

# 物理演示实验期中报告

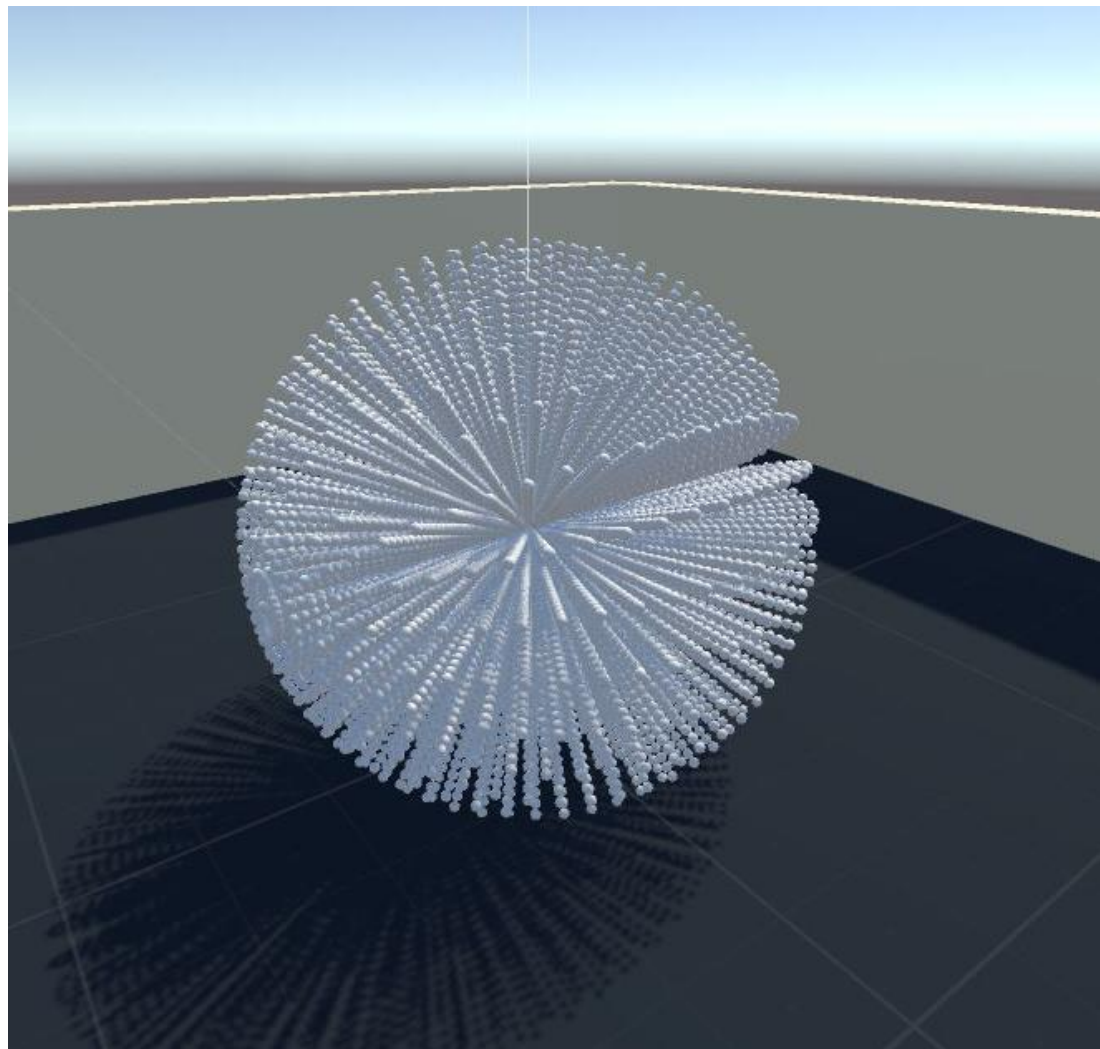
——电子云模型在VR中的展示

胡琼

指导老师：魏心源

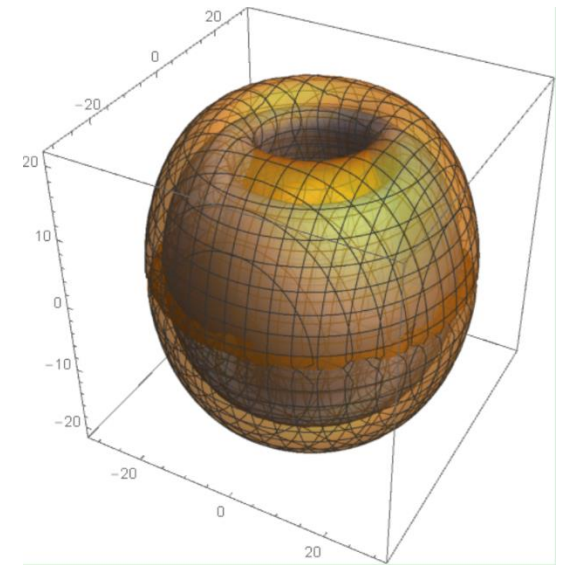
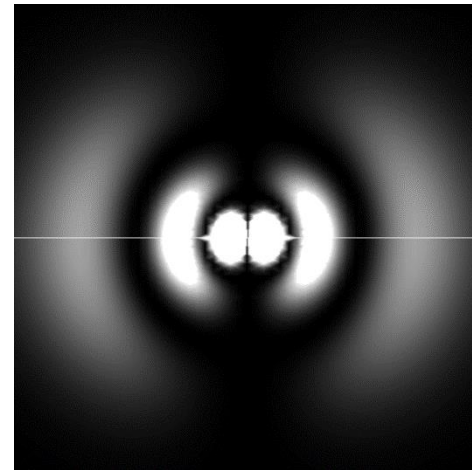
# 目录

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# 动机

- VR的优势：
- 身临其境，近距离观察现实中不可能存在/很难观察的事物
- 小到原子电子
- 大到星球宇宙
- 都能近在眼前
- 原子物理电子云模型：难以直观想象或用二维图像来理解



# 原理

- 氢原子薛定谔方程的解

- 径向方程:  $R(r)^{(2)} + \left(\frac{2\mu}{\hbar^2} \left(E + \frac{e^2}{r}\right) - \frac{l(l+1)}{r^2}\right)R(r) = 0$

- 通解:  $R_{nl}(r) = N_{nl} e^{-\frac{\zeta}{2}r} \zeta^l F(-n+l+1, 2l+2, \zeta r),$

- $\left( \text{其中 } \zeta = \frac{2Zr}{na}, N_{nl} = \left(\frac{2Z}{a}\right)^{\frac{3}{2}} \frac{1}{n^2(2l+1)!} \sqrt{\frac{(n+1)!}{(n-l-1)!}} \right)$

- 球谐函数:  $Y_{lm}(\theta, \varphi) = (-1)^m \sqrt{\frac{(2l+1)(l-m)!}{4\pi(l+m)!}} \cdot P_l^m(\cos\theta) e^{im\varphi},$

- $\left( \text{其中 } \theta = \arctan\left(\frac{\sqrt{x^2+y^2}}{z}\right) \right)$

# 原理

- 氢原子波函数:

- $$\psi_{nlm} = \sqrt{\left(\frac{2}{na}\right)^3 \frac{(n-l-1)!}{2n((n+l)!)^3}} e^{-\frac{Zr}{na}} \left(\frac{2Zr}{na}\right)^l \left(L_{n-l-1}^{2l+1}\left(\frac{2Zr}{na}\right)\right) Y_l^m(\theta, \phi),$$

- 概率密度分布函数:

- $$W_{nlm}(r, \theta, \varphi) = |R_{nl}(r)Y_{lm}(\theta, \varphi)|^2$$

# 原理

$$\bullet W_{100} = \frac{1}{\pi} * \frac{1}{a^3} e^{-\frac{2r}{a}}$$

$$\bullet W_{200} = \frac{1}{8\pi} * \frac{1}{a^3} \left(1 - \frac{r}{2a}\right)^2 e^{-\frac{r}{a}}$$

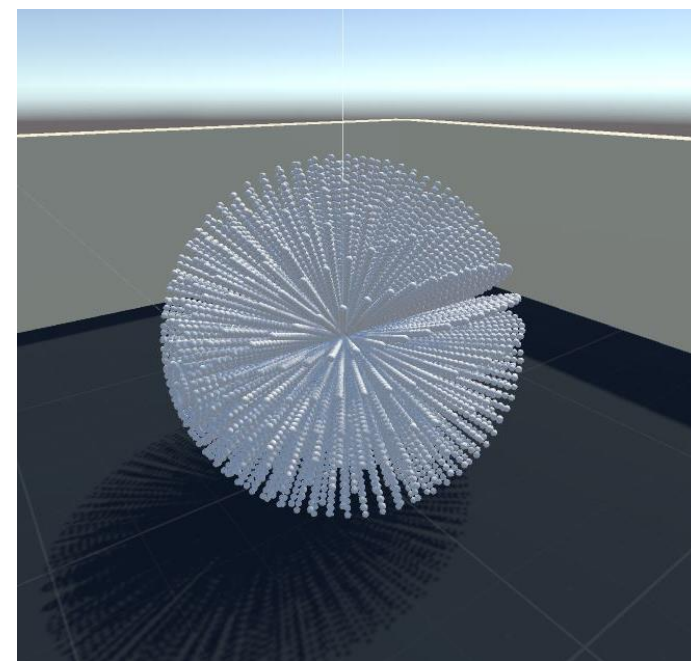
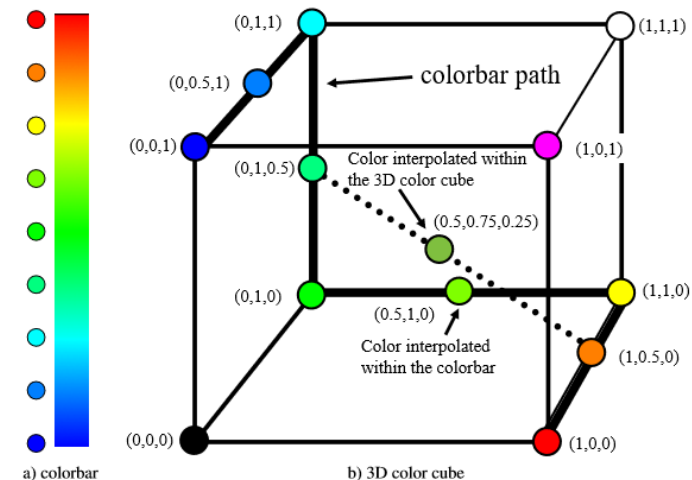
$$\bullet W_{210} = \frac{1}{32\pi} * \frac{1}{a^5} * r^2 * e^{-\frac{r}{a}} * \text{Cos}[\theta]^2$$

$$\bullet W_{211} = \frac{1}{64\pi} * \frac{1}{a^5} * r^2 e^{-\frac{r}{a}} * \text{Sin}[\theta]^2$$

$$\bullet n=3, n=4 \dots \dots$$

# 算法

- 两种搜索方式：球坐标、直角坐标
- 三种表现电子密度的方法：球的大小、颜色、透明度
- 概率密度函数有e指数关系，
- 大的太大、小的太小
- 用一定的函数关系缓和这种变化：
- 取对数、开根号等

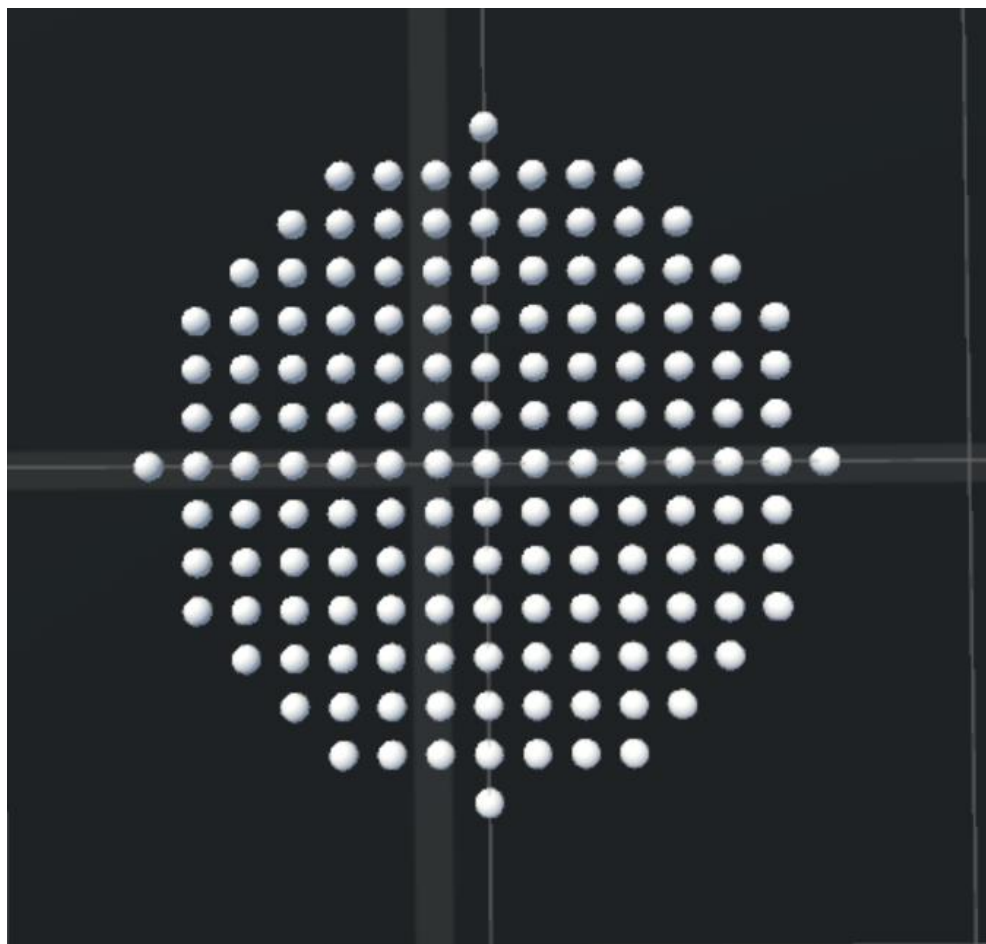


# 算法

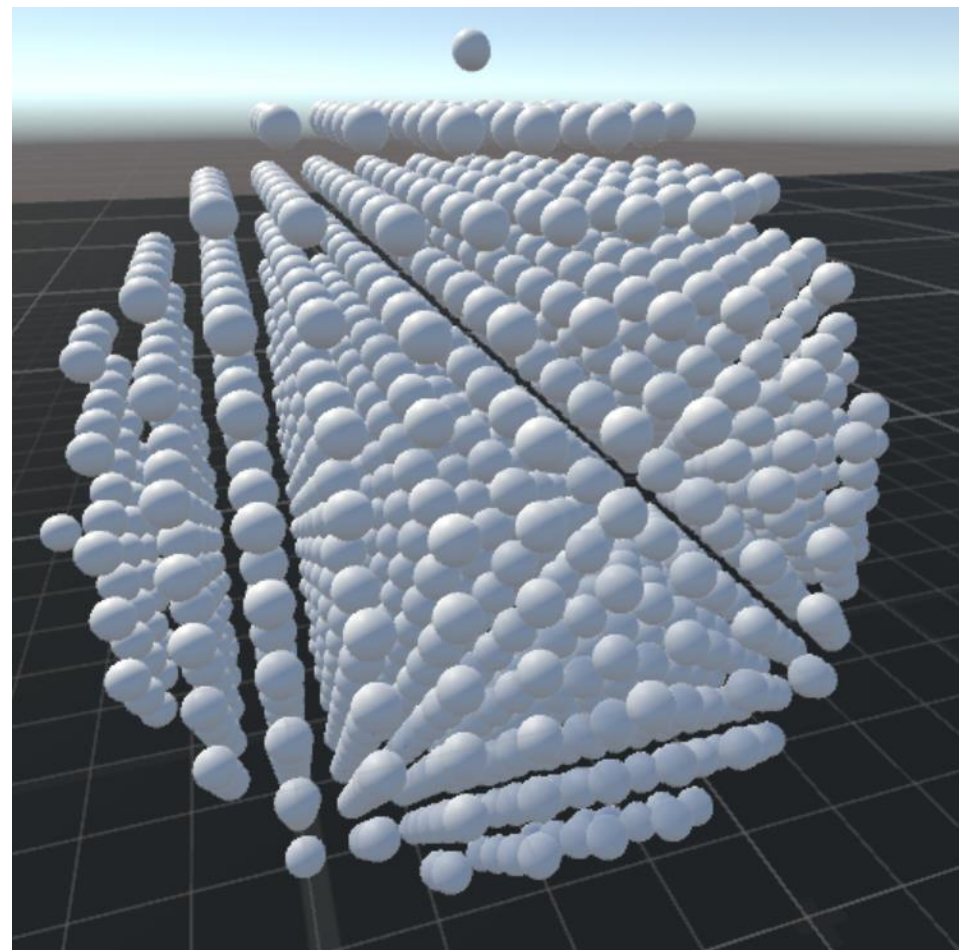
- 定义球坐标与直角坐标的转换函数
- 定义概率密度分布函数
- 引擎初始化
- 搜索每个小球，计算概率密度，修改对应的大小/颜色等性质
- 画出小球



均匀分布，  
按直角坐标搜索

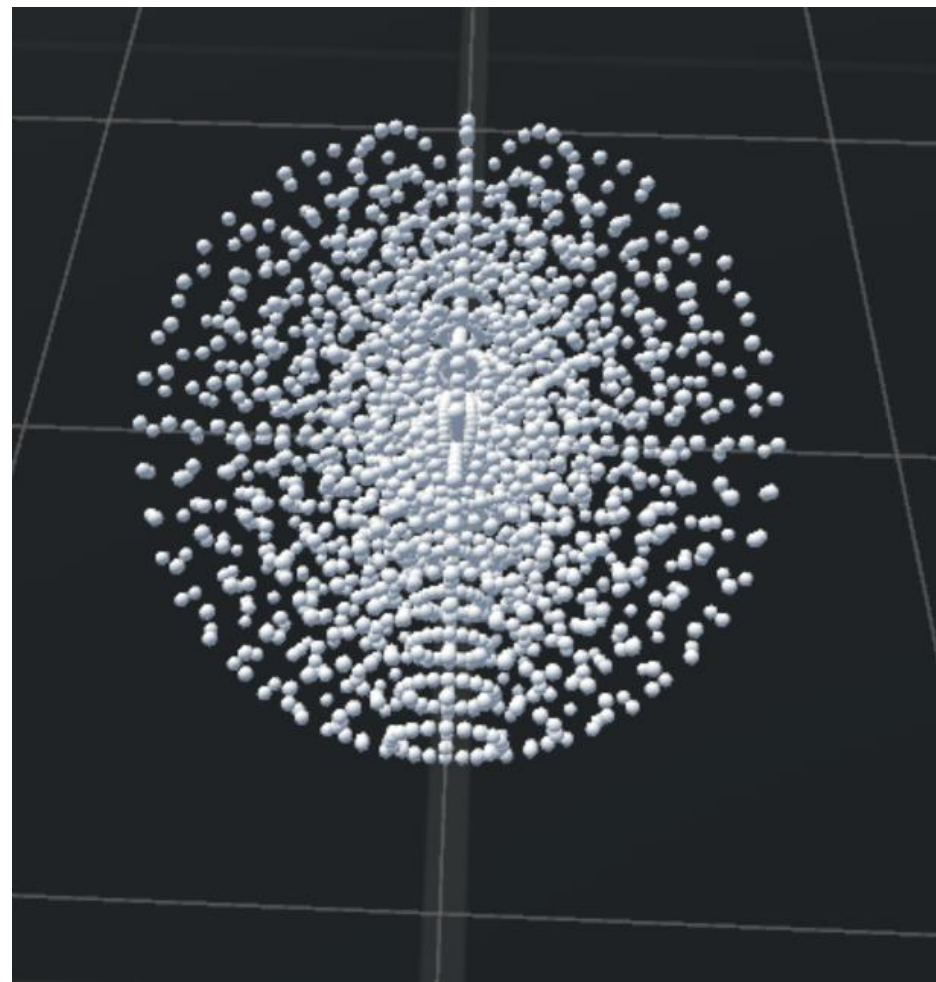
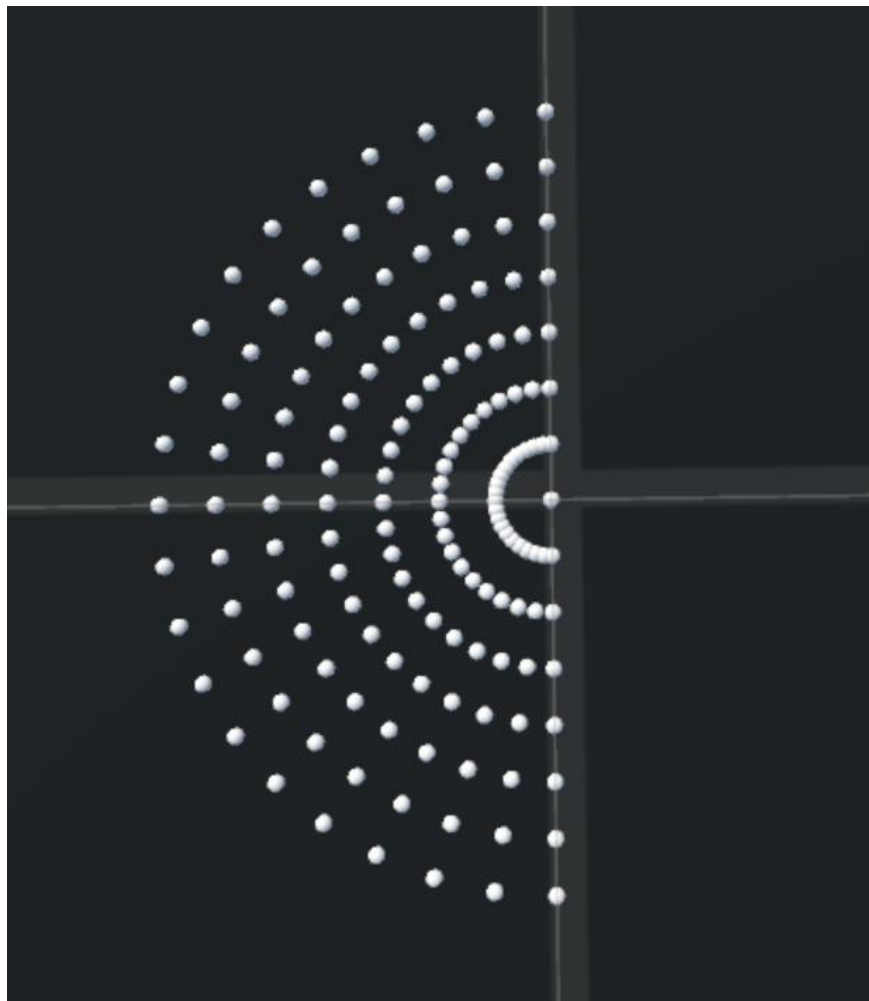


结果

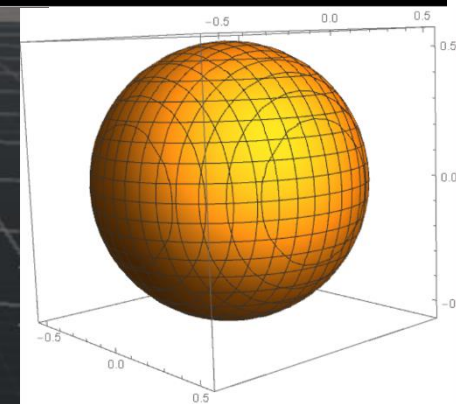
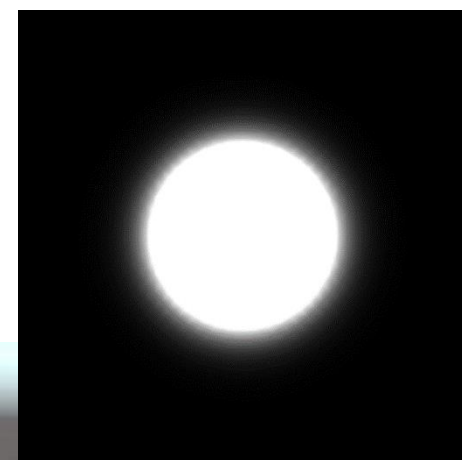
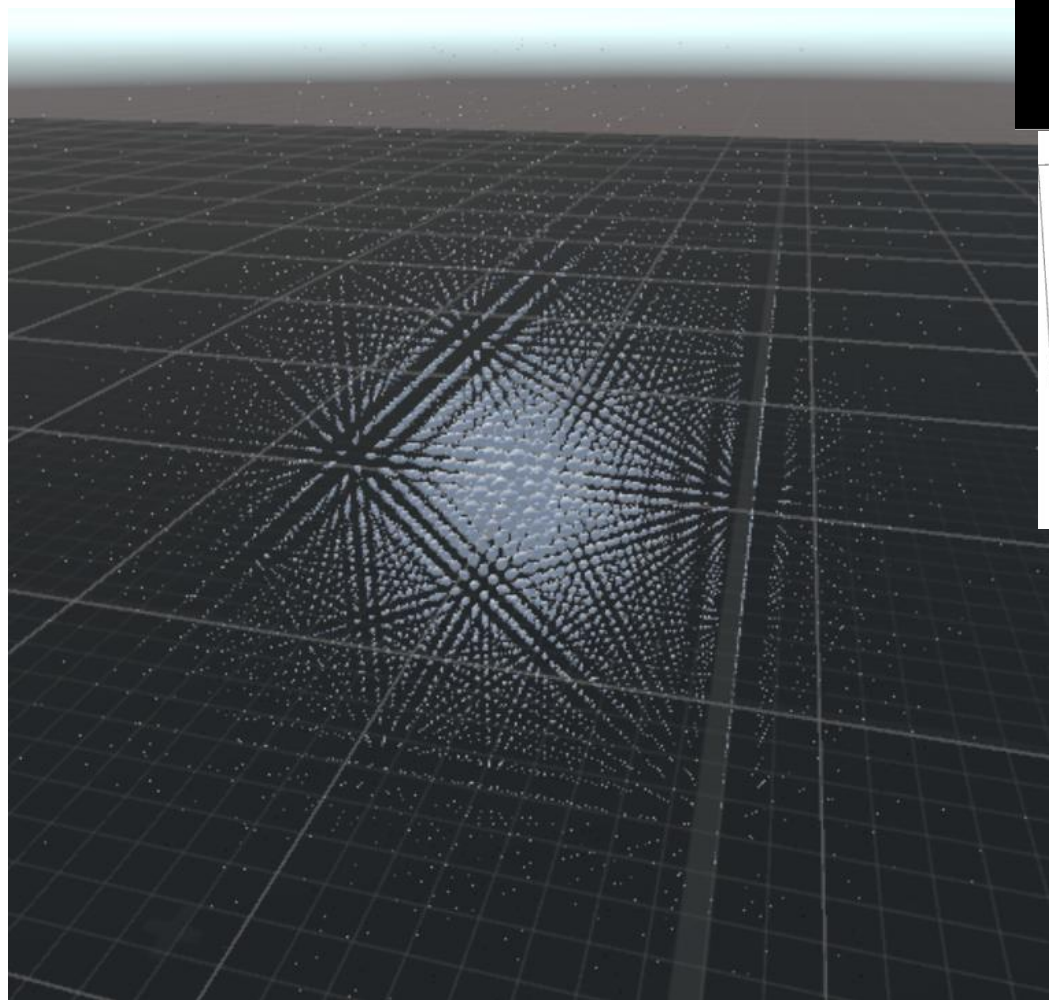
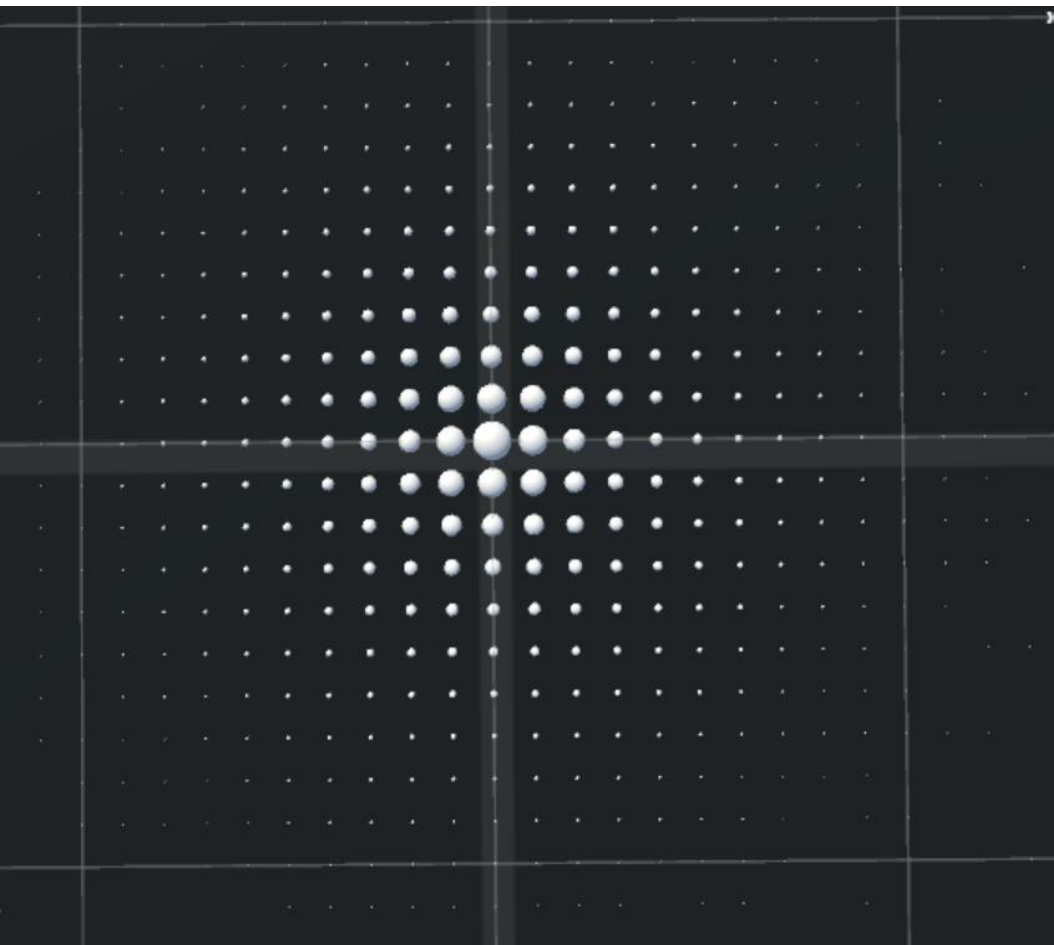


均匀分布，  
按球坐标搜索

结果

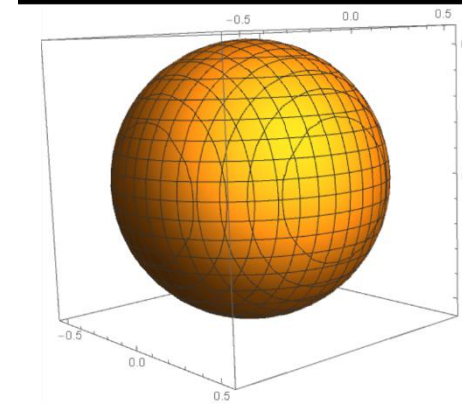
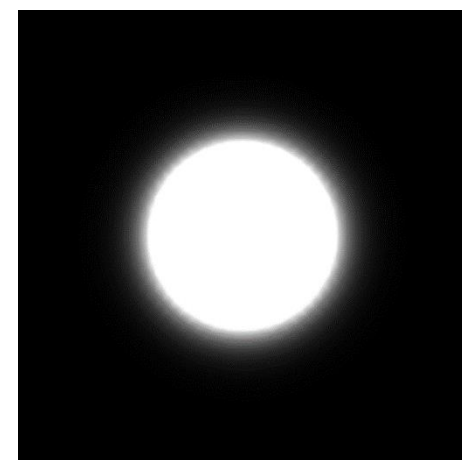
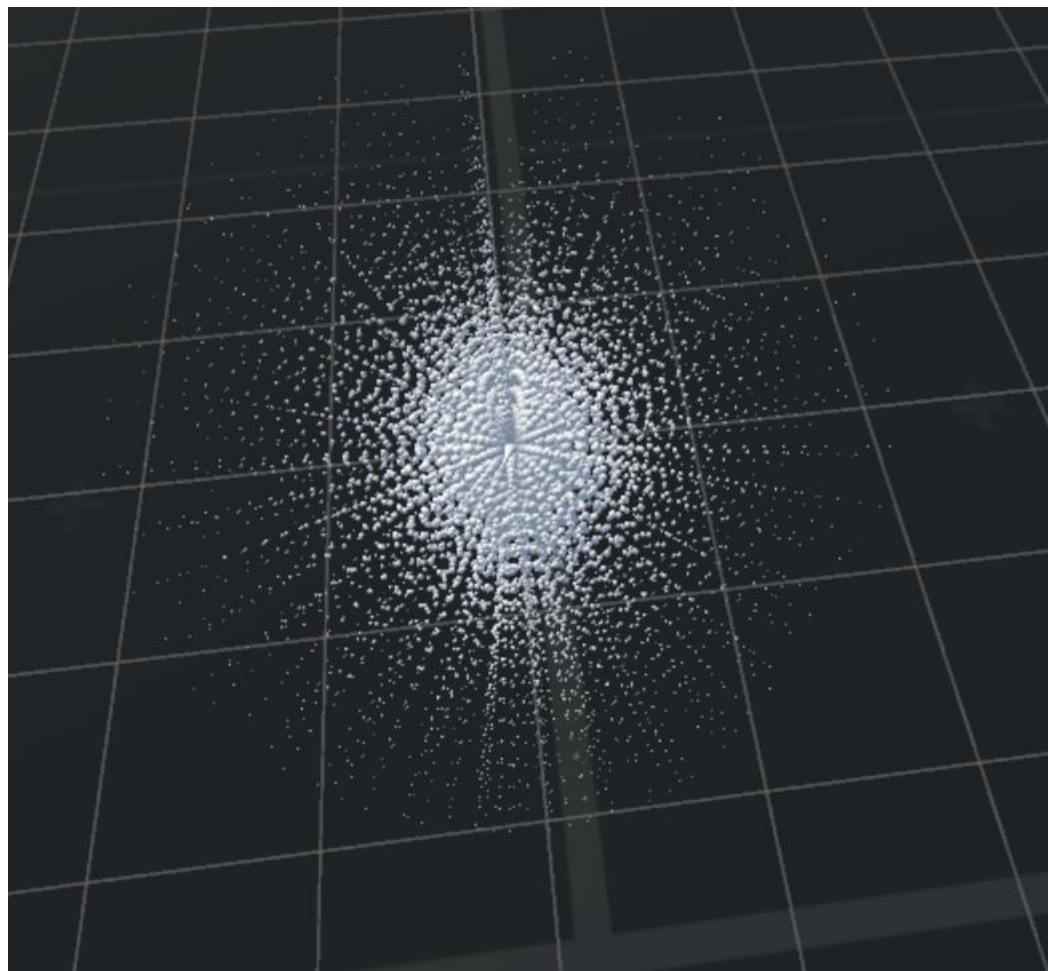
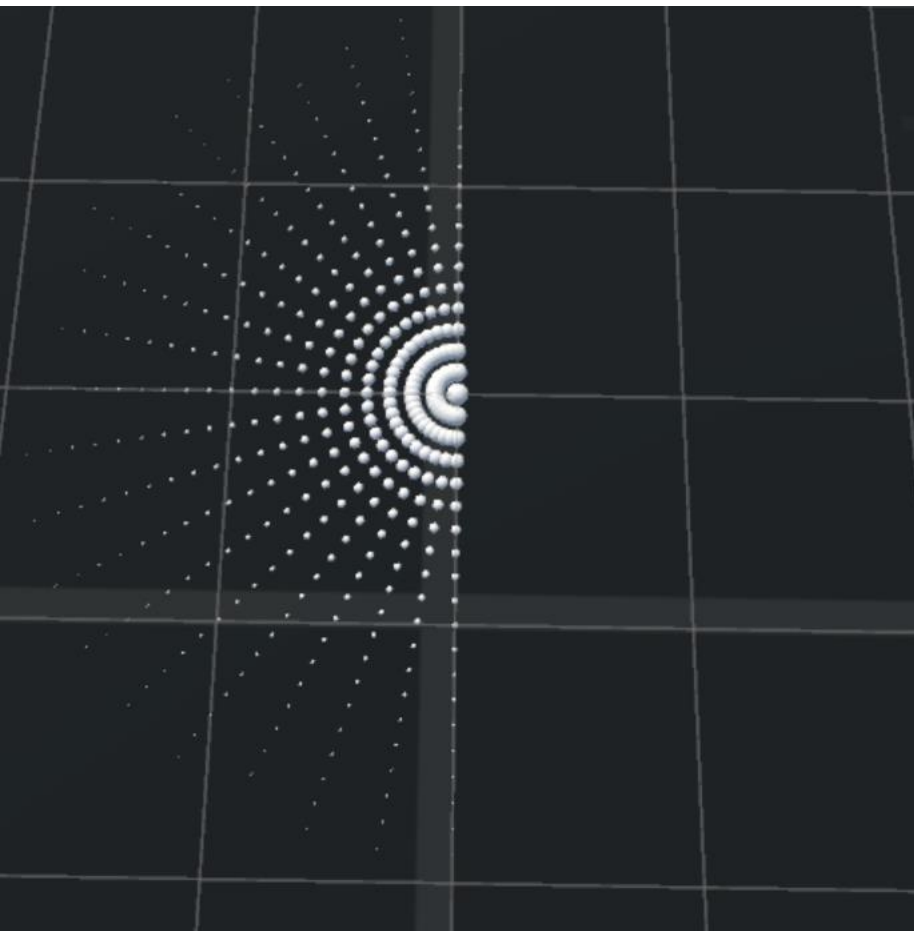


# 1,0,0, 按直角坐标搜索

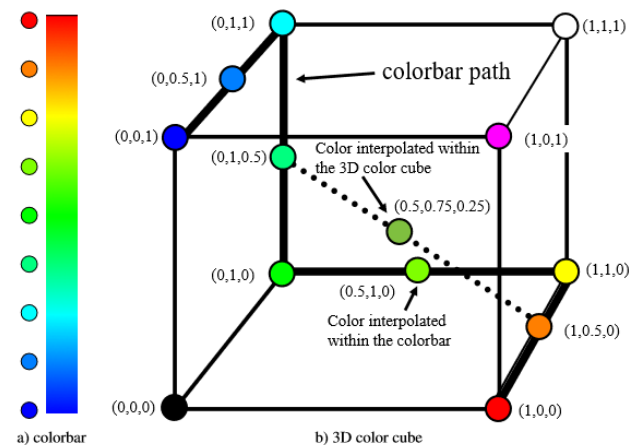
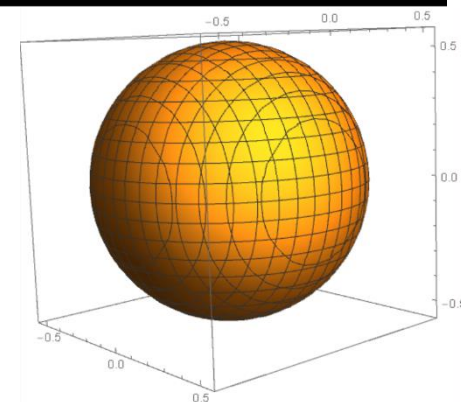
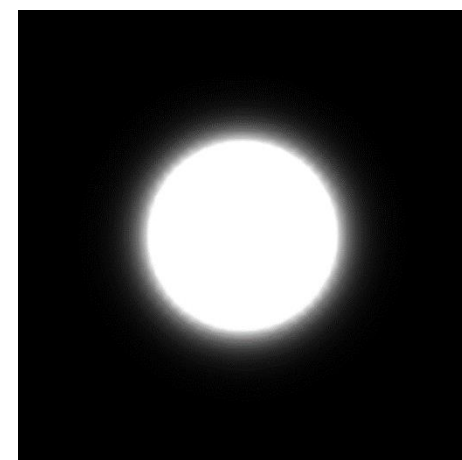
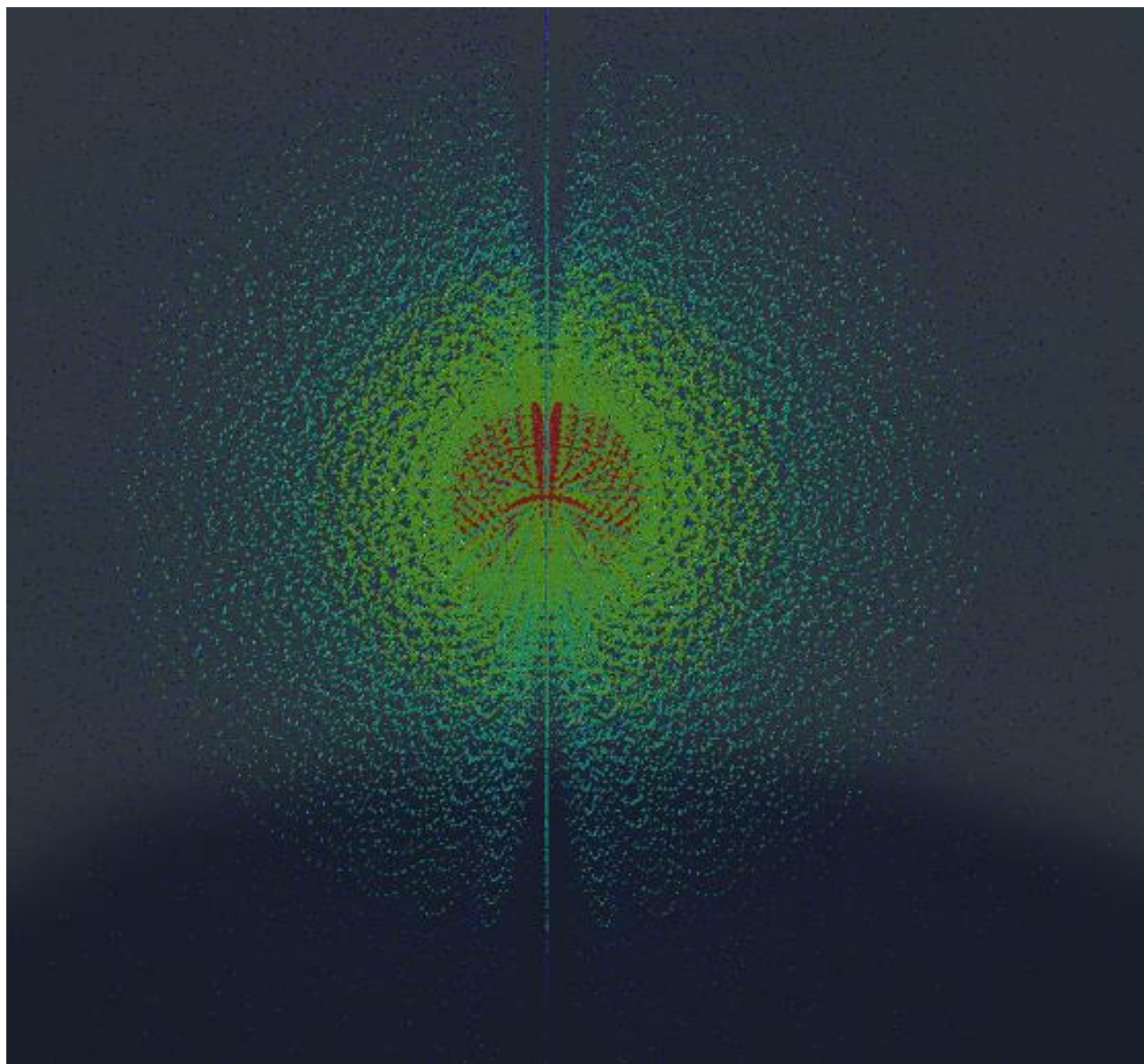




# 1,0,0, 按球坐标搜索

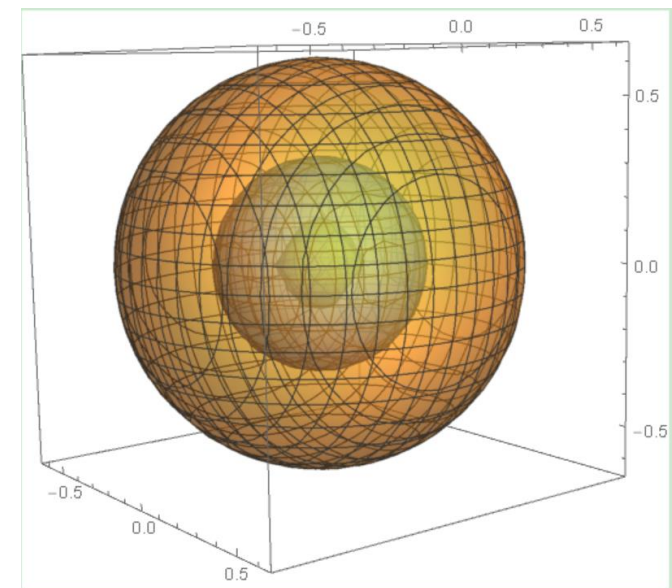
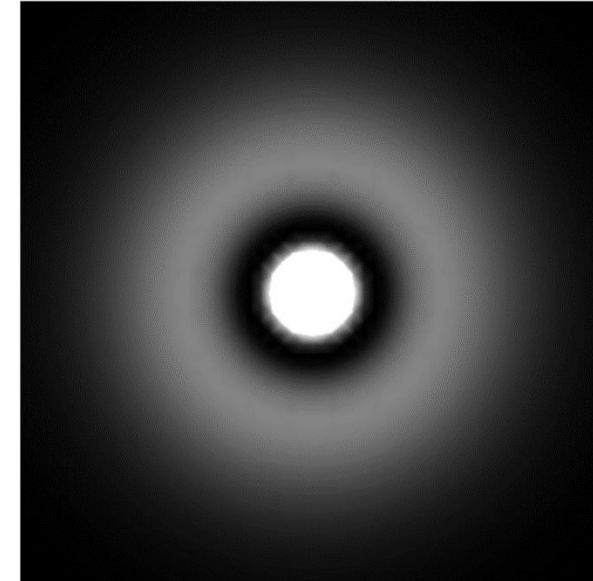
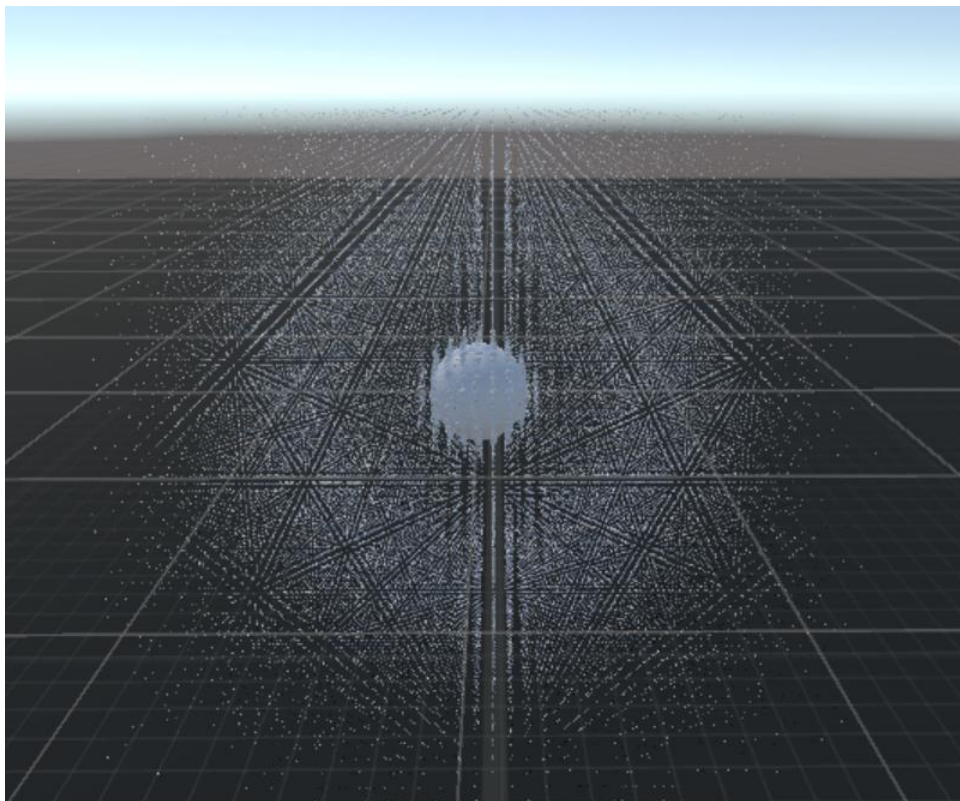
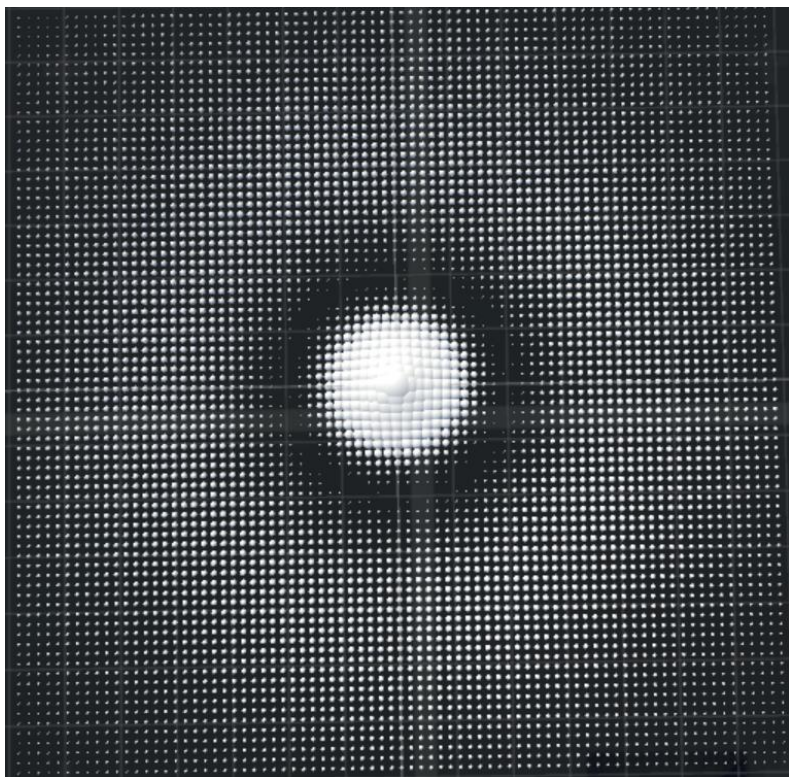


# 1,0,0, 按球坐标搜索, 用颜色来展示



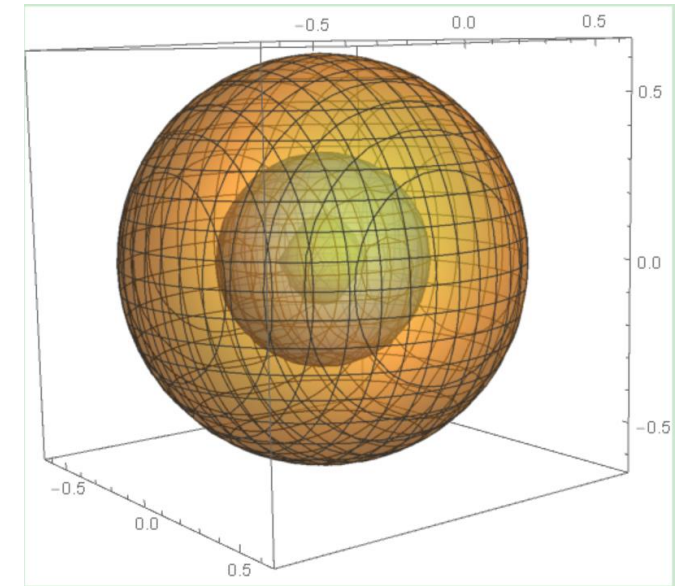
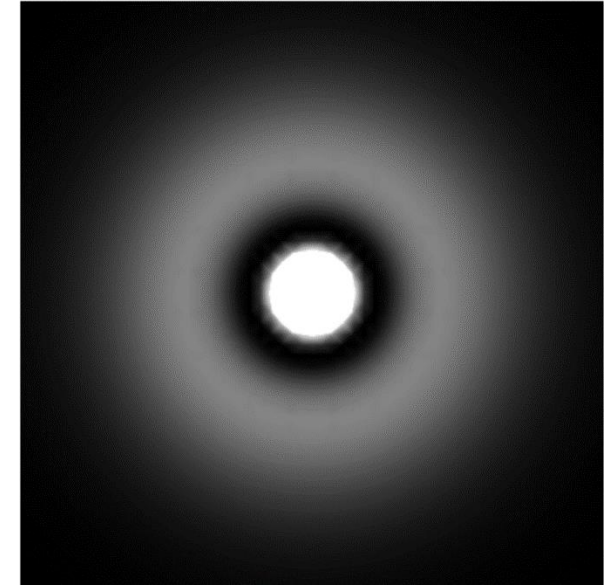
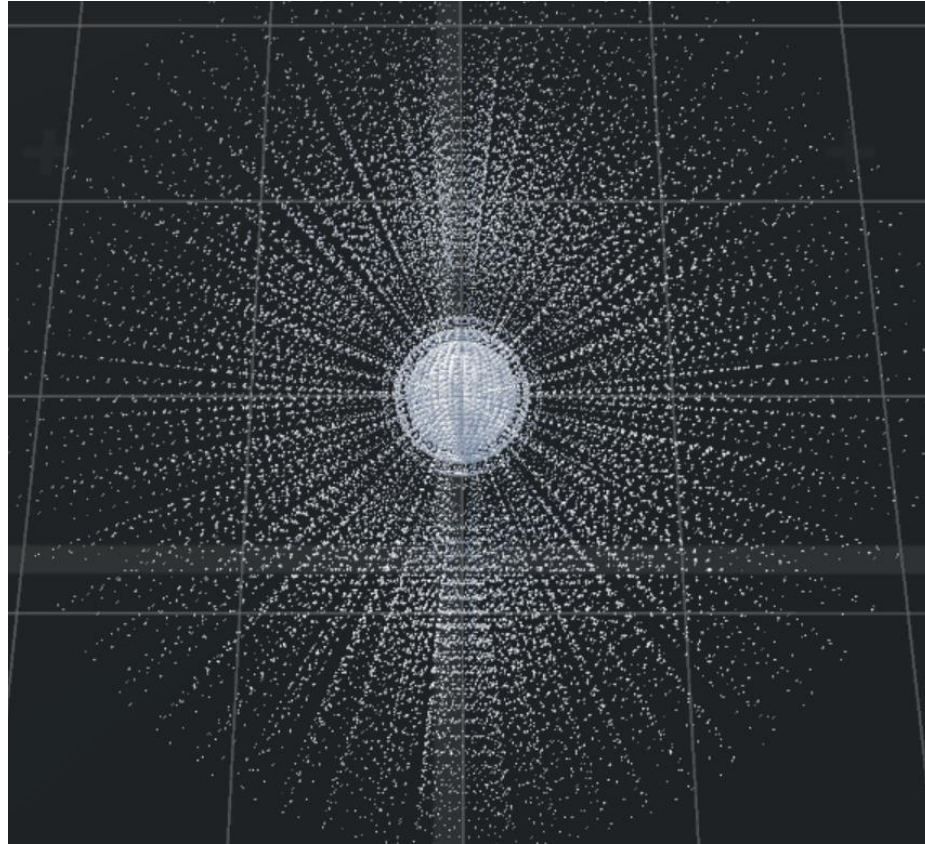
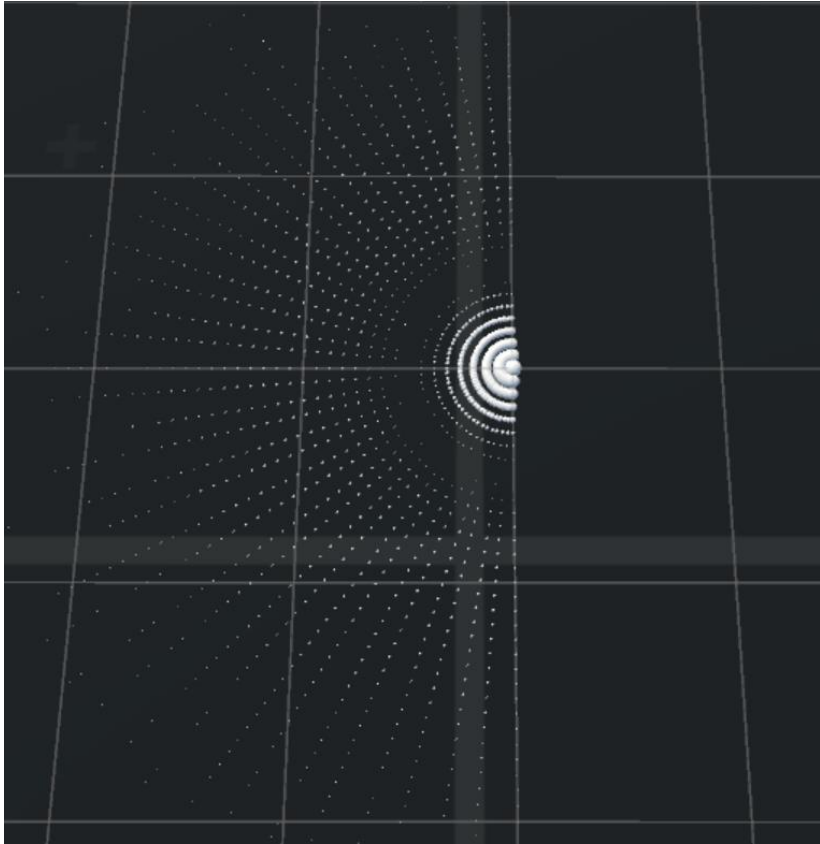


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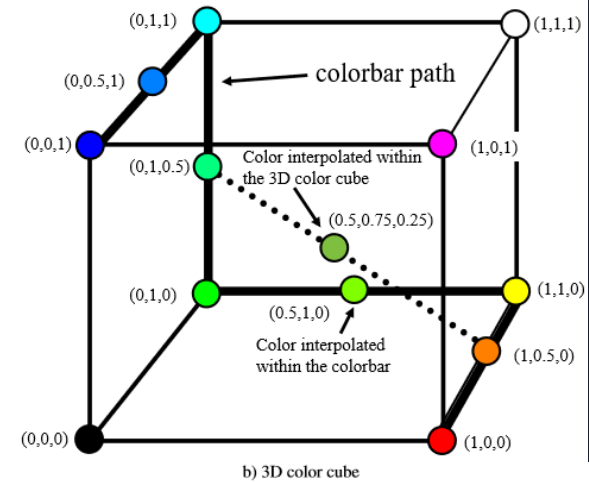
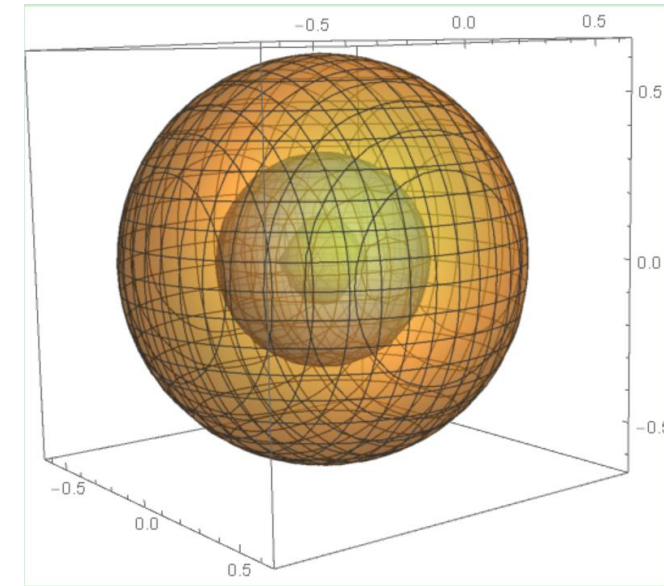
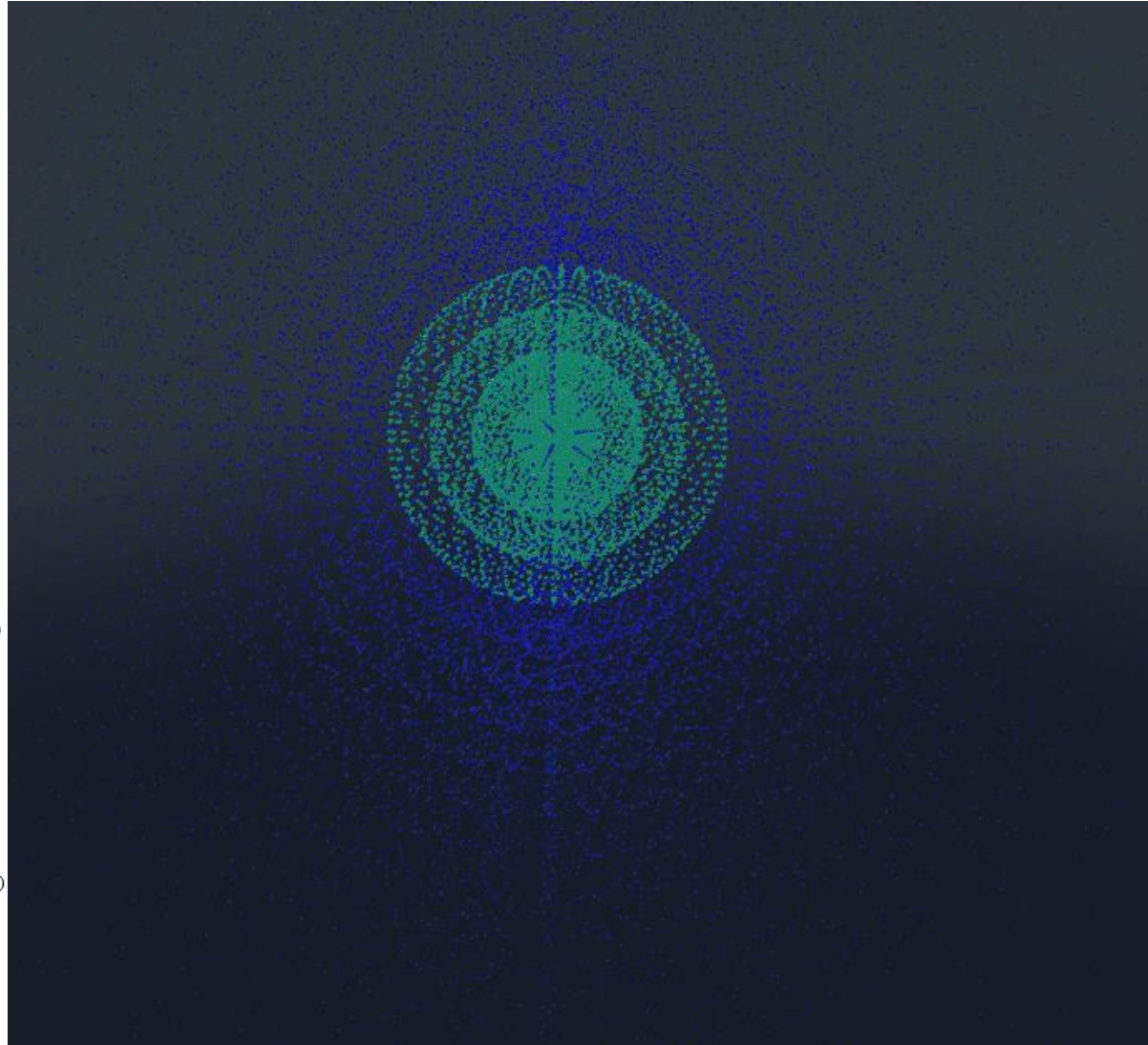
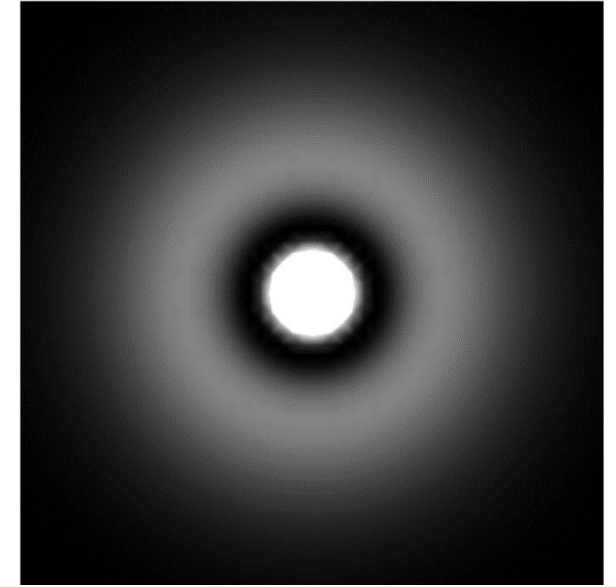




# 2,0,0, 按球坐标搜索

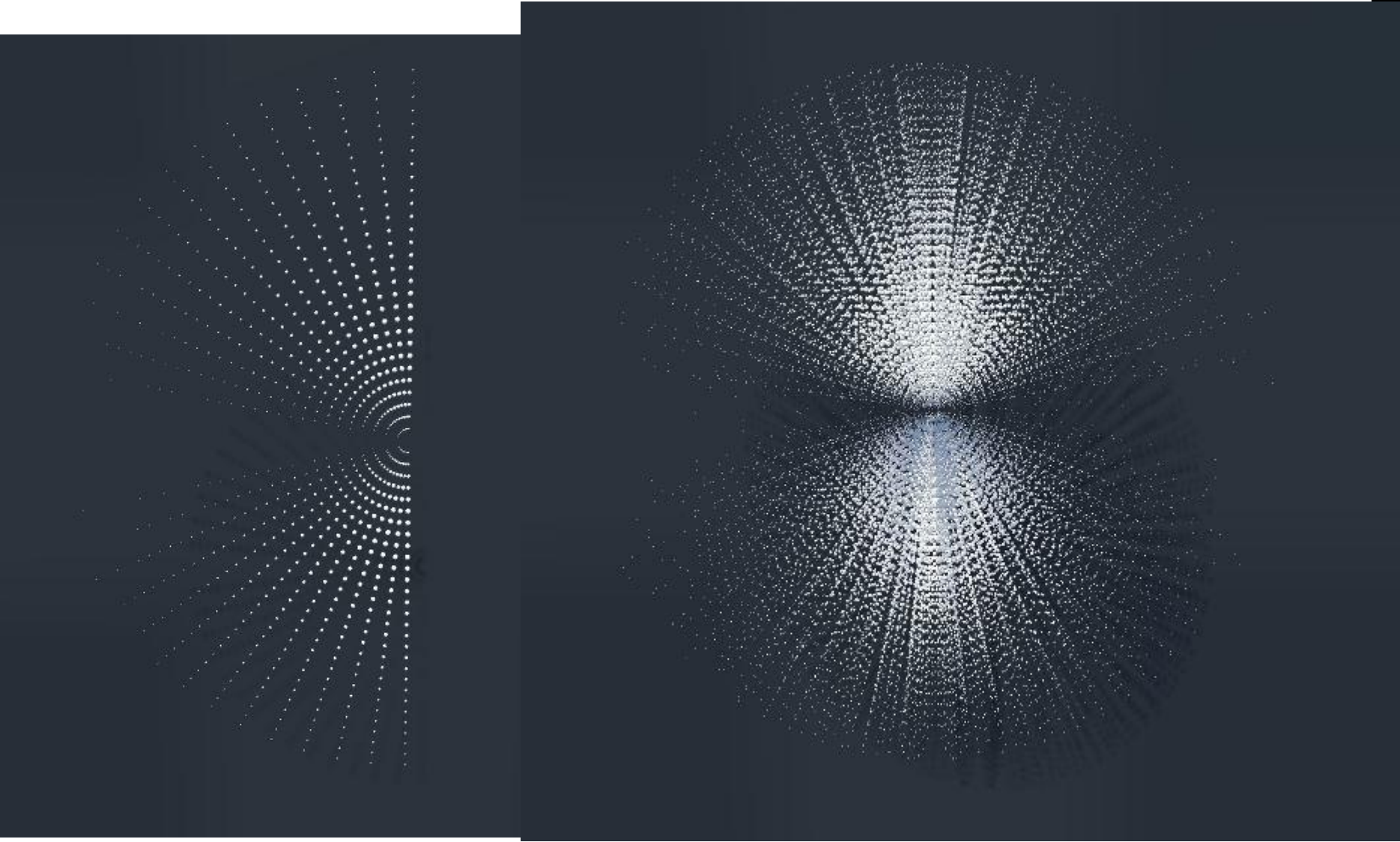
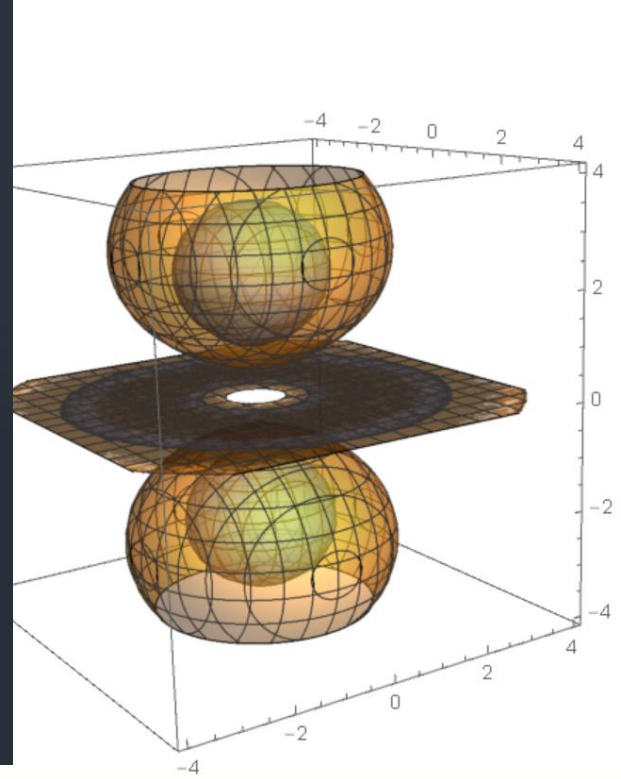
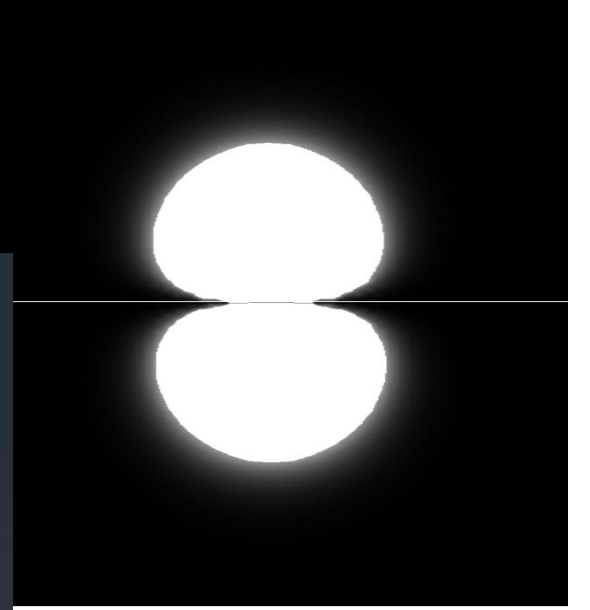


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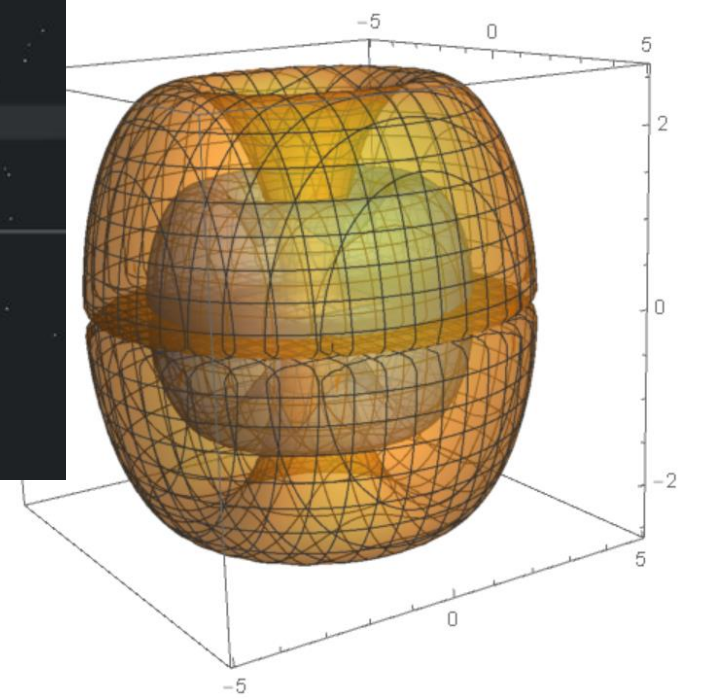
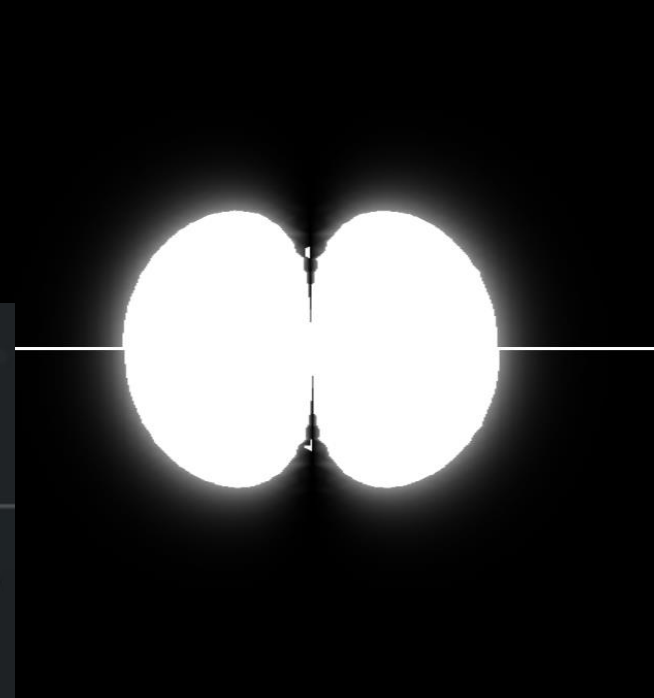
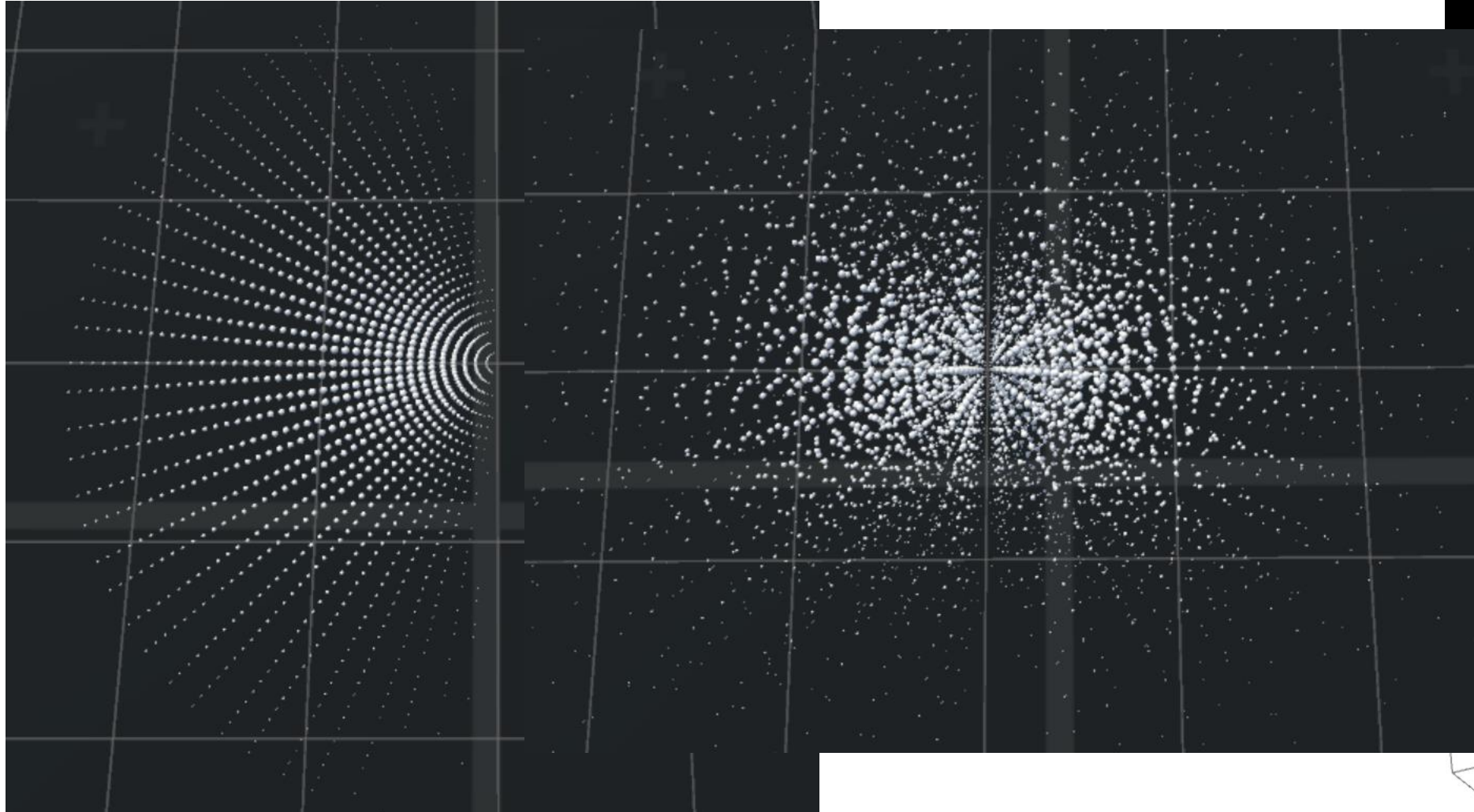




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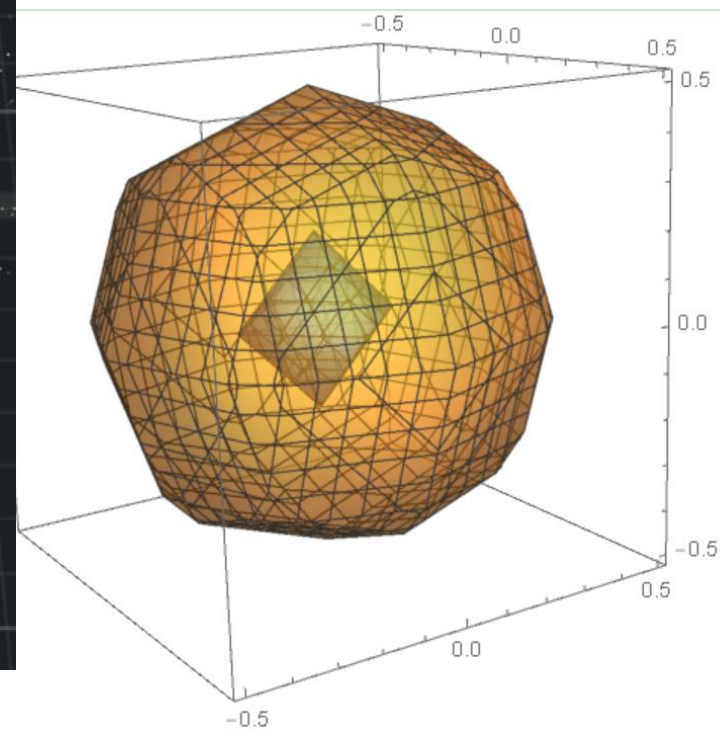
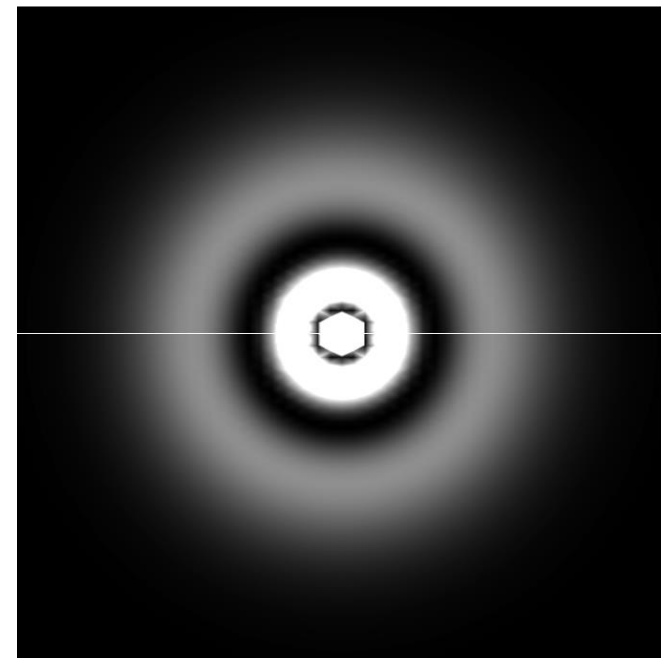
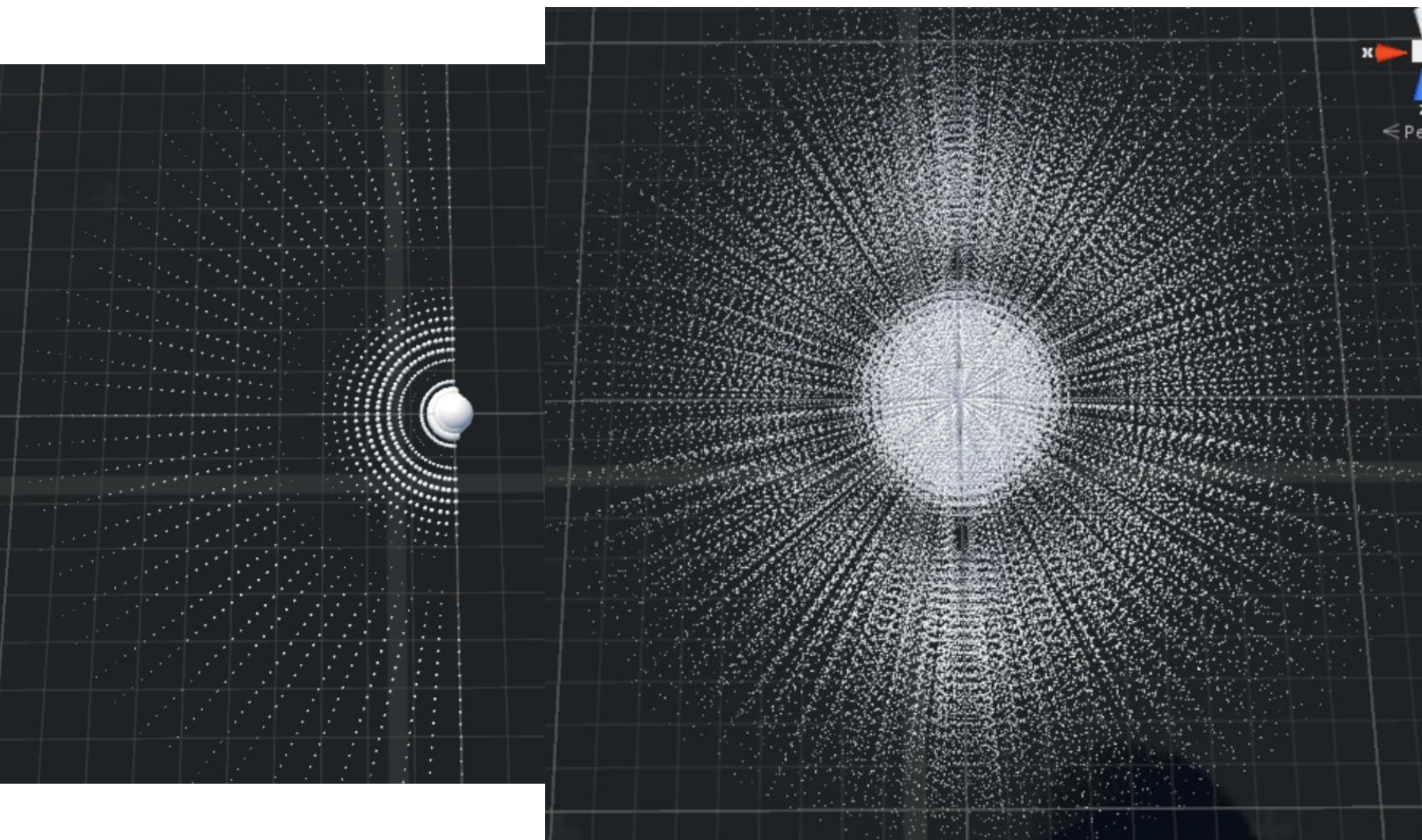


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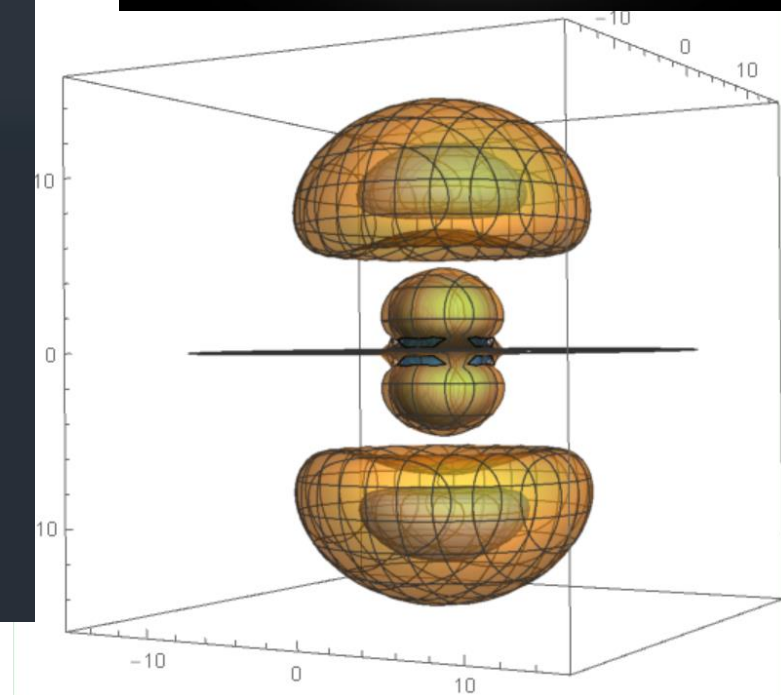
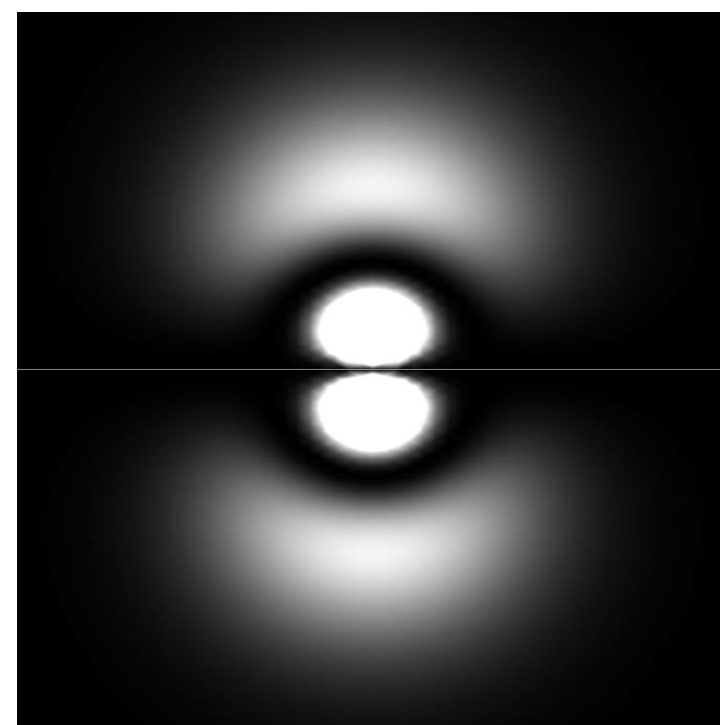
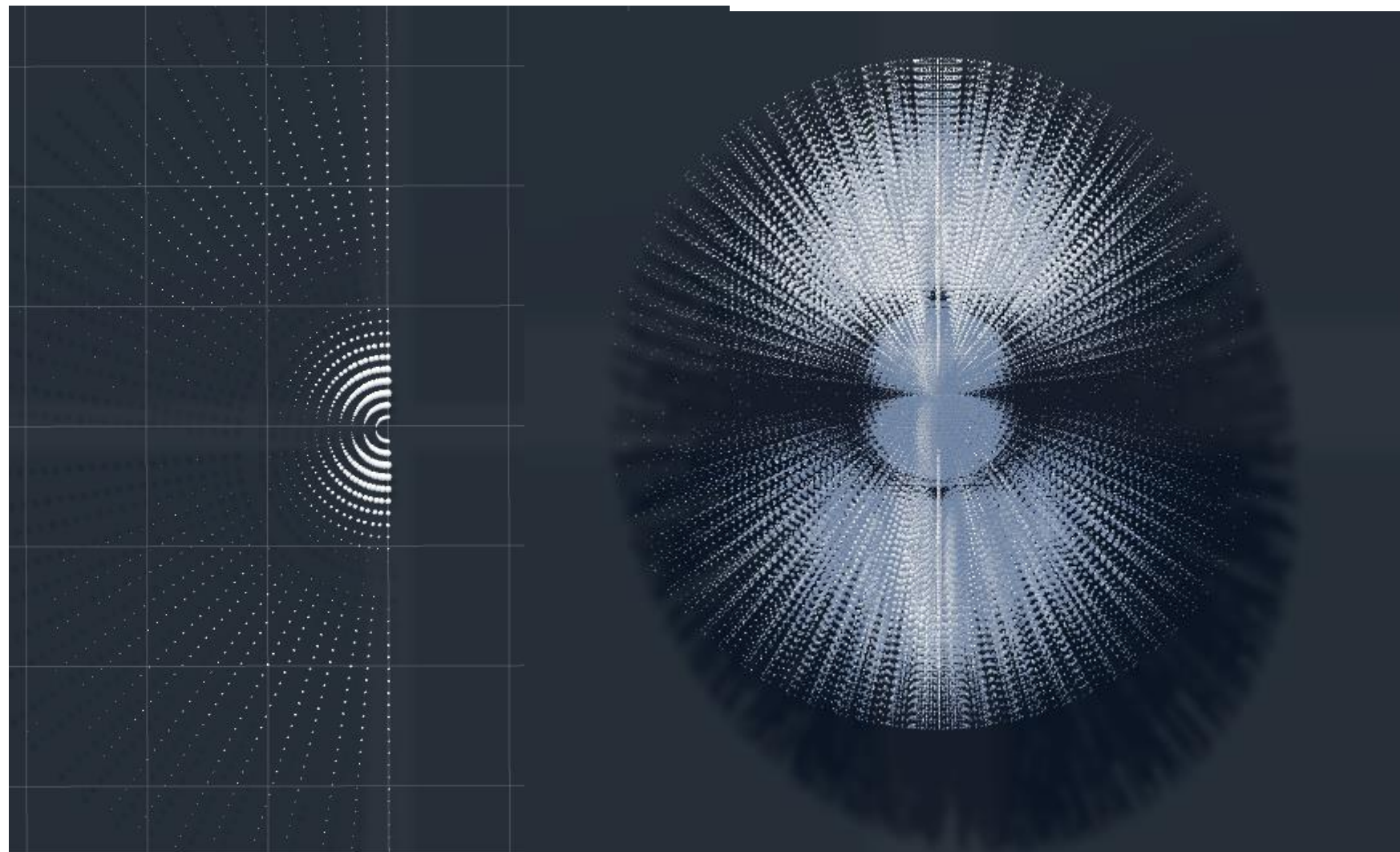




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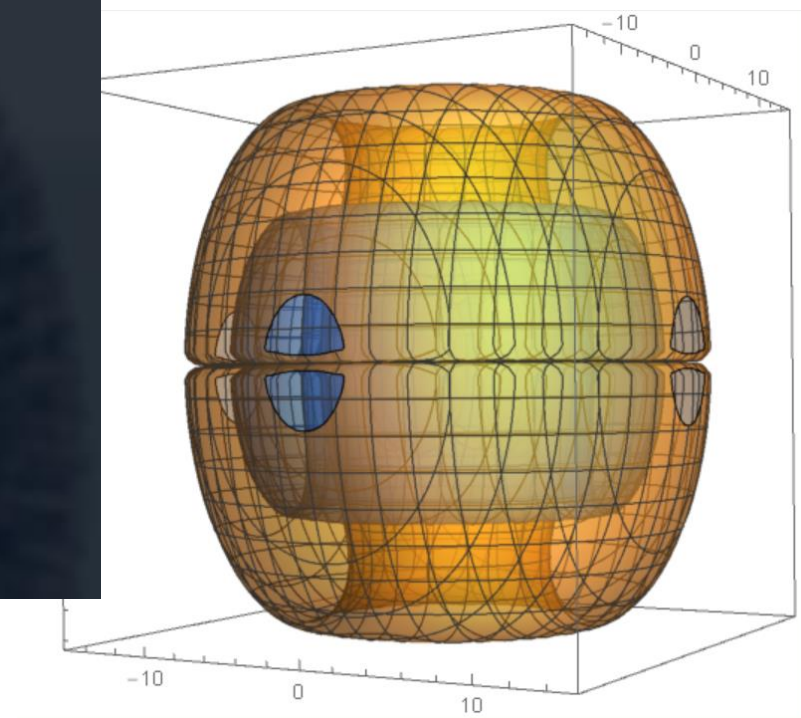
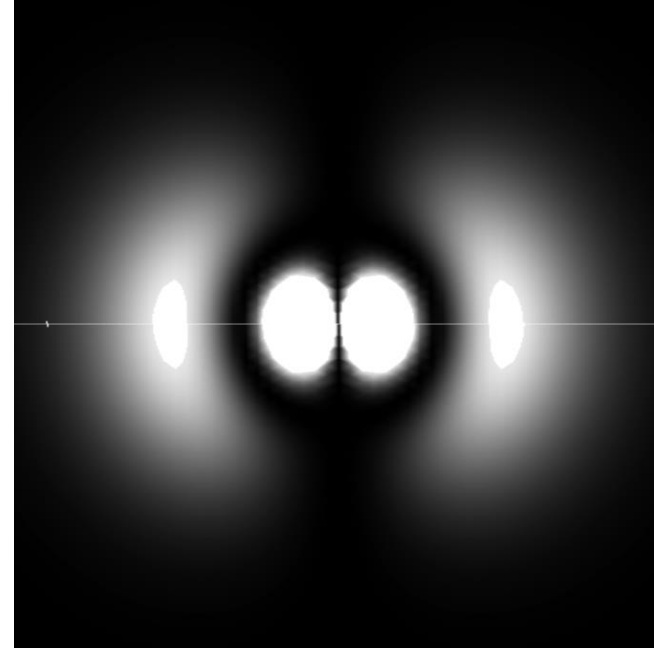
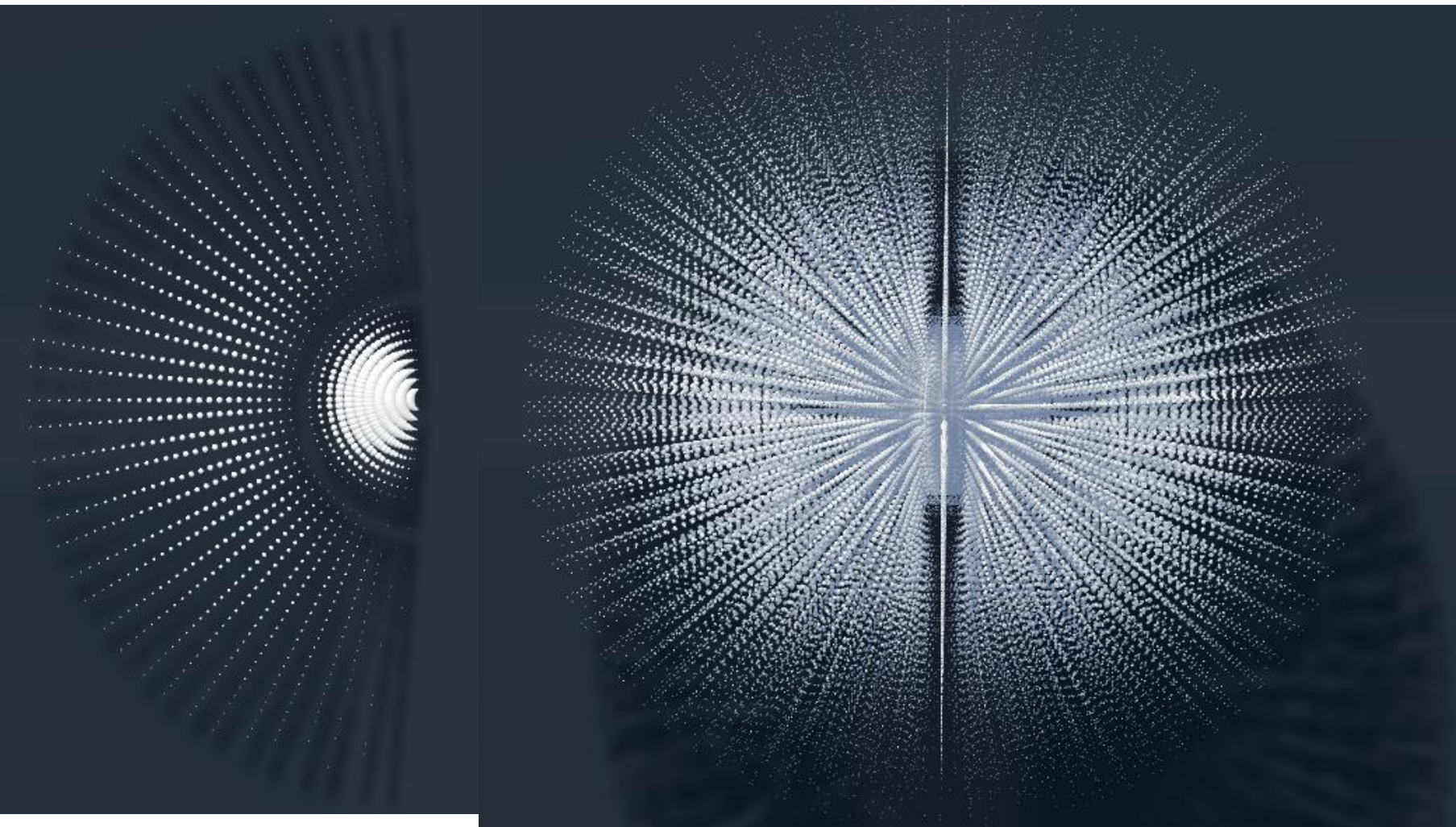


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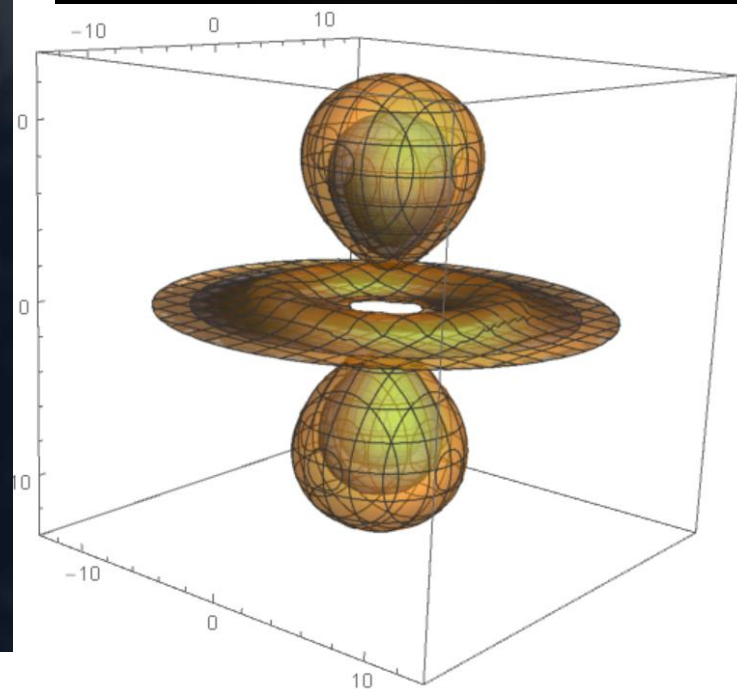
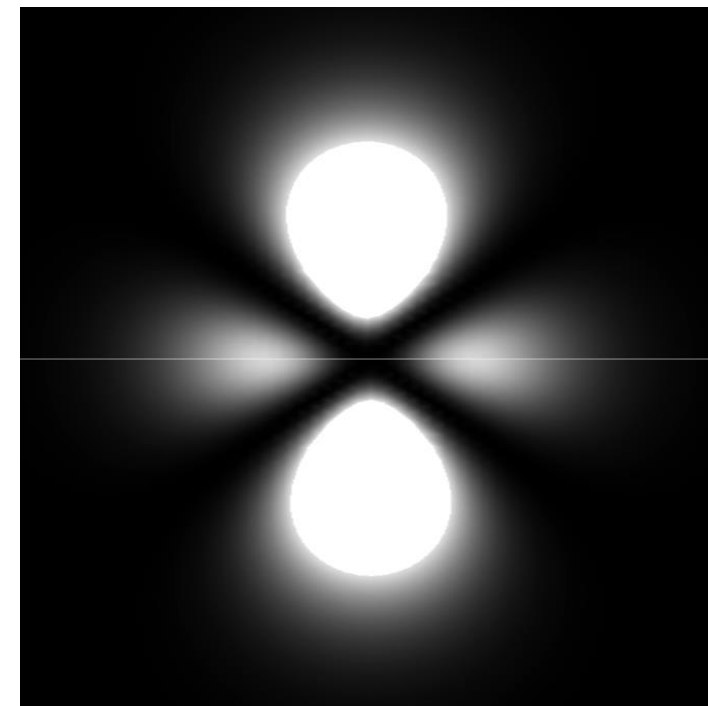
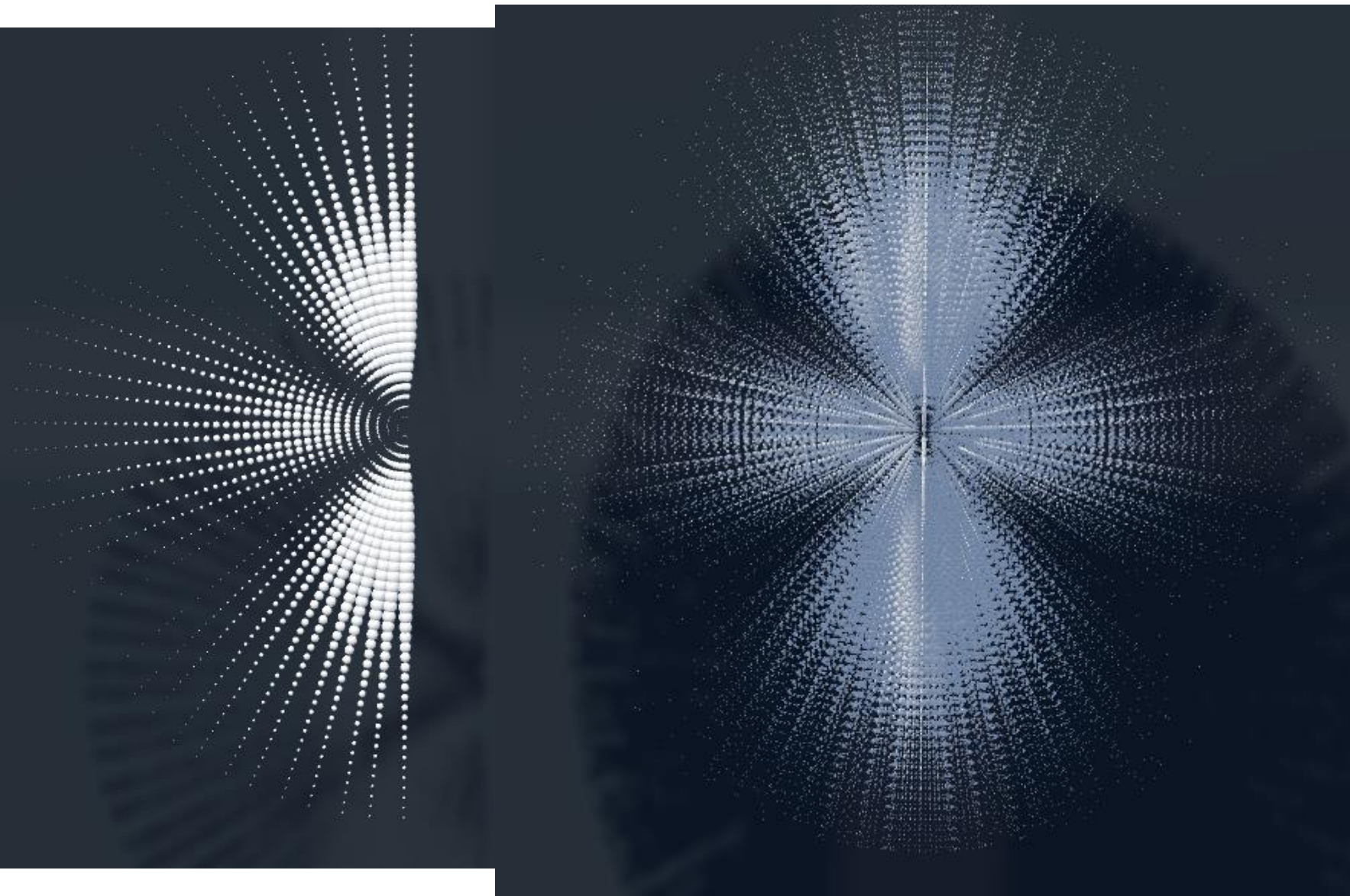


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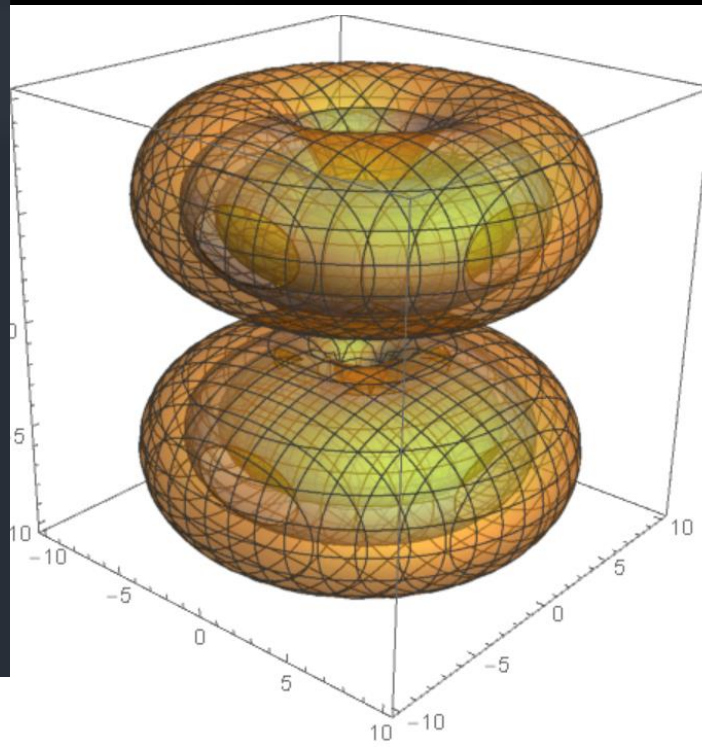
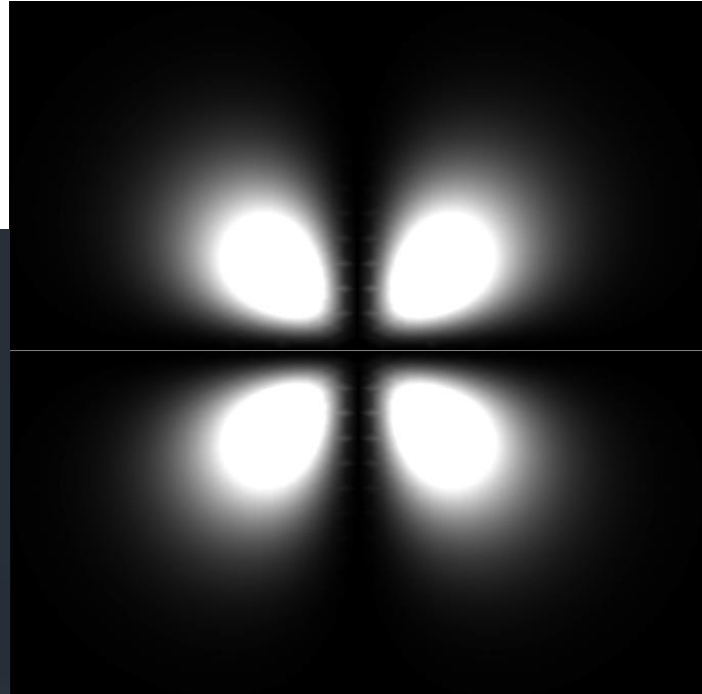
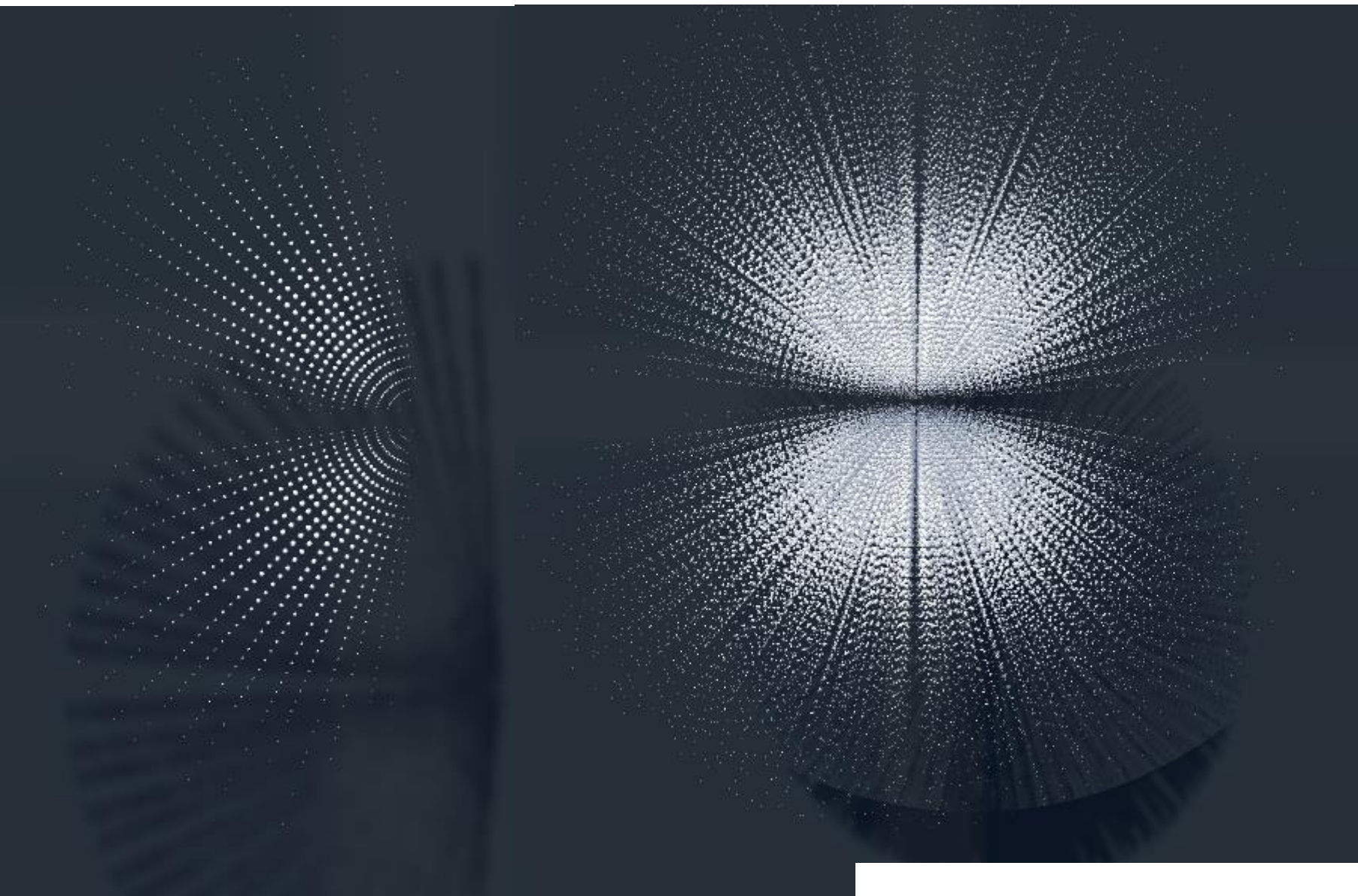


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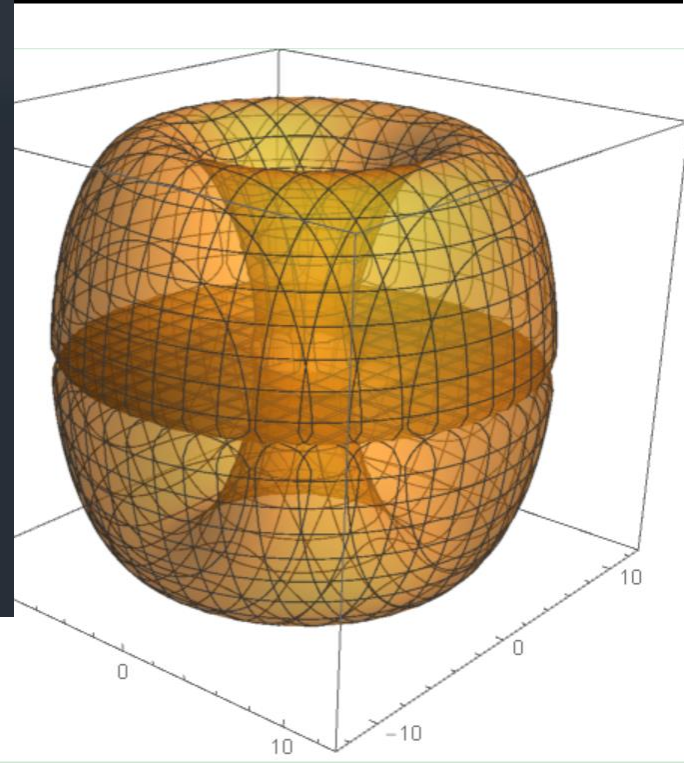
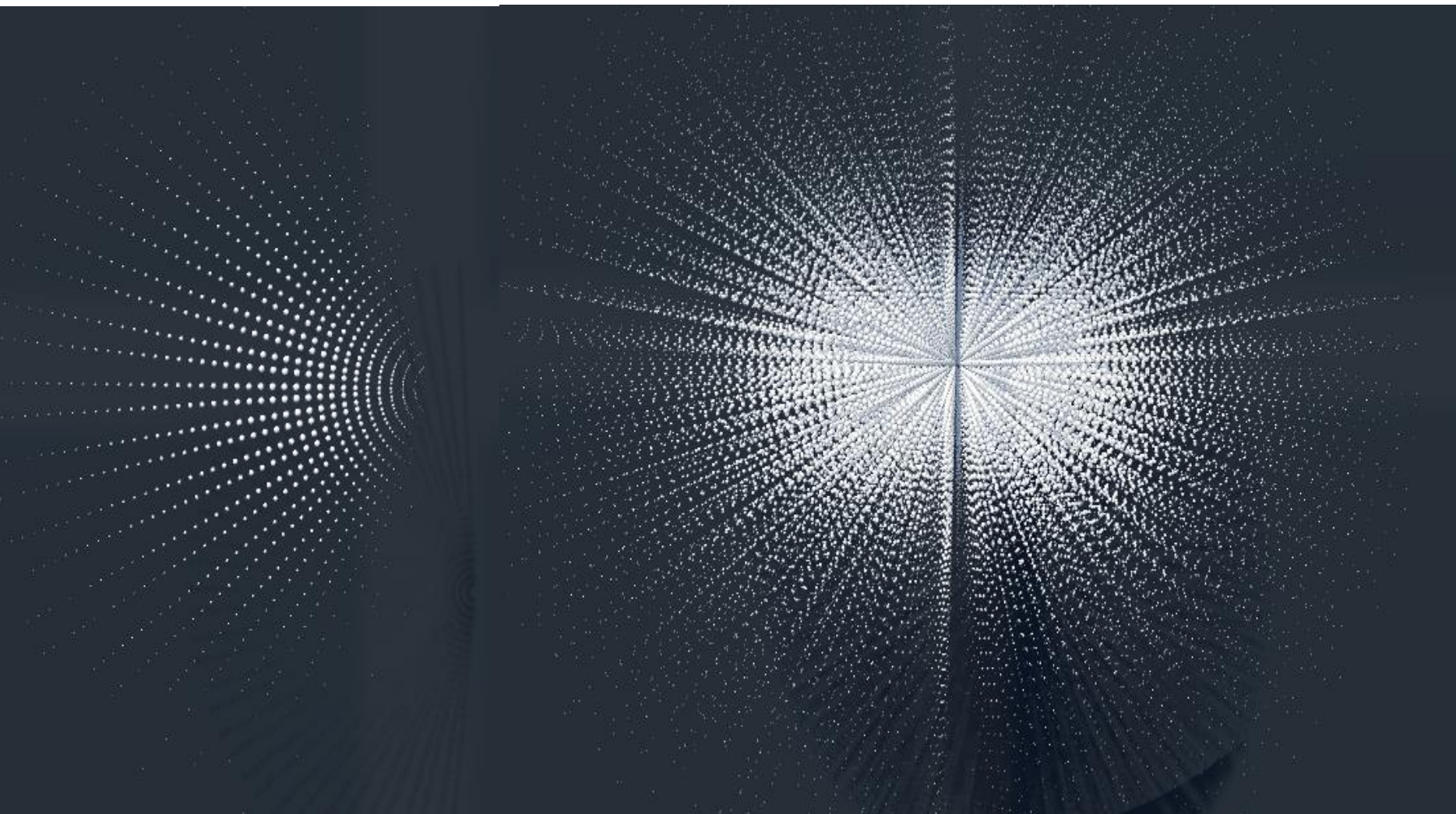


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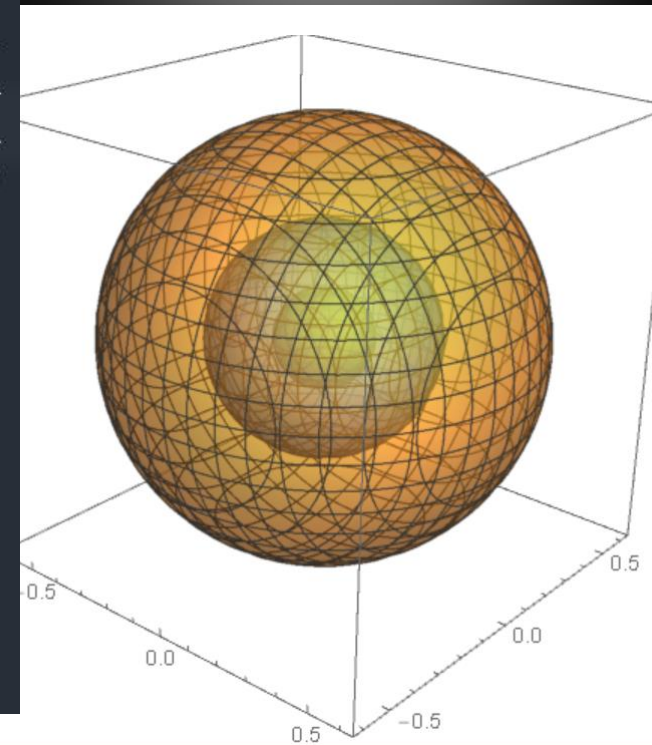
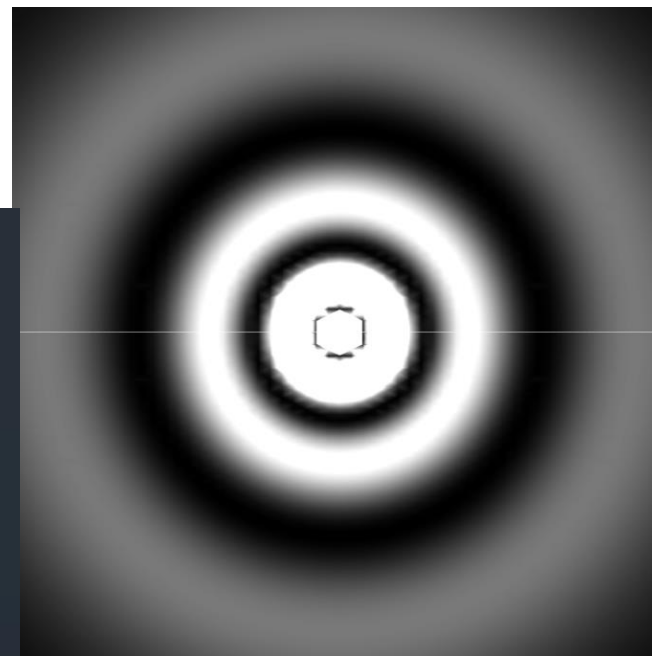
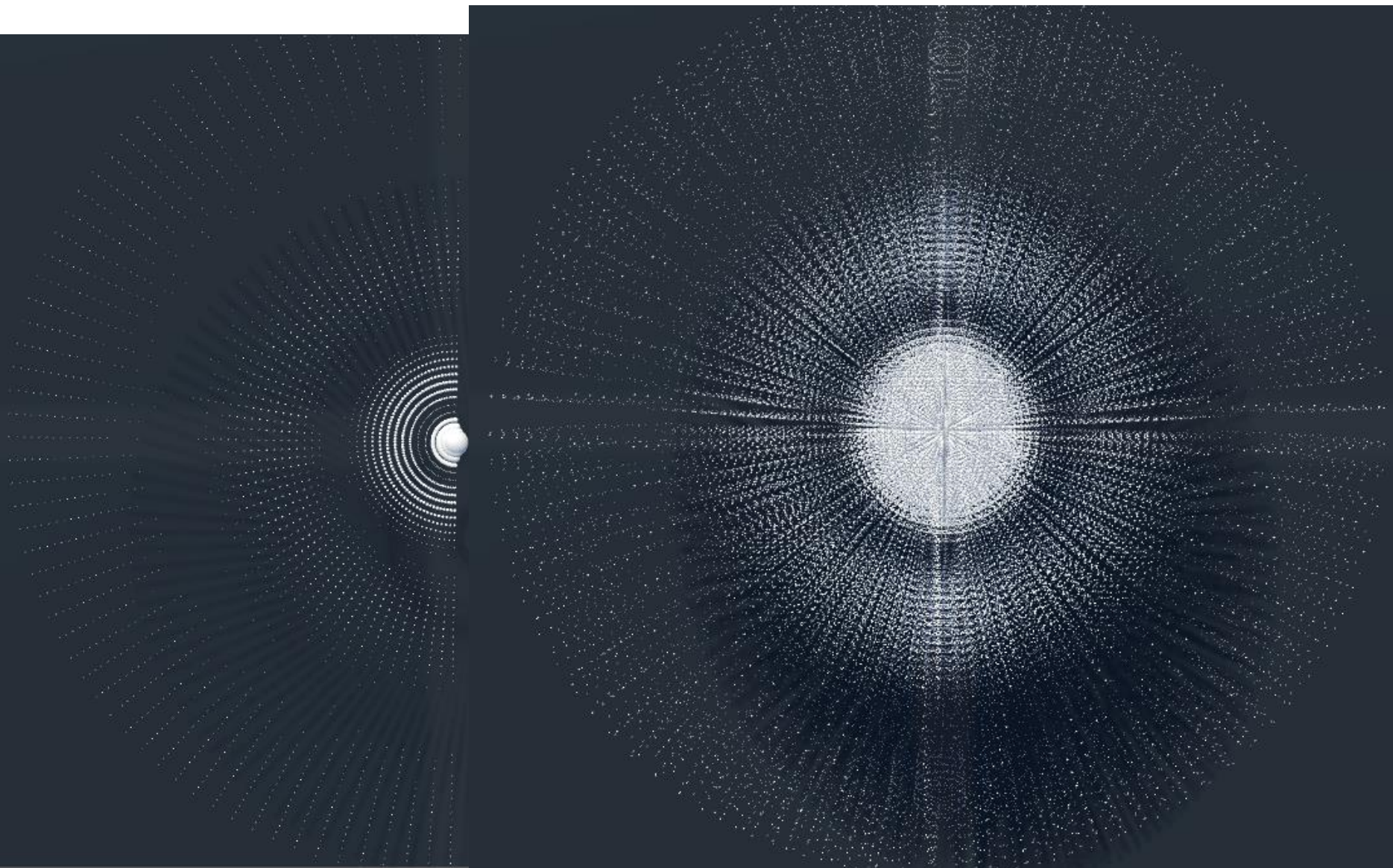


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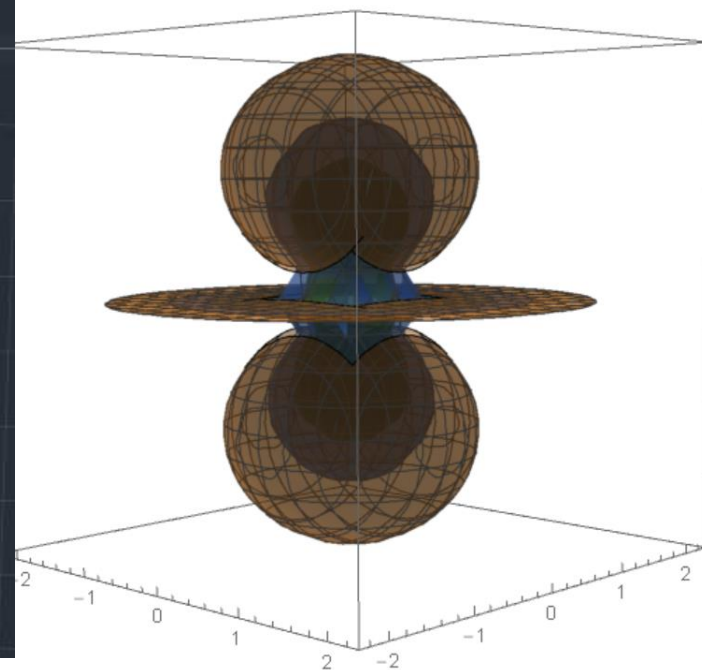
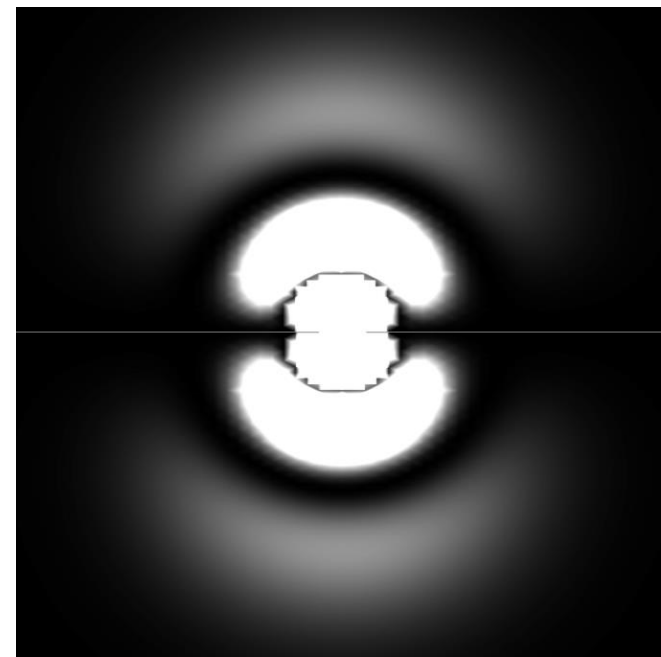
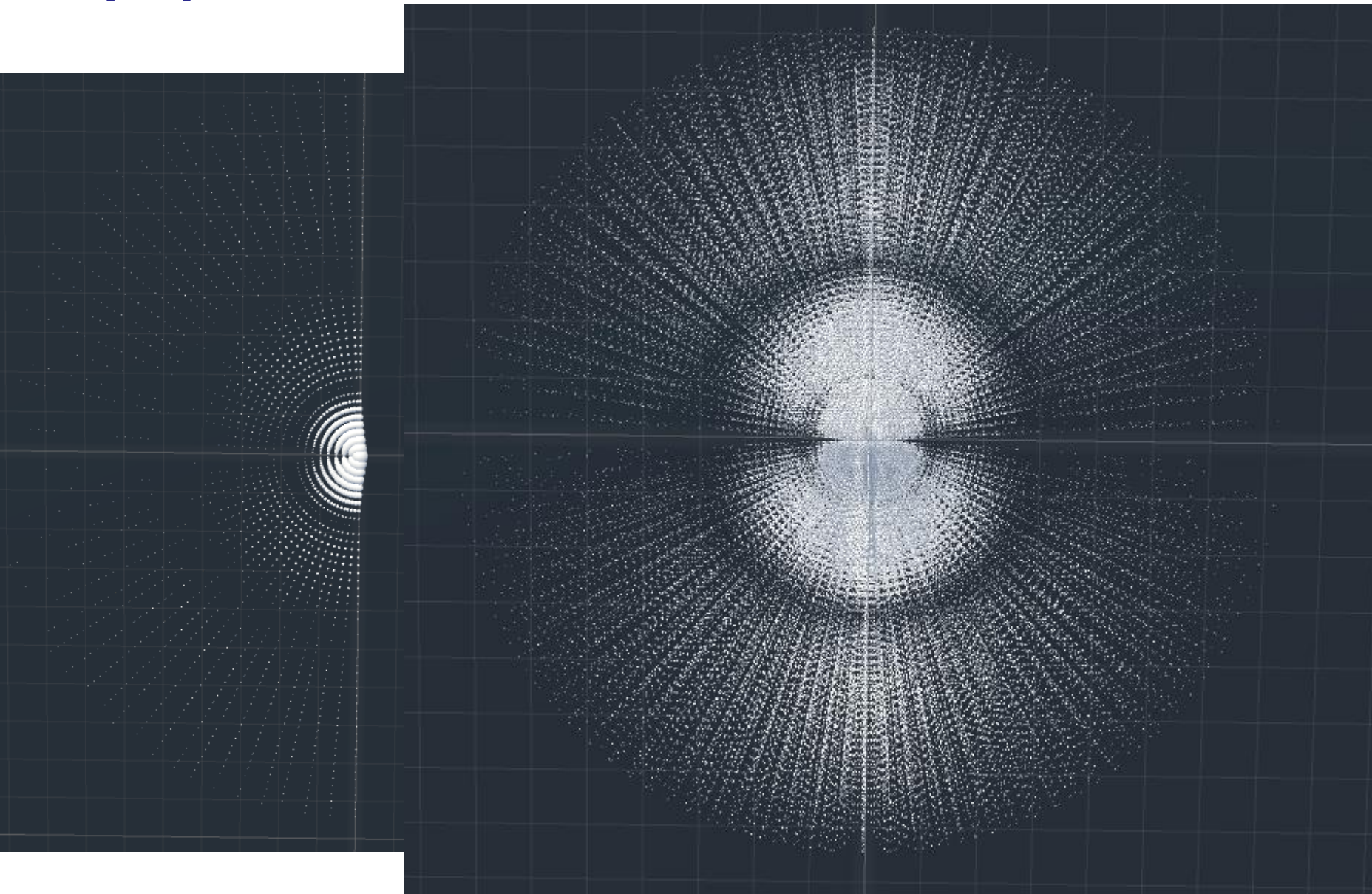


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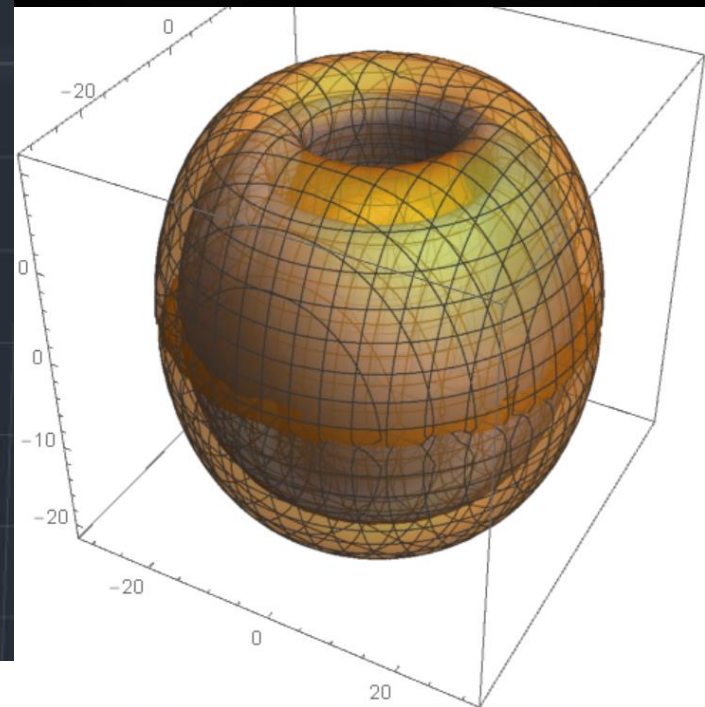
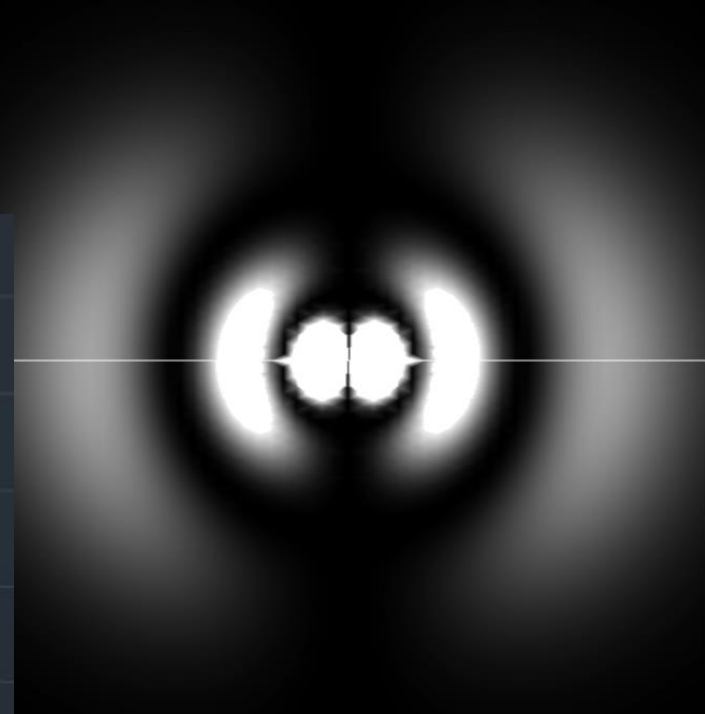
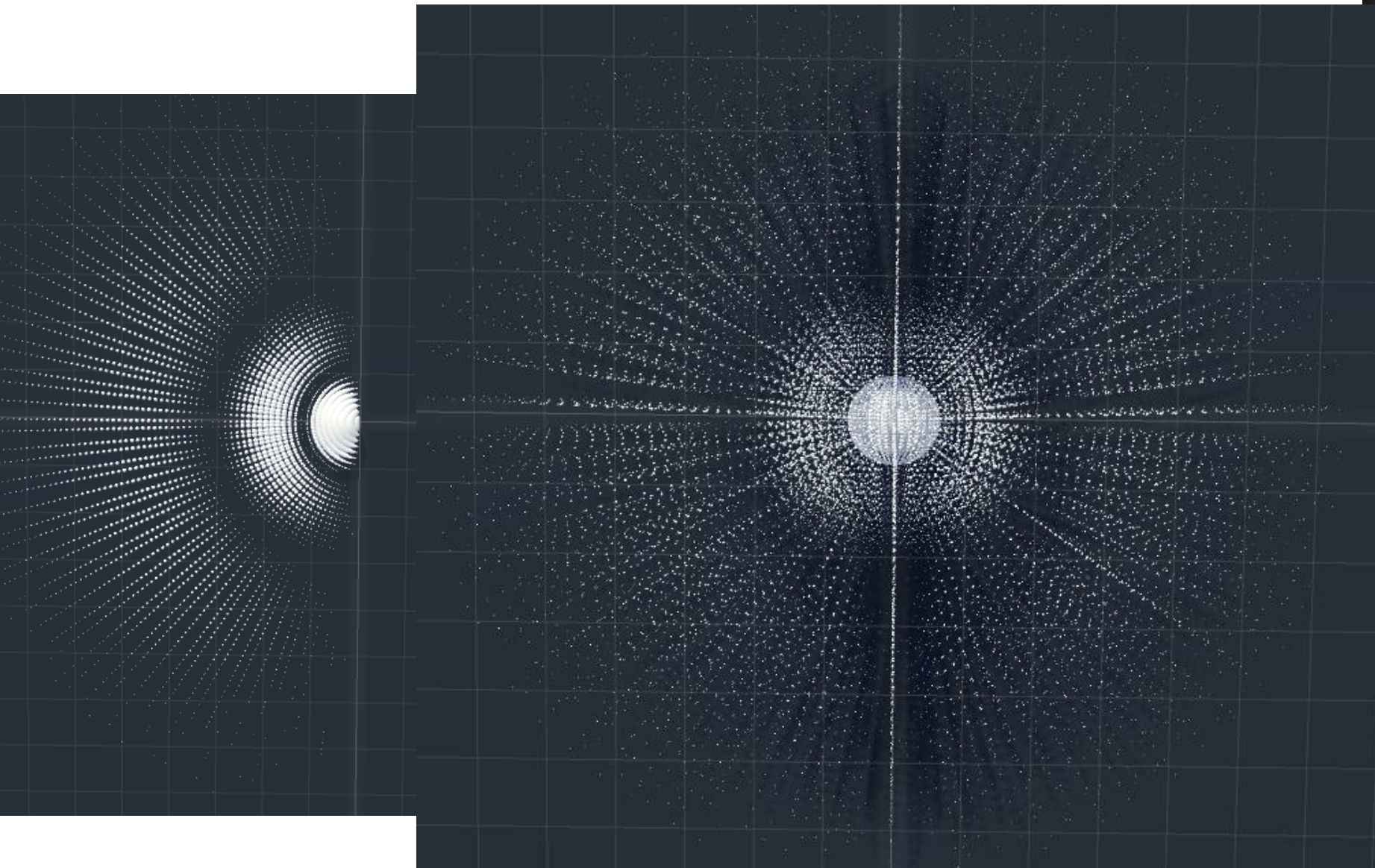


# 4,1,0, 按球坐标搜索



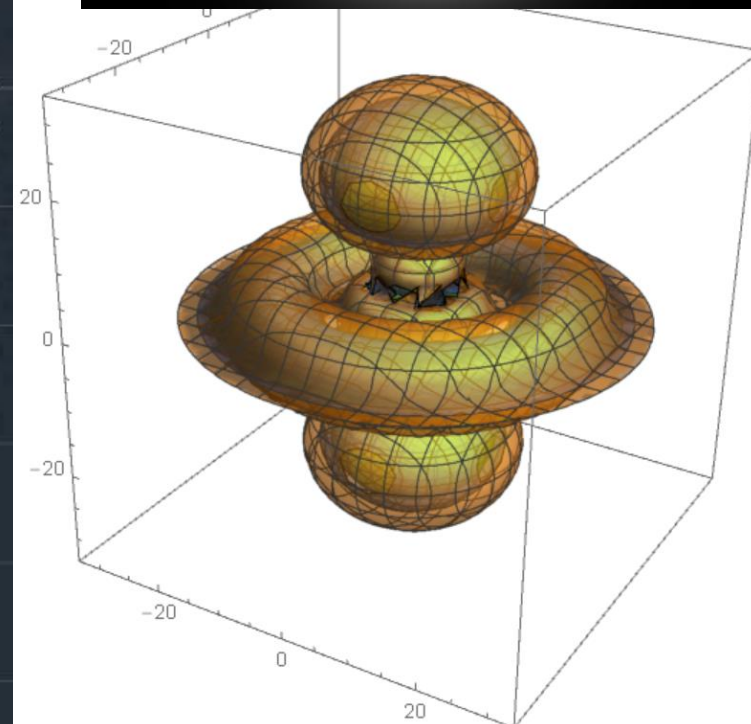
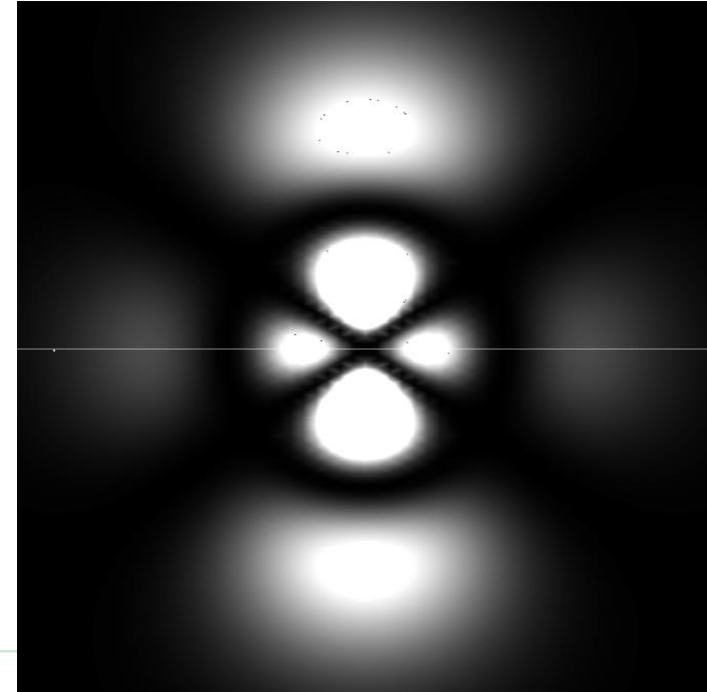
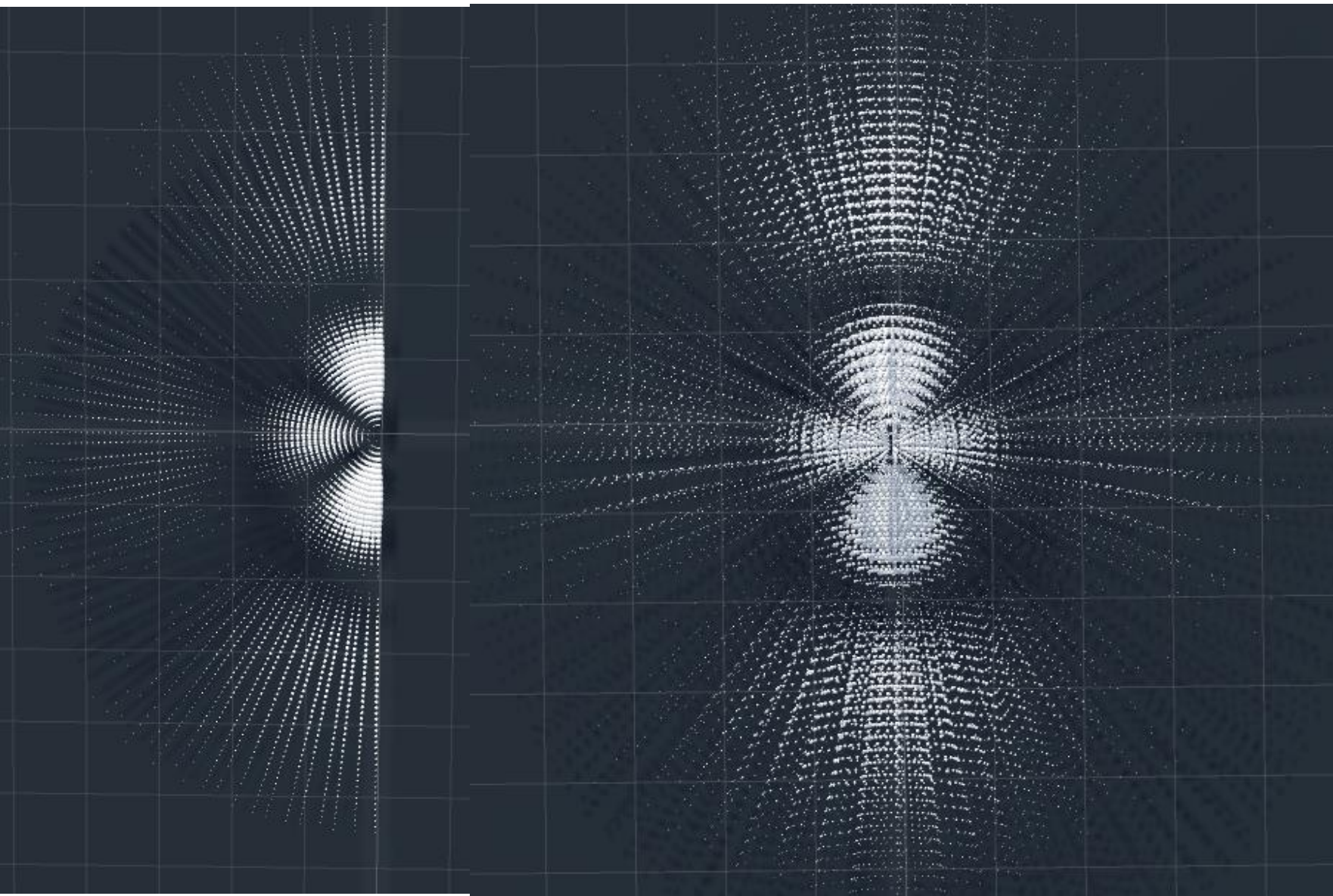


# 4,1,1, 按球坐标搜索



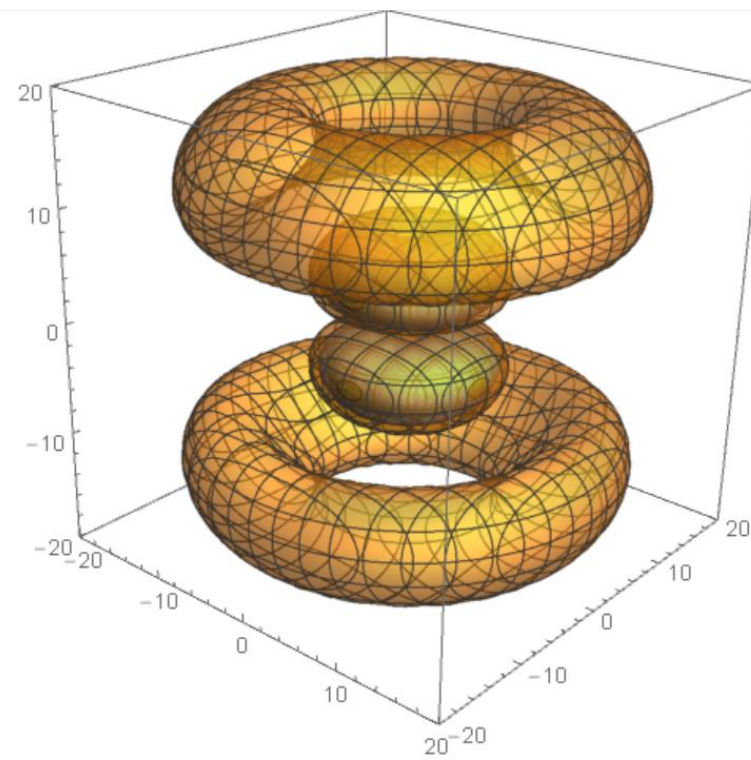
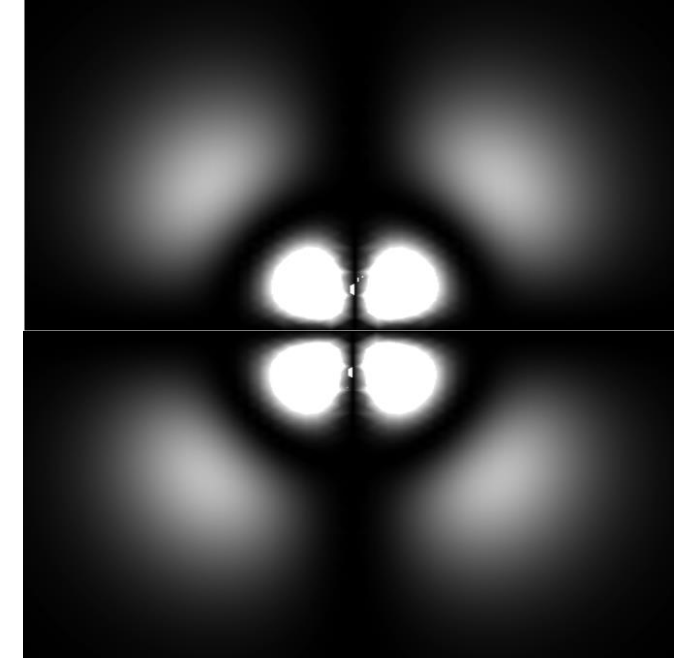
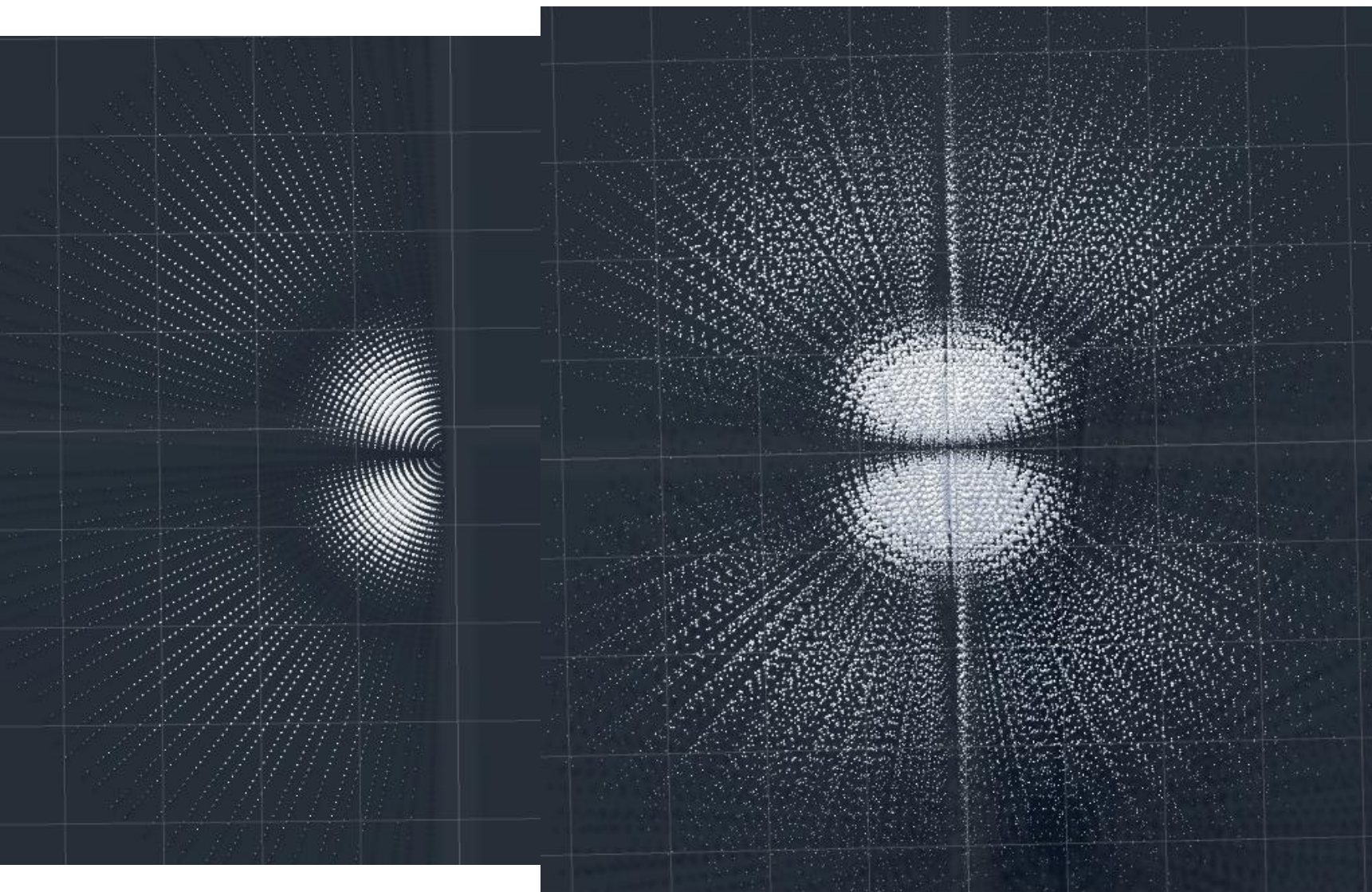


# 4,2,0, 按球坐标搜索



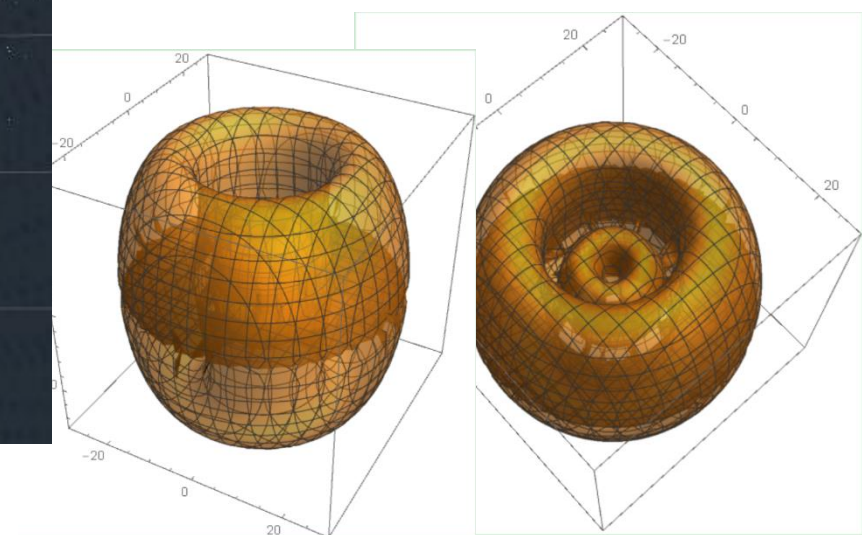
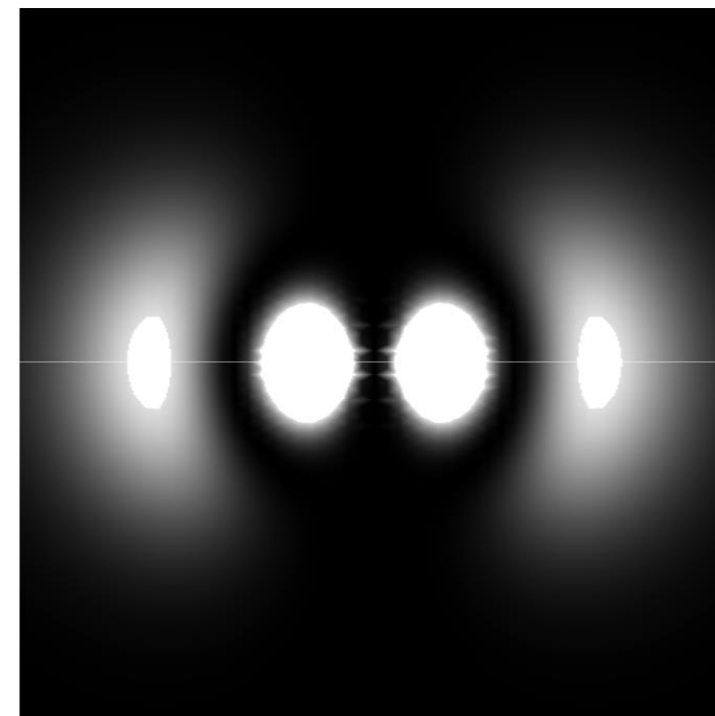
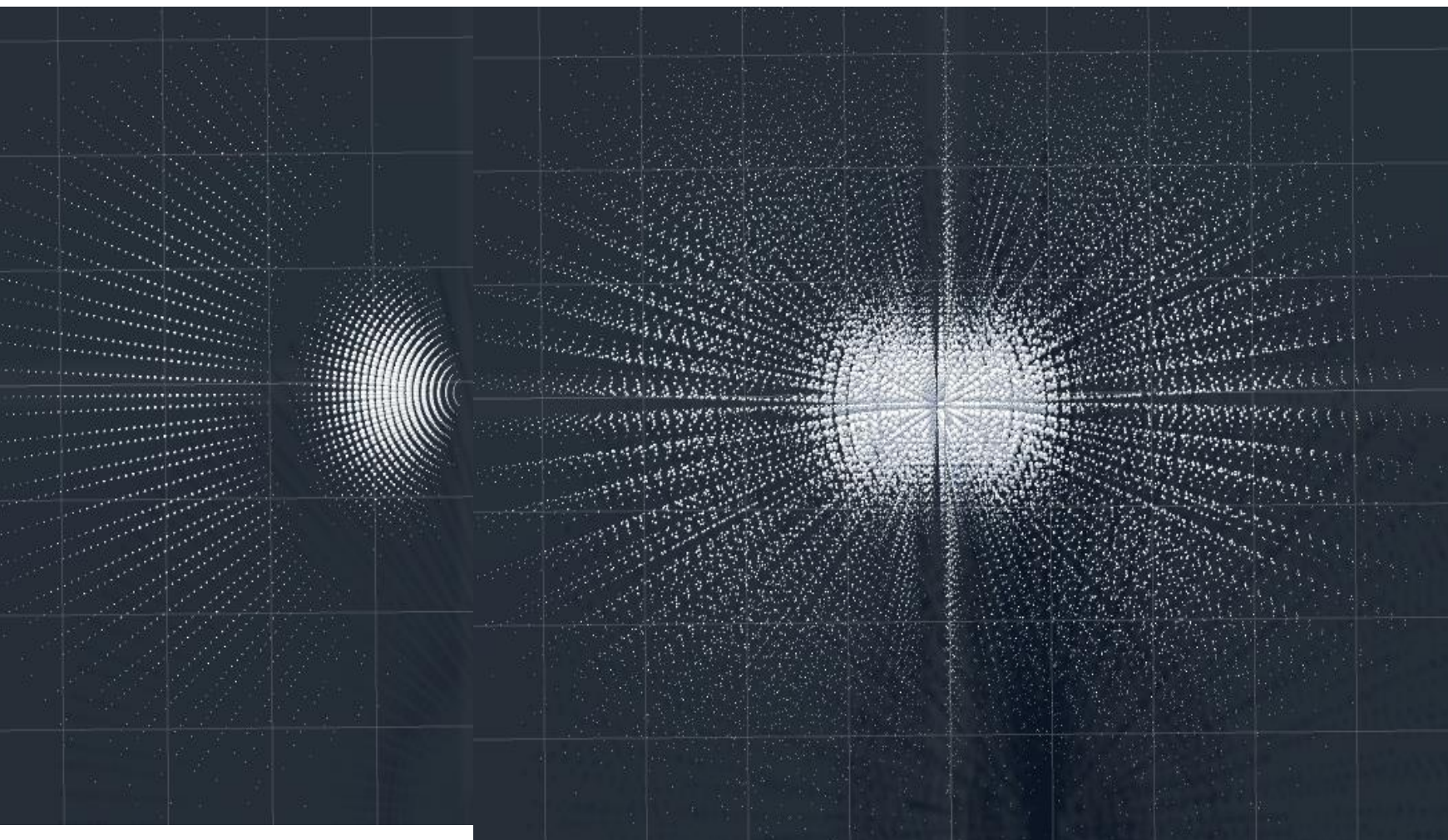


# 4,2,1, 按球坐标搜索



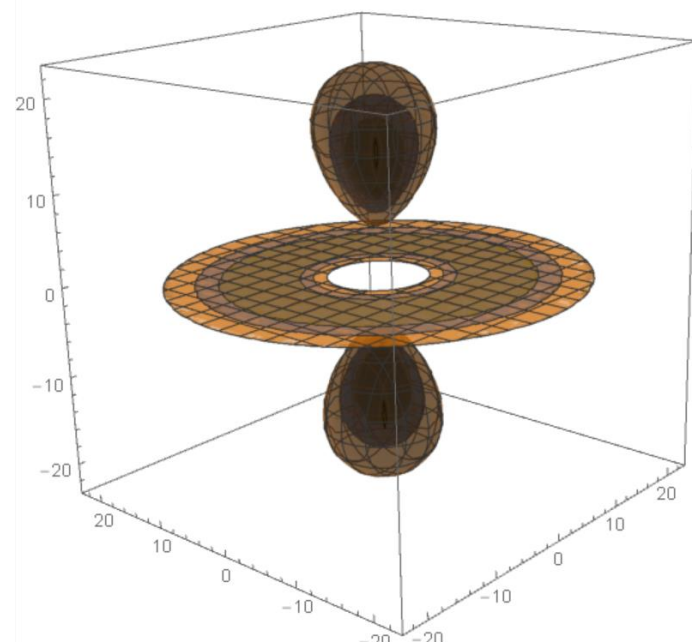
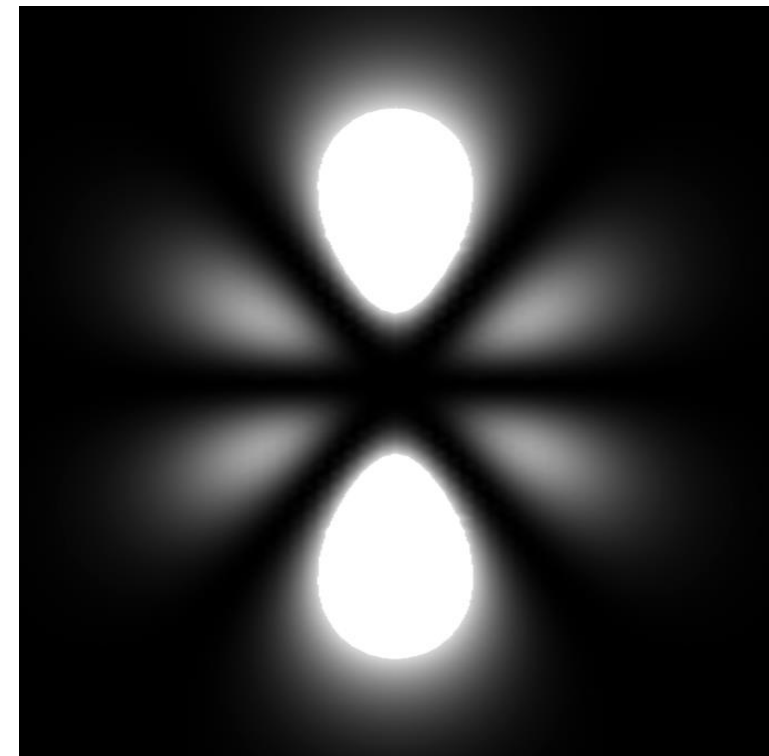
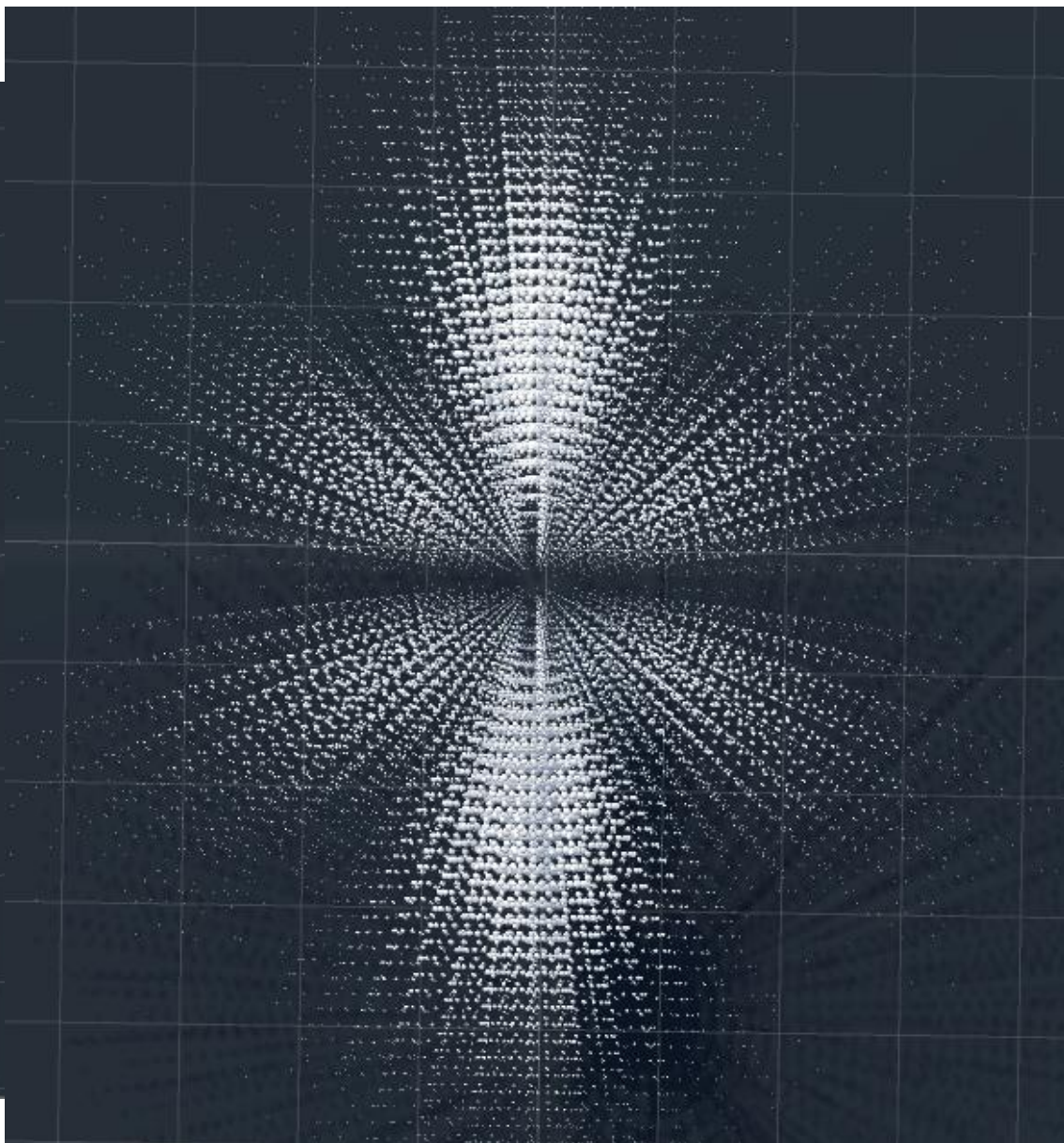
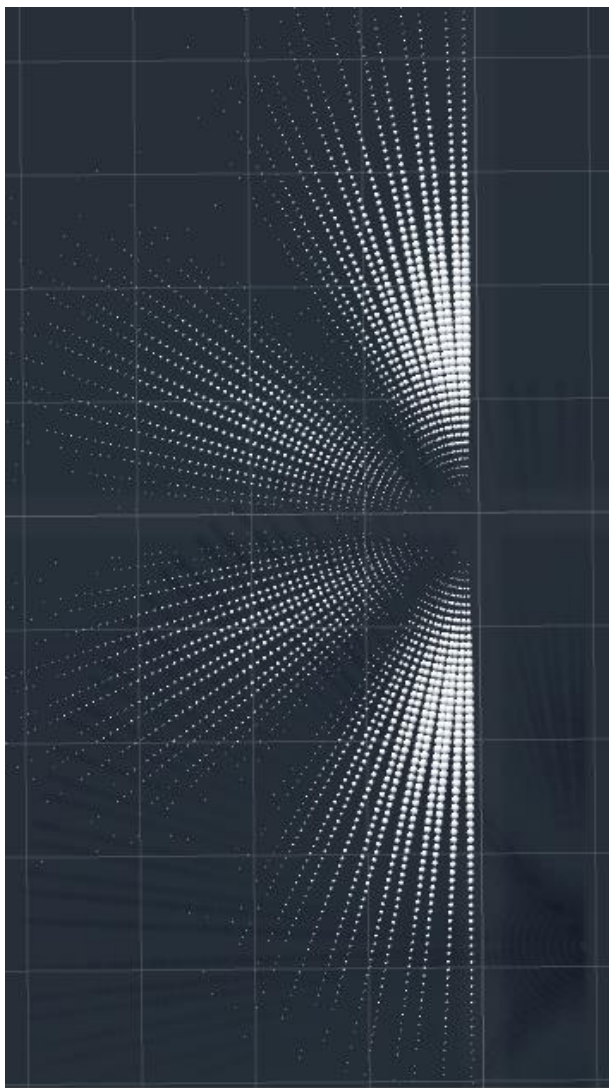


# 4,2,2, 按球坐标搜索



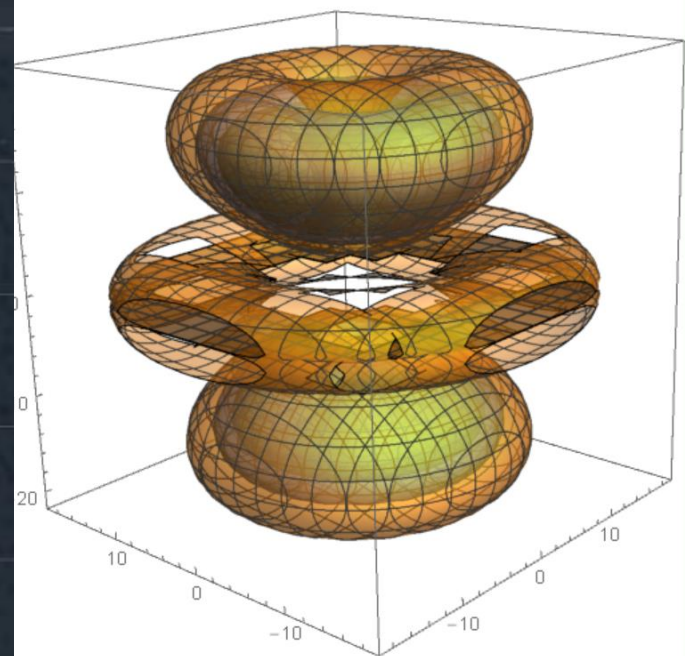
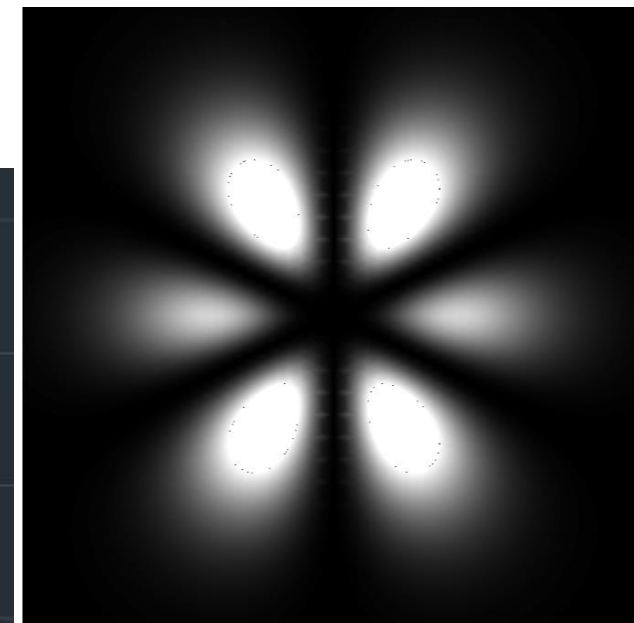
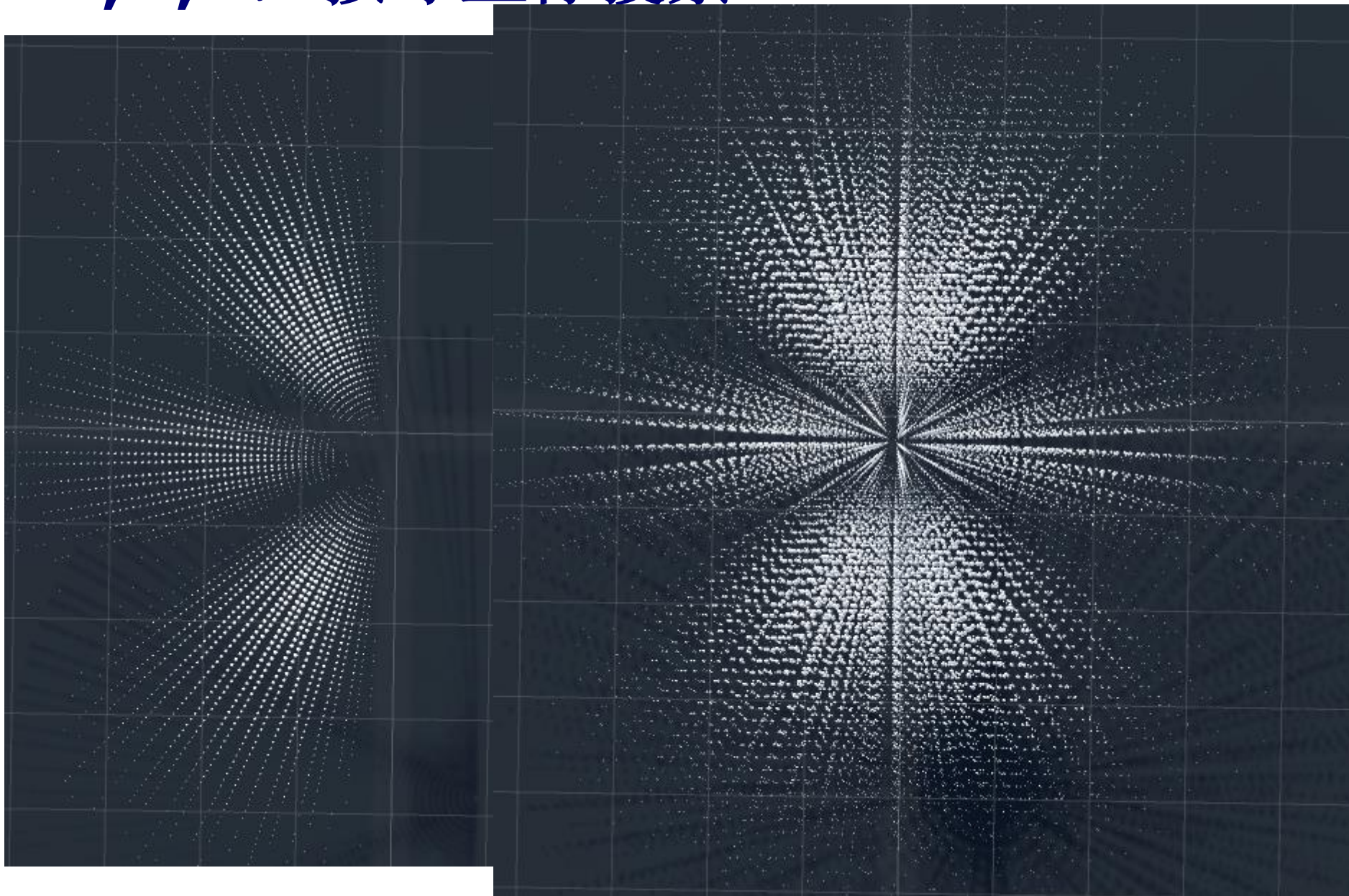


# 4,3,0, 按球坐标搜索



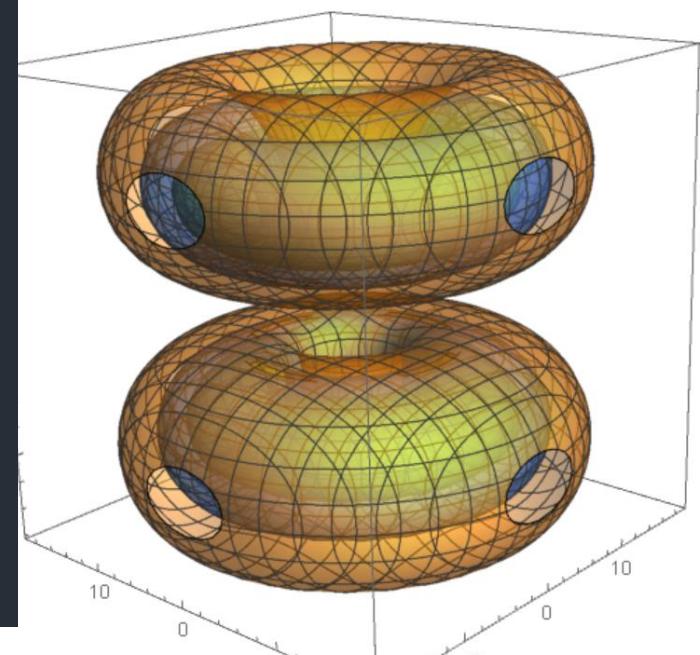
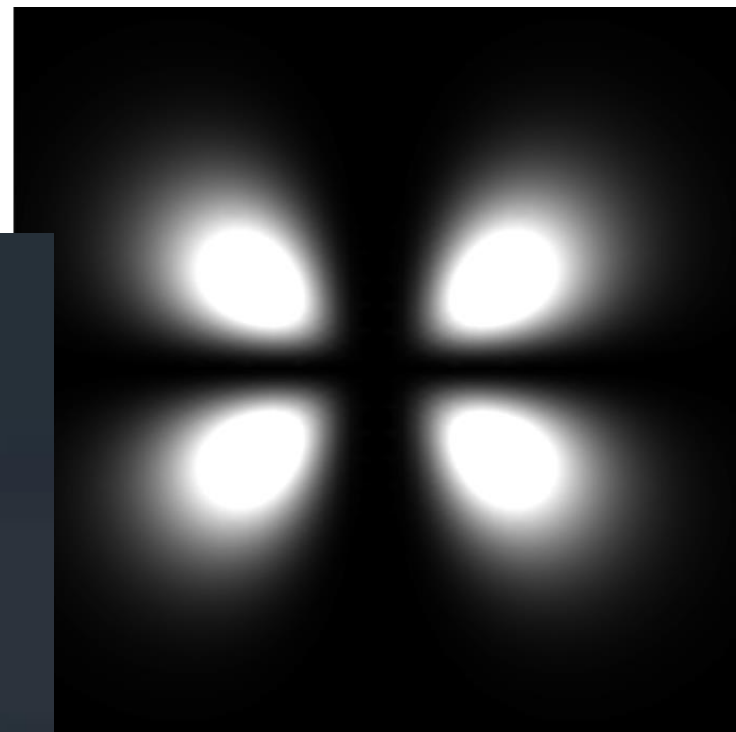
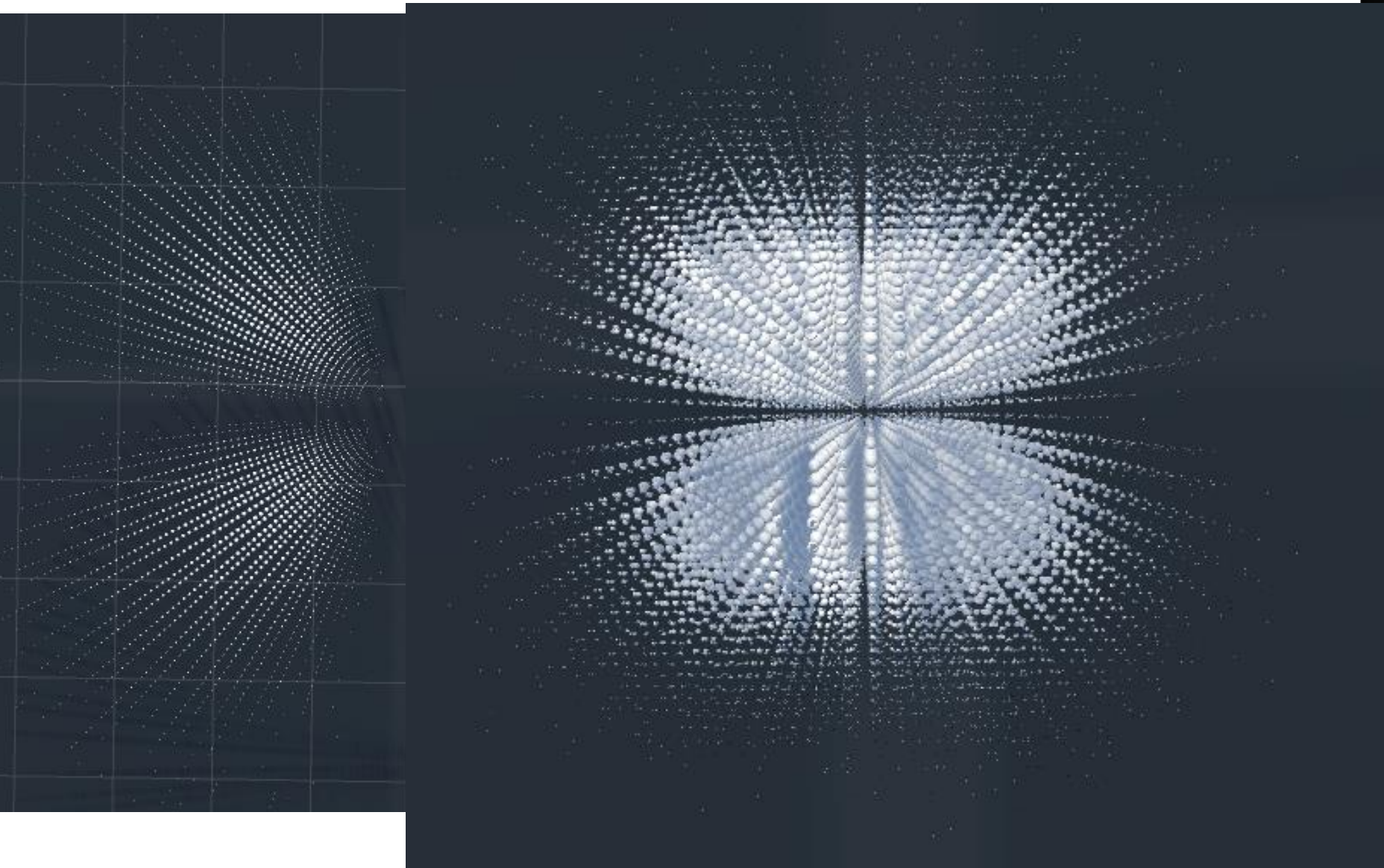


# 4,3,1, 按球坐标搜索



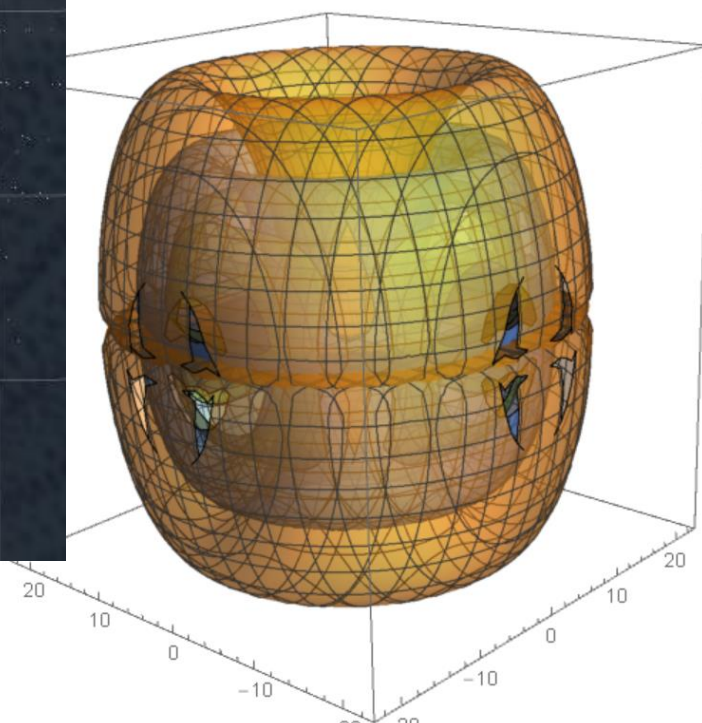
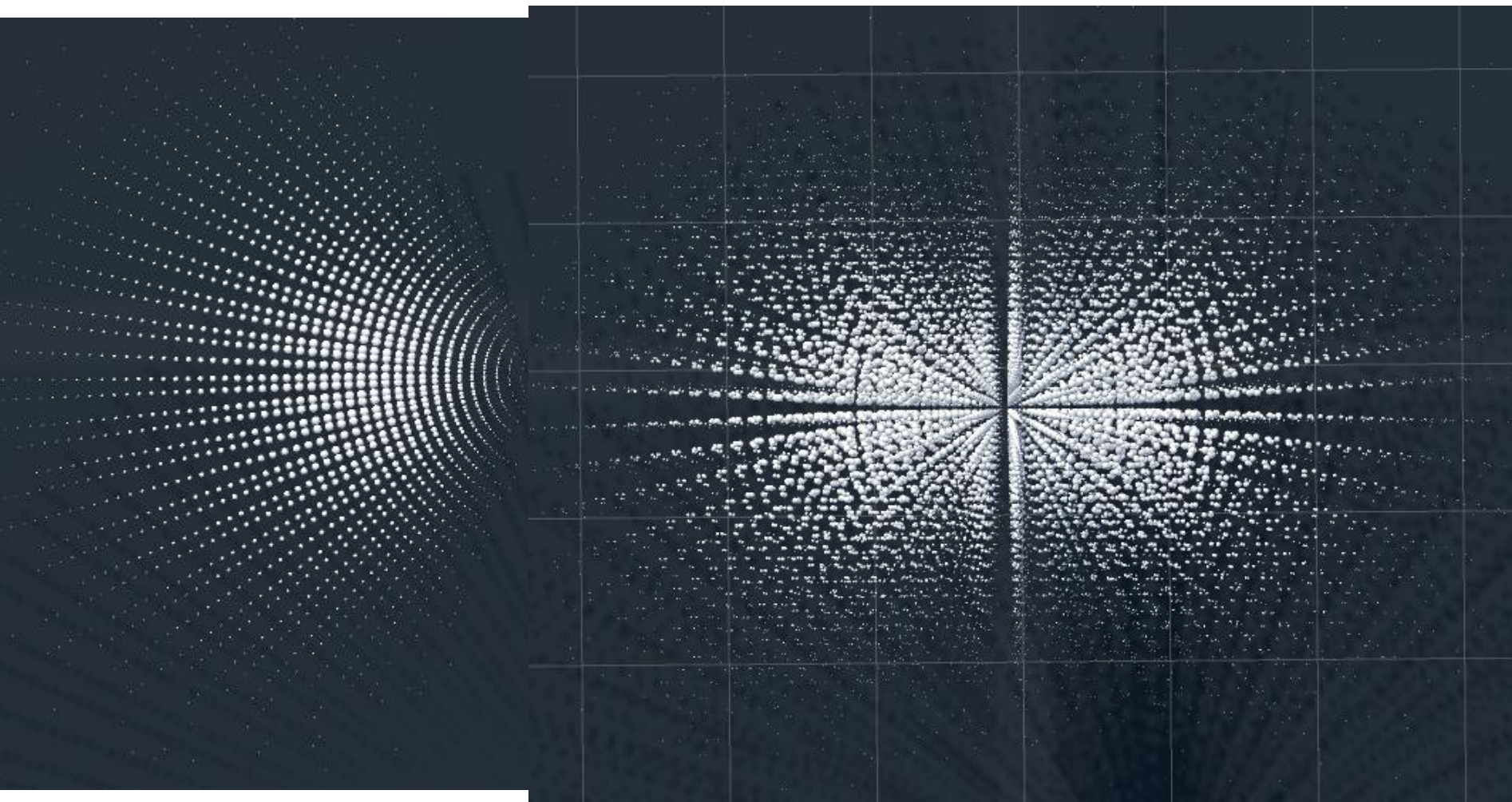


# 4,3,2, 按球坐标搜索





# 4,3,3, 按球坐标搜索



# 后期计划

- 现有结果的优化
- 贴图切片方法
- 人的操纵互动
- 多电子原子
- 共价键的演示
- .....

# 致谢

- 感谢魏老师、黄文凯学长的指导
- 感谢吕老师、沈寒非助教的支持
- 感谢许叶融同学上学期的课题帮助入门

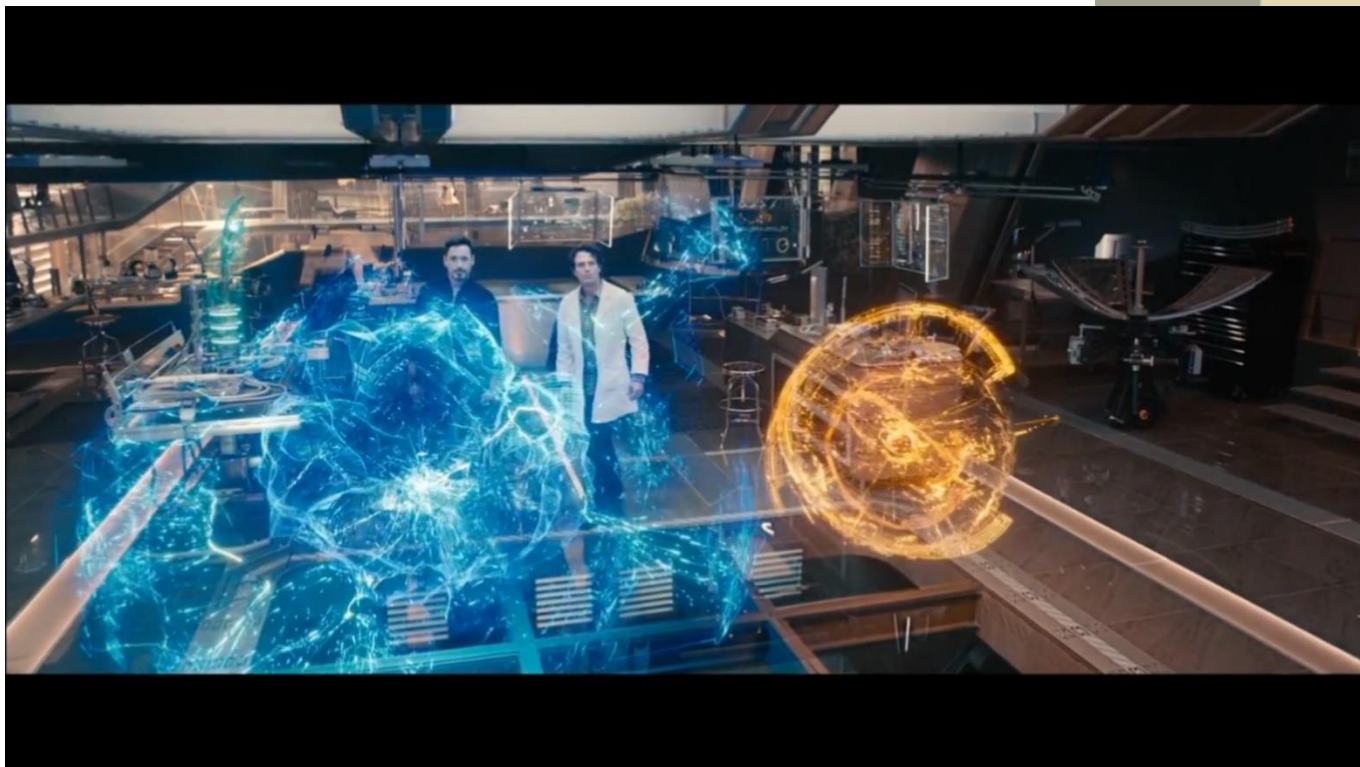
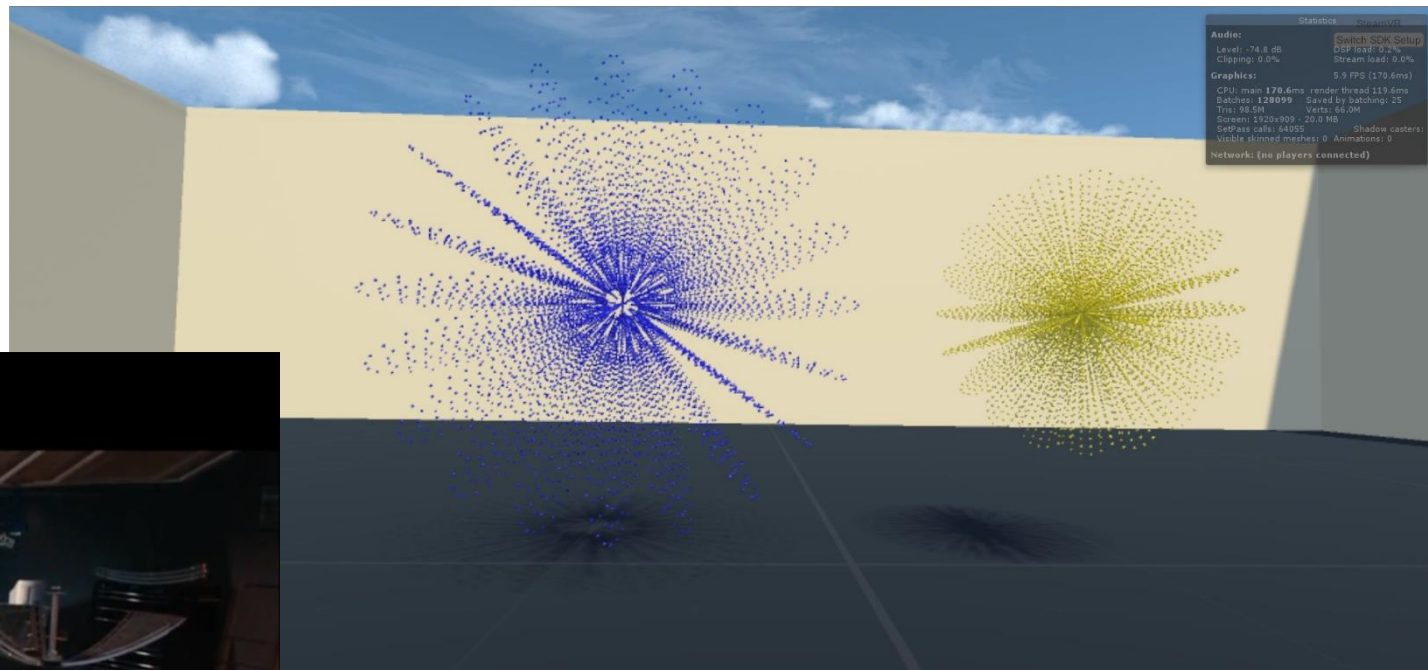
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谢 谢 !



# 彩蛋



# 演示

- 欢迎到隔壁房间去体验