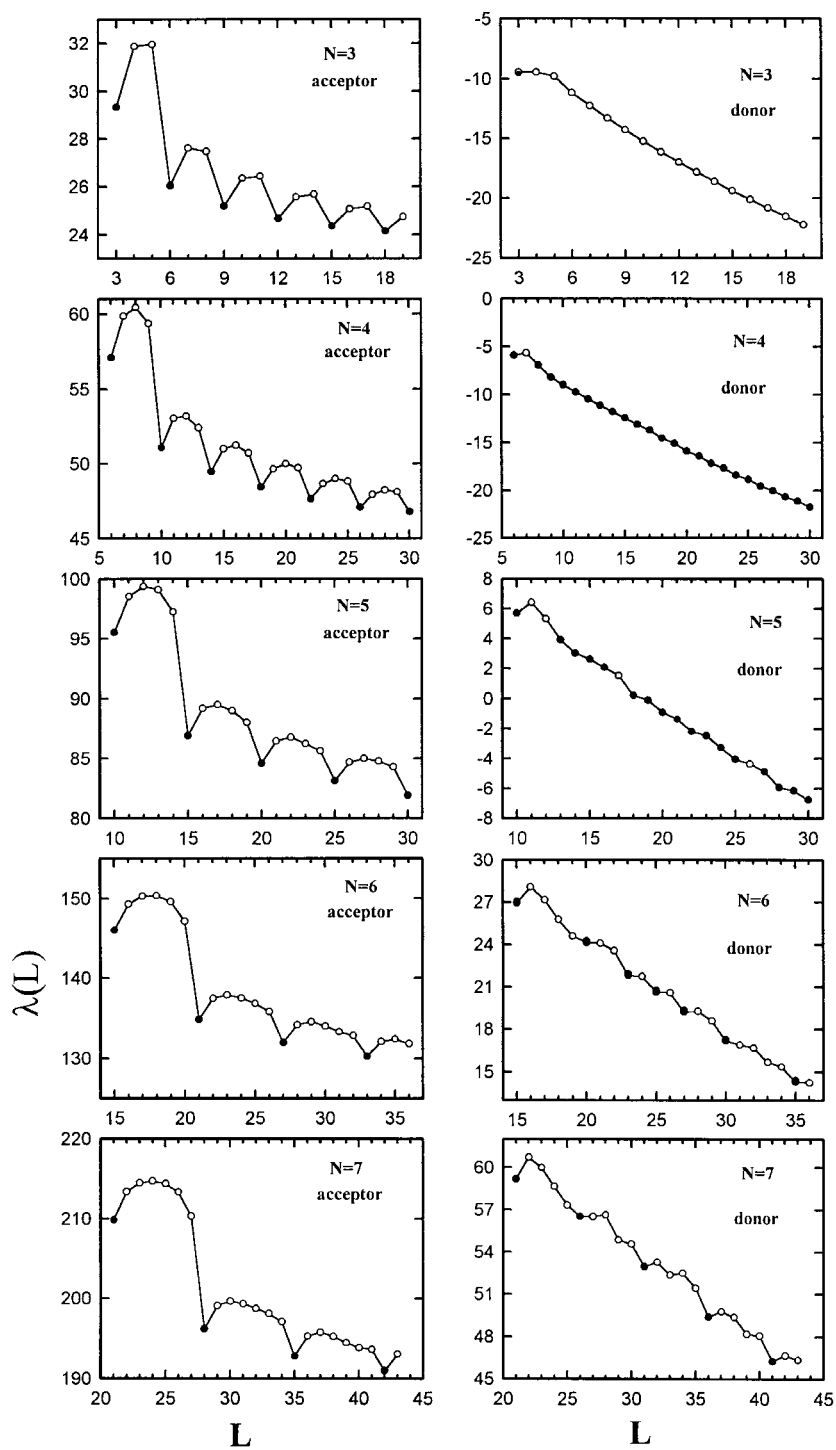
The two sequences overlap at  $L = 15$  and  $35$ , etc.  $L = 19$  and  $31$  are in the sequence  $L_{(2,4)}$ . They do not show a significant downward cusp since they are respectively adjacent to  $L = 20$  and  $30$  in the sequence  $L_{(1,5)}$ . Structurally, it is impossible for two adjacent values of  $L$  to show cusps.

As a generalization of equations (15) and (16), consider a state of  $N$  electrons,  $n$  of them filling the inner orbits  $l = 0, 1, 2, \dots, n - 1$  and the other  $(N - n)$  compactly filling some outer orbits  $l = j, (j + 1), \dots, (N - n + j - 1)$ ; the state will have a total angular momentum

$$L_{(n, N-n)} = [n(n - 1) + (N - n - 1)(N - n)]/2 + (N - n)j \quad (j = n, n + 1, n + 2, \dots). \quad (17)$$

With the aid of equation (17), it is easy to classify the magic numbers for other values of  $N$  into sequences. In the case of  $N = 7$ , the magic numbers  $L = 21, 26, 31, 36, 41, \dots$  form a sequence  $L_{(2,5)}$ . In the case of  $N = 8$ , the magic numbers  $L = 28, 34, 40, 46, \dots$  form a sequence  $L_{(2,6)}$ ; the magic numbers,  $L = 38, 43, 48, \dots$  form a sequence  $L_{(3,5)}$ . In the case of  $N = 9$ , the magic numbers  $L = 36, 42, 48, 54, 60, 66, \dots$  form a sequence  $L_{(3,6)}$ . In the case of  $N = 10$ , the magic numbers  $L = 45, 52, 59, 66, 73, \dots$  form a sequence  $L_{(3,7)}$ ; the magic numbers  $L = 57, 63, 69, 75, \dots$  form a sequence  $L_{(4,6)}$ . In the case of  $N = 11$ , the magic numbers  $L = 55, 62, 69, 76, 83, 90, \dots$  form a sequence  $L_{(4,7)}$ ; the magic numbers  $L = 67, 73, 79, 85, \dots$  form a sequence  $L_{(5,6)}$ ; the magic numbers  $L = 71, 79, 87, \dots$  form a sequence  $L_{(3,8)}$ . In the case of  $N = 12$ , the magic numbers  $L = 66, 74, 82, 90, 98, \dots$  form a sequence  $L_{(4,8)}$ ; the magic numbers  $L = 80, 87, 94, 101, \dots$  form a sequence  $L_{(5,7)}$ .

To summarize, we have calculated the ground-state energies of several interacting electrons occupying the lowest Landau level of a parabolic dot with centred Coulomb impurities. The hyperspherical coordinates have been introduced to separate each of the interaction energies into a product of a size factor and a correlation factor, the latter clearly exhibiting the existence of magic values of the total angular momentum  $L$ . In the presence of an acceptor ion, the regularity of the magic numbers is easily seen, while in the presence of a donor ion, the regularity appears complicated. Keeping in mind that electrons tend to form compact bunches, we have successfully classified all of the magic numbers into simple sequences.



**Figure 1.** The correlation factors in the lowest states,  $\lambda_1(L)$ , are presented as functions of  $L$  for  $N = 3-12$ . Filled circles denote states that can form the ground state in a varying magnetic field.

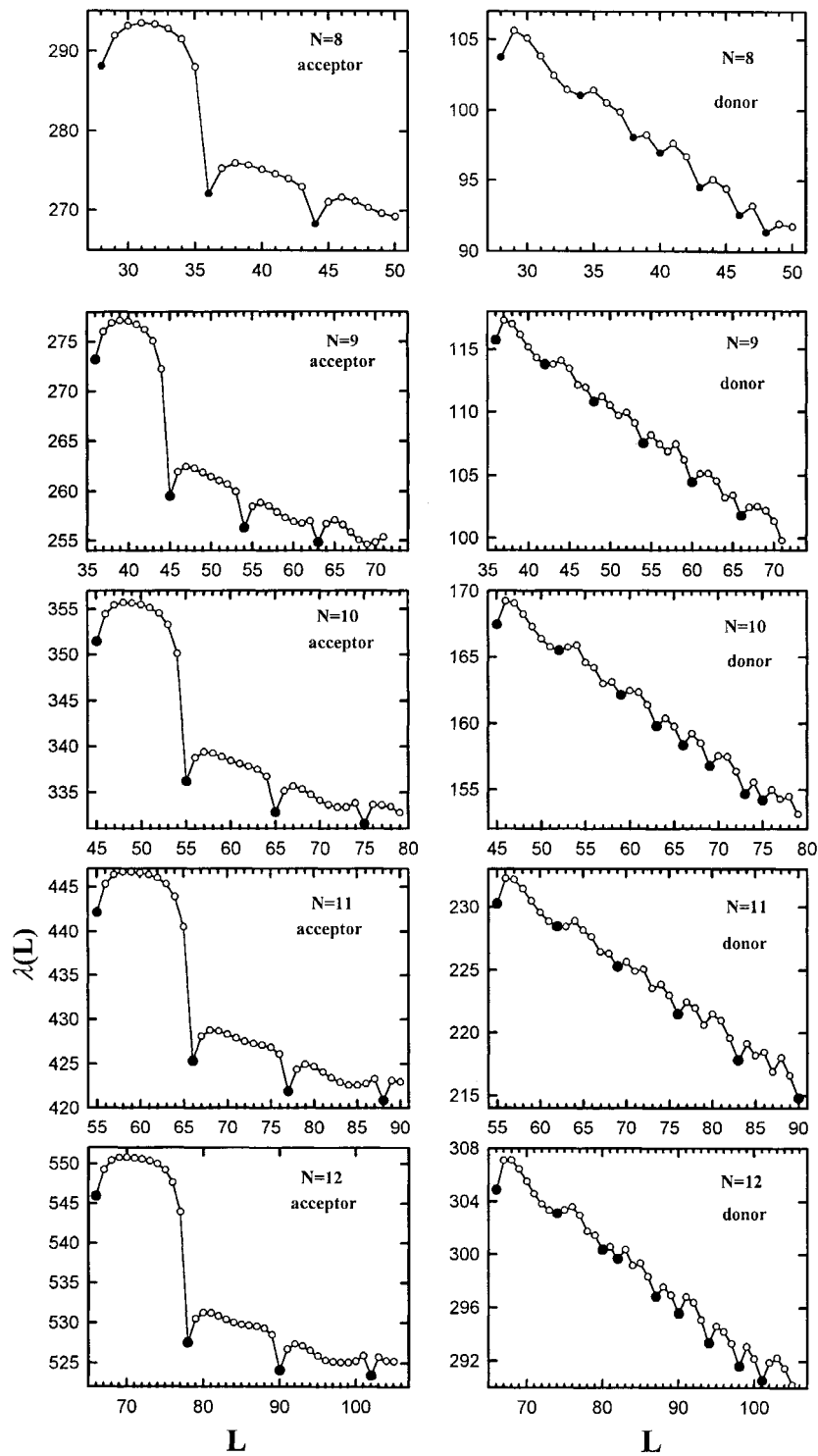


Figure 1. (Continued)



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