Capture-zone areas in submonolayer nucleation: Effects of dimensionality and short-range interactions

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Simulation results for the asymptotic scaled capture-zone distribution (CZD) for the case of irreversible nucleation and growth of point islands are presented for substrate dimension $d=1$, 2, 3, and 4 and compared with a recent conjecture based on the Wigner distribution. Poor agreement is found between the predicted Wigner distributions and the asymptotic CZD in the limit of infinite D/F (corresponding to the ratio of monomer hopping rate D to deposition rate F). Our results also indicate that for $d=2$ and 3 the asymptotic CZD for point islands is independent of model details and dimension. However, for $d=1$ and $d=4$ the resulting distribution is significantly more sharply peaked. We also find that in contrast to the island-size distribution, for which mean-field-like behavior is observed in $d=3$ and above, the asymptotic CZD is significantly broadened by fluctuations even in $d=4$.

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I. INTRODUCTION

The organization and ordering of islands in the submonolayer regime of thin-film growth can play an important role in determining the multilayer growth behavior [1]. Consequently, island nucleation and growth has been the subject of much recent interest (for a recent review see Ref. [2]). One quantity of particular interest is the island-size distribution (ISD) which may be written in the form

$$f(s/S) = N_s(\theta)S^2/\theta, \tag{1}$$

where $N_s(\theta)$ is the density (per site) of islands of size s at coverage θ, $S=\Sigma_{s\geqslant 2}sN_s/\Sigma N_{s\geqslant 2}$ is the average island size, and $f(s/S)$ is the scaled ISD. In particular, simulations [3] have shown that the asymptotic scaled ISD corresponding to large values of D/F (where D is the monomer hopping rate and F is the deposition rate) in the precoalescence regime depends on the size i of the critical nucleus, which corresponds to one less than the size of the smallest stable cluster. While no exact analytical form exists even for the simplest case corresponding to irreversible growth ($i=1$), a variety of approximate expressions and/or methods have been proposed [3–9] for calculating the ISD.

A related quantity [4,5] which is indirectly linked to the scaled ISD is the scaled capture zone size distribution (CZD). The capture zone of an island coincides roughly with the island's Voronoi polygon, and may be defined as the region surrounding that island in which a diffusing particle or monomer is more likely to attach to that island than to any other existing island. Since the size of an island's capture zone is directly related to its capture number or propensity to capture diffusing particles, the ISD is indirectly related to the CZD [5]. As a result, determining the dependence of the CZD on the critical island size is a subject of some interest.

Recently, it has been suggested [10] that the scaled capture-zone size distribution may be accurately represented using a Wigner distribution [11,12] of the form

$$P_\beta(u) = a_\beta u^\beta \exp(-b_\beta u^2), \tag{2}$$

where the parameter β depends on the substrate dimension d and critical island size i, via the expression [13] $\beta=(2/d)(i+1)$ for $d=1,2$. It was also suggested that for $d>2$, the value of β is the same as for $d=2$, i.e., one has $\beta=i+1$. Using this expression, good agreement with simulation results was demonstrated [10] for the scaled CZD for compact islands with $i=0$ and $i=1$ in $d=2$. However, poor agreement between simulation results and the predicted $P_2(u)$ was found for the case of point islands with $i=1$ in $d=2$, and instead much better agreement [14] was found with $P_4(u)$. Therefore, it is of interest to study in more detail the asymptotic scaled CZD for point islands as well as the dependence on substrate dimension d in order to determine the asymptotic behavior.

Here we present the results of extensive kinetic Monte Carlo (KMC) simulations carried out to obtain the asymptotic capture-zone size distribution for the case of irreversible growth ($i=1$) of point islands with $d=1-4$. In order to determine the asymptotic distribution, results are presented for values of D/F ranging from 10^5 to 10^{10}. In addition, to understand the dependence of the CZD on the short-range interaction, results are also presented for two different point-island models with and without short-range interactions.

This paper is organized as follows. In Sec. II, we discuss the models used in our simulations while our results are presented in Sec. III. Finally, we discuss our results in Sec. IV.

II. MODEL AND SIMULATIONS

To understand the dependence on substrate dimension we have studied the scaling of the capture-zone distribution on a one-dimensional lattice ($d=1$), as well as on square and triangular lattices ($d=2$), and cubic ($d=3$) and hypercubic

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($d=4$) lattices for the case of irreversible growth ($i=1$) of point islands. In our simulations, monomers were deposited randomly with a (per site) deposition rate F, and were assumed to diffuse to nearest-neighbor sites with hopping rate D. The size of an island's capture zone was determined by counting the number of empty sites or sites occupied by monomers whose distance from the island is less than the distance to any other island. If a site is found to be equally distant to two or more closest islands, then its contribution to the capture zone is divided equally between those islands. This is essentially equivalent to a Voronoi construction around each island. Once the capture zone for each island was determined, the scaled capture-zone distribution (CZD) $C(z/Z)$ was calculated using the expression

$$C(z/Z) = ZN_z \Big/ \sum_z N_z, \tag{3}$$

where N_z is the number of capture zones of size z and Z is the average capture zone size.

We note that in previous point-island model simulations of the ISD and capture-number distribution (CND) for the case of irreversible growth in $d=3$ and $d=4$ carried out by Shi, Shim, and Amar (SSA model) [15,16], if a monomer is deposited on or hops onto an already occupied site then that monomer is irreversibly captured by the island. Similarly, if a monomer hops onto another monomer then a dimer island is nucleated at that site. However, in the two-dimensional (2D) point-island simulations of the capture-zone distribution carried out by Evans and Bartelt [8] (EB) the short-range interaction was treated differently. In particular, in the EB point-island model (see also Ref. [17]) if a monomer is deposited at or diffuses to a site which is nearest neighbor to an occupied site, then that monomer is immediately captured by the nearby monomer or island. Thus, while the SSA model is a model which has no short-range interaction, the EB model has a short-range (nearest-neighbor) attractive interaction and thus is more similar to that for a compact or fractal island model (e.g., less point-island-like).

Since these differences involve only the short-range interaction, we expect that in the asymptotic limit of large D/F there will be no differences between the scaled CZD obtained for both models. However, for comparison in all cases we have carried out simulations using both the EB and SSA versions of the point-island model.

In order to determine the asymptotic behavior, simulations were carried out for values of D/F ranging from 10^5 to 10^{10}, and the CZD and ISD were calculated for coverages ranging from $\theta=0.1$ to $\theta=0.4$. Our simulations in $d=1$ were carried out on systems of size $L=10^6$ with results averaged over 200–1000 runs. Simulations in $d=2$ were carried out for both square and triangular lattices with systems of size $L=1024$, while for $d=3$ and $d=4$, simulations were carried out on cubic lattices of size 160 and 50, respectively. In order to obtain good statistics, our results for $d=2-4$ were averaged over 40–200 runs.

III. RESULTS

A. Results for $d=2-4$

We first consider the dependence of the scaled CZD on coverage and D/F in $d=2-4$. Figure 1(a) shows typical results for the dependence on coverage for $d=3$ ($D/F=10^9$) for the SSA model, while Fig. 1(b) shows the corresponding results for the dependence on D/F ($\theta=0.1$). Similar results have been obtained in $d=2$ and $d=4$. As can be seen, while there is essentially no coverage dependence, in general the peak of the scaled CZD decreases with increasing D/F. This latter behavior indicates that the asymptotic scaled CZD distribution only occurs for significantly larger D/F. Accordingly, here we focus on the dependence of the scaled CZD on D/F for $\theta=0.1$ since there is essentially no coverage dependence.

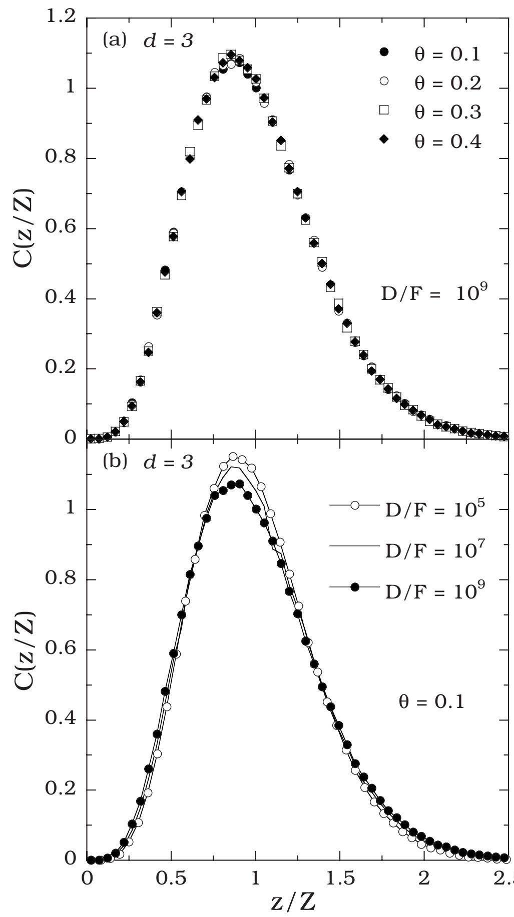

FIG. 1. Scaled CZD $C(z/Z)$ (where Z is the average capture zone size) obtained from simulations of SSA model in $d=3$. (a) Coverage dependence; (b) dependence on D/F.

We now consider the dependence of the CZD on the details of the short-range interaction. Figure 2 shows a comparison between results obtained using the SSA model (filled symbols) and EB model (open symbols) in $d=2$ for $D/F=10^7$ and $\theta=0.1$. We note that the results of the scaled ISD and CZD for the EB model in Fig. 2 is in excellent agreement with the corresponding previous result given in Ref. [7]. As can be seen, for finite D/F there is a clear disagreement between the scaled CZD obtained using the two models. In contrast, as shown in Fig. 2 the ISDs are in perfect agreement. These results indicate that for finite D/F the scaled CZD depends more sensitively on the details of the short-range interaction than the scaled ISD. They also indicate that the connection between the CZD and the ISD is

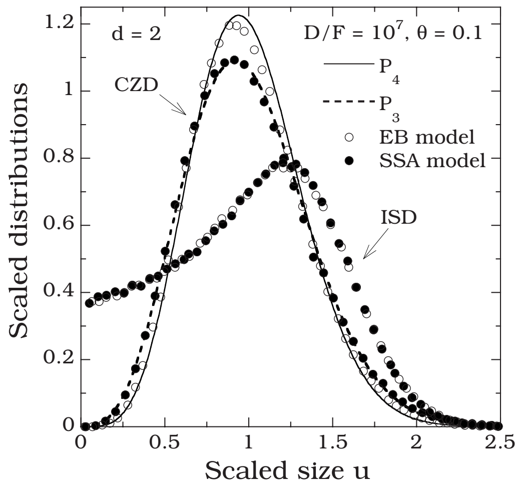

FIG. 2. Comparison of scaled CZD $C(z/Z)$ and ISD $f(s/S)$ obtained for SSA and EB point-island models in $d=2$ for $D/F=10^7$ and $\theta=0.1$ along with Wigner distributions $P_3(u)$ and $P_4(u)$.

more indirect than might have previously been considered. It is worth noting that with the same set of parameters given in Fig. 2 (e.g., $D/F=10^7$ and $\theta=0.1$) the CZD for extended (square) islands [7] is significantly broader and has a lower peak value ($\simeq 1.07$) than for the EB point-island model.

We now consider the dependence of the scaled CZD on dimension for large D/F. Figure 3(a) shows our SSA model results for $d=2-4$ for $D/F=10^9$ and $\theta=0.1$. As can be seen, the scaled capture-zone distribution for $d=2$ is very close to that for $d=3$, in good agreement with the prediction of Ref. [10] that for $i=1$ the scaled CZD should be independent of dimension for $d \geqslant 3$. However, in both cases the scaled CZD is much closer to the Wigner distribution with $\beta=3$ rather than the predicted value of $\beta=2$ (dotted curve). Furthermore, for $d=4$ the scaled CZD appears to be significantly different from the distribution for $d=2$ and 3 and is instead close to the Wigner distribution with $\beta=4$. Similar results for the EB model are shown in Fig. 3(b). While the peak values for the scaled CZD are somewhat higher than for the SSA model, we still find that the scaled CZD is approximately independent of dimension for $d=2$ and 3 and is significantly closer to the Wigner distribution with $\beta=3$ than the predicted distribution corresponding to $\beta=2$.

To determine the asymptotic behavior of the scaled CZD we have also studied the dependence of the peak height on D/F. Figure 4 shows our results for the CZD peak height as a function of D/F for square, cubic, and hypercubic lattices in $d=2$, 3, and 4, respectively, and for a triangular lattice ($d=2$) for both the SSA and EB models, for values of D/F ranging from 10^6 to 10^{10}. In order to extrapolate to the asymptotic behavior, the CZD peak height C_{pk} was fit to the form $C_{pk}(D/F)=C_{pk}(\infty)+a(D/F)^{-\gamma}$. The value of γ ($\gamma \simeq 0.1$) was chosen which gives the best overall fit for both models for $d=2-4$. For comparison, the peak heights for the Wigner distributions with $\beta=3$ and $\beta=4$ are also shown. A summary of our results is shown in Table I. We note that the power-law fitting form used to extract the asymptotic value of $C_{pk}(\infty)$ is an empirical form which explains our results very well, as shown in Fig. 4. Similar expressions were also

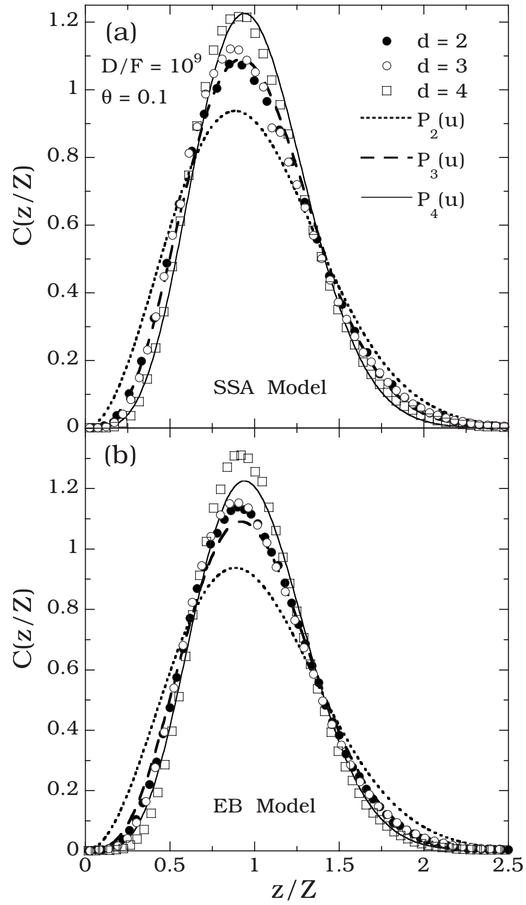

FIG. 3. Scaled CZD for SSA model (a) and EB model (b) for $D/F=10^9$ and $\theta=0.1$ for $d=2$ (filled circles), $d=3$ (open triangles), and $d=4$ (open squares) along with Wigner distributions for $\beta=2$, 3, and 4.

used in Refs. [15,16] to extract the asymptotic behavior of the scaled ISD as well as capture number distributions and the results of fittings elucidated the difference and similarity between the results of rate-equation approach and KMC simulations in $d=3$ and 4.

As can be seen, due to the longer range of interaction, the dependence on D/F is stronger for the EB model than for the SSA model. However, for a given value of d the asymptotic values of the peak heights for both models agree within error bars (see Table I). In addition, for $d=2$ and 3 the extrapolated asymptotic value $C_{pk}(\infty)$ is roughly independent of dimension. Thus, our results indicate that for $d=2$ and 3 the asymptotic scaled CZD is independent of dimension and/or model details, in good agreement with the prediction of Ref. [10] that for $d \geqslant 2$ the scaled CZD should be independent of dimension. However, the asymptotic peak value of the CZD for $d=2$ and 3 is significantly higher than the predicted value corresponding to $\beta=2$ $[P_2(x_{pk})=0.937]$ and is somewhat lower than that corresponding to $\beta=3$ $[P_3(x_{pk})=1.09]$.

Surprisingly, in $d=4$, we find that for both models the asymptotic peak value is even higher. In particular, for the SSA model we find $C_{pk}^{\mathrm{SSA}}(\infty,d=4)=1.17\pm0.04$ while for the EB model we find $C_{pk}^{\mathrm{EB}}(\infty,d=4)=1.13\pm0.06$. Averaging over both models, we obtain $C_{pk}^{\mathrm{av}}(d=4)=1.15\pm0.04$. We note

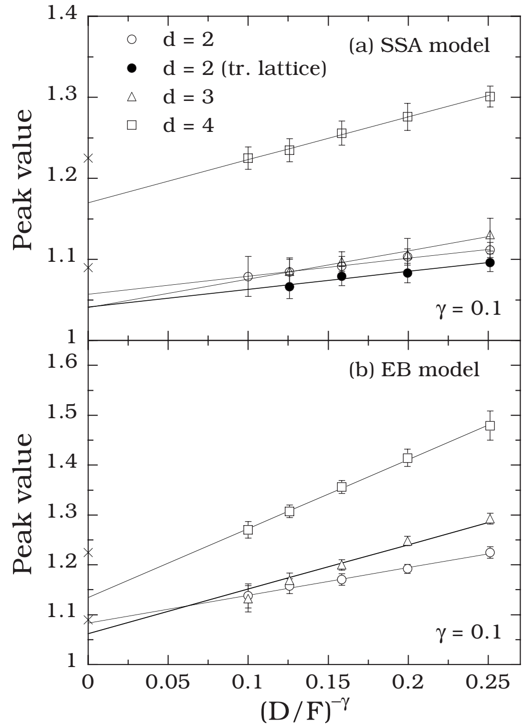

FIG. 4. Peak height of scaled CZD as function of D/F for SSA model (a) and EB model (b) in $d=2-4$. Upper and lower $\times$'s on y axes correspond to $P_4(x_{pk})=1.225$ and $P_3(x_{pk})=1.09$, respectively.

that this value is in between the peak values corresponding to $\beta=4$ (1.225) and $\beta=3$ (1.09).

B. Results for $d=1$

In order to get a more complete picture of the dependence on dimension, we have also carried simulations in $d=1$ for both the EB and SSA models. Figure 5(a) shows our results for the SSA model for different values of D/F. We note that for comparable values of D/F these results are in good agreement with previous results obtained in Ref. [4] using a similar point-island model. However, somewhat surprisingly we find that, in contrast to our results for higher dimensions, in $d=1$ the peak of the CZD increases with D/F. In addition, we note that while the scaled CZD for $D/F=10^7$ is relatively close to the prediction of Ref. [10] corresponding to $P_4(u)$, for $D/F=10^9$ the peak of the scaled CZD is somewhat higher. In order to obtain the asymptotic peak height for both the EB and SSA models, we have plotted in Fig. 5(b) the peak height as a function of $(D/F)^{-\gamma}$ (where $\gamma=0.2$ was found to be the best fit for both models) for values of D/F ranging from 10^5 to 10^9. As can be seen, while the peak height for the EB model tends to be lower than that for the SSA model for finite D/F, the asymptotic peak height for both models is essentially the same (1.31 ± 0.01) and is significantly larger than the peak value corresponding to $\beta=4$ (1.225). Thus, our results indicate that although the predicted distribution $P_4(u)$ is close, it is still significantly lower than the asymptotic CZD for point islands in $d=1$.

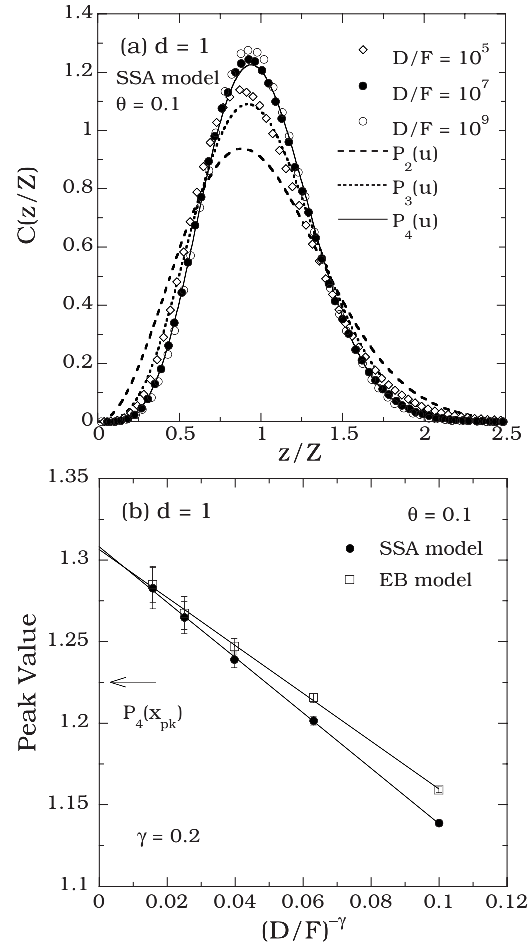

FIG. 5. (a) D/F dependence of scaled CZD obtained from simulations of SSA model in $d=1$. (b) Asymptotic peak heights for both EB and SSA models. Arrow indicates peak height for $P_4(u)$.

TABLE I. Simulation results for asymptotic peak heights $C_{pk}(\infty)$ for SSA and EB models, along with average $C_{pk}^{av}(\infty)$ in different dimensions d. For comparison, predicted values for β and peak height $P_\beta(x_{pk})$ from Ref. [10] are also shown. $P_d(x_{pk})$ corresponding to peak height for $\beta=d$ is also shown for reference.

d	$C_{pk}^{SSA}(\infty)$	$C_{pk}^{EB}(\infty)$	$C_{pk}^{av}(\infty)$	β	$P_\beta(x_{pk})$	$P_d(x_{pk})$
1	1.31 ± 0.01	1.31 ± 0.01	1.31 ± 0.01	4	1.225	0.760
2	1.04 ± 0.04	1.08 ± 0.04	1.06 ± 0.03	2	0.937	0.937
3	1.04 ± 0.05	1.06 ± 0.04	1.05 ± 0.04	2	0.937	1.09
4	1.17 ± 0.04	1.13 ± 0.06	1.15 ± 0.03	2	0.937	1.225

IV. DISCUSSION

We have carried out extensive simulations of point-island models of irreversible nucleation and growth in $d=1-4$ for values of D/F ranging from 10^5 to 10^{10} in order to determine the asymptotic scaled CZD and compare with recent predictions [10] based on random matrix theory. In addition, to determine the dependence on the short-range interaction and also check for universality, we have studied two different models, the EB model with short-range attractive interaction (in which any particle within a nearest-neighbor distance is automatically incorporated into an island) and the SSA model without short-range interaction (for which only particles which land on an existing monomer or island are incorporated into the island). We have also carried out simulations on two different lattices in $d=2$, a triangular lattice and a square lattice, in order to determine the dependence on lattice geometry. In each case, by extrapolating to infinite D/F we have estimated the asymptotic peak height for the scaled CZD.

In general, we find good scaling as a function of coverage, i.e., the CZD is essentially independent of coverage for fixed D/F. However, we also find that the CZD depends on D/F for finite D/F. In particular, for $d=2-4$ we find that the peak height of the scaled CZD decreases with increasing D/F, while for $d=1$ it increases. We also note that for $d=2-4$, the dependence of the peak height on D/F and lattice dimension tends to be stronger for the EB model than for the SSA model. This is perhaps not surprising since the interaction range is larger for the EB model than for the SSA model. However, somewhat surprisingly, for $d=1$ the dependence of the peak height on D/F is larger for the SSA model than for the EB model.

When extrapolating to the asymptotic limit our results indicate that, for $d=2$ and 3, the asymptotic CZD is independent of model details and dimension, in good qualitative agreement with the prediction of Ref. [10]. This behavior is in strong contrast to that of the scaled ISD which depends strongly on dimension and corresponds to a finite distribution in $d=2$ [8], while diverging with increasing D/F in $d=3$ [15]. We also note that our estimate for the asymptotic value of the peak of the CZD in $d=2$ and 3 ($C_{pk}^{d=2,3} \simeq 1.06 \pm 0.03$) is significantly lower than obtained in previous 2D point-island model simulations for finite D/F [8], but is still significantly higher than the predicted peak value [10] [$P_2(x_{pk})=0.937$] corresponding to the Wigner distribution with $\beta=2$. However, it is relatively close to the peak value [$P_3(x_{pk})=1.09$] corresponding to the Wigner distribution with $\beta=3$. In contrast, for $d=1$ the peak height of the asymptotic CZD is significantly larger than for $d=2$ and $d=3$. For this case, while our results for small D/F agree with previous results [4], for which good agreement with the Wigner distribution with $\beta=4$ was found [10], both the peak height for larger D/F as well as the asymptotic peak height ($C_{pk}^{d=1}=1.31 \pm 0.01$) are noticeably higher than the value [$P_4(x_{pk})=1.225$] corresponding to the Wigner distribution with $\beta=4$.

We have also obtained results for $d=4$. In this case, we found somewhat surprisingly that the asymptotic peak height ($C_{pk}^{d=4} \simeq 1.15 \pm 0.03$) is significantly higher than in $d=2$ and $d=3$. However, it is still somewhat lower (e.g., outside the error bars) than the peak height of the Wigner distribution with $\beta=4$ [$P_4(x_{pk})=1.225$]. We note that while the system sizes in $d=4$ were somewhat limited compared to our simulations for smaller d, there was no evidence for a finite-size effect in this case, since the average island separation for the highest value of D/F studied ($D/F=10^9$) was several times smaller than the system size L.

In summary, our results indicate that for point-island models, while the scaled CZD depends strongly on D/F as well as on the short-range interaction for finite D/F, the asymptotic CZD is relatively independent of model details such as the short-range interaction. In addition, we find good agreement between the asymptotic CZD in $d=2$ and $d=3$ as suggested in Ref. [10]. However, in general we do not find good agreement between the Wigner distribution using the predicted value of β [$\beta=(2/d)(i+1)$] given in Ref. [10] and our asymptotic simulation results. In particular, in $d=2$ and 3 we find better agreement with the Wigner distribution with $\beta=3$ than the predicted value of $\beta=2$. Similarly, the peak height of the asymptotic CZD in $d=1$ is noticeably higher than the Wigner distribution with $\beta=4$.

It is also of interest to compare our results for the asymptotic CZD of point islands with $i=1$ in $d=2$ with previous results obtained for extended islands. As already noted in the Introduction, for the case of circular islands [5] with $D/F=10^6$ the peak of the CZD was significantly lower than for the point-island models studied here, and good agreement was found [10] with the predicted Wigner distribution with $\beta=2$ [$P_2(x_{pk}) \simeq 0.94$] for this case. Thus, it would appear that there may be significant differences between the asymptotic CZD for point islands and extended islands, and that the theory of Pimpinelli and Einstein [10] may be more applicable to extended islands. In this connection it is also worth noting that simulations by Evans and Bartelt of the EB model with $i=1$ in $d=2$ (see Ref. [8]) indicate that for point islands the ISD depends more strongly on D/F than the CZD. This is in contrast to the relatively weak dependence of the ISD on D/F found for extended islands. Thus, it would appear that there are significant differences between the point-island and extended-island models which may lead to different asymptotic behavior for both the ISD and the CZD. On the other hand, it should be noted that in simulations [7] of square islands in $d=2$ with a larger value of D/F ($D/F=10^7$) than for the circular islands studied in Ref. [5] the peak height of the CZD (1.06) was found to be relatively close to the asymptotic value (1.06 ± 0.03) obtained from our point-island simulations. Thus, further work will be needed to understand the similarities and/or differences between extended island and point-island models in the asymptotic limit.

Finally, it is interesting to discuss in somewhat more detail our results for the dimensionality dependence of the scaled CZD, and compare with previous results obtained for the scaled ISD. We note that we have previously shown [15,16] that for the point-island model the ISD diverges in $d=3$ and above, due to the fact that both the average capture zone and average capture number for a given island size become independent of island size. These results also indicate [16] that $d=4$ is the critical dimension for pure mean-field (MF) behavior for the ISD as well as for the capture-number distribution (CND). In contrast, the results presented here indicate that the asymptotic scaled CZD in $d=3$ and 4 does not diverge with increasing D/F, and thus does not correspond to pure MF behavior, for which a δ-function like CZD would be expected. The difference in the behaviors is due to the effects of fluctuations, which tend to "broaden" the CZD even for large d, but which tend to "cancel out" when calculating quantities such as the average capture zone or capture number for a given island size. Thus, our results further underline the fact that, as indicated in Ref. [5], the connection between the CZD and the ISD is indirect, since, for example, one can have a MF ISD in $d=4$ while the CZD does not exhibit MF behavior.

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