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## Complex rovibrational dynamics of the Ar·NO<sup>+</sup> complex

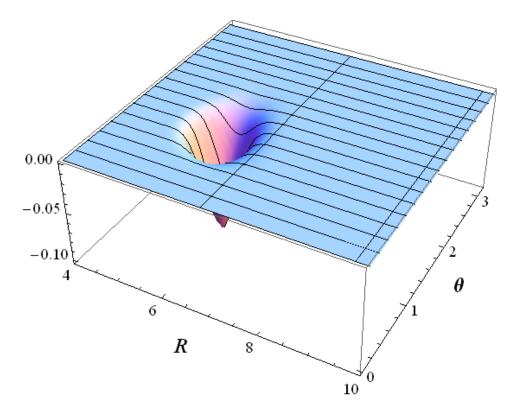
Dóra Papp,<sup>1</sup> János Sarka,<sup>1</sup> Tamás Szidarovszky,<sup>1</sup> Attila G. Császár,<sup>1, a)</sup> Edit Mátyus,<sup>2</sup> Majdi Hochlaf,<sup>3</sup> and Thierry Stoecklin<sup>4, b)</sup>
<sup>1)</sup> MTA-ELTE Complex Chemical Systems Research Group, H-1117 Budapest, Pázmány Péter sétány 1/A, Hungary
<sup>2)</sup> Institute of Chemistry, Eötvös Loránd University, H-1117 Budapest, Pázmány Péter sétány 1/A, Hungary
<sup>3)</sup> Université Paris-Est, Laboratoire Modélisation et Simulation Multi Echelle, MSME UMR 8208 CNRS, 5 bd Descartes, 77454 Marne-la-Vallée, France
<sup>4)</sup> Institut des Sciences Moléculaires, Université de Bordeaux, CNRS UMR 5255, 33405 Talence Cedex, France

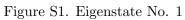
## Bound state wave function plots

2D cuts of the wave functions of all the 200 vibrational bound states of the Ar–NO<sup>+</sup> complex along the R and  $\theta$  Jacobi coordinates obtained from variational GENIUSH computations. The third r coordinate is held fixed at its equilibrium value. Energies corresponding to the eigenstates reported here can be found in the text file of the Electronic Supplementary Information.

<sup>&</sup>lt;sup>a)</sup>csaszar@chem.elte.hu

<sup>&</sup>lt;sup>b)</sup>thierry.stoecklin@u-bordeaux.fr





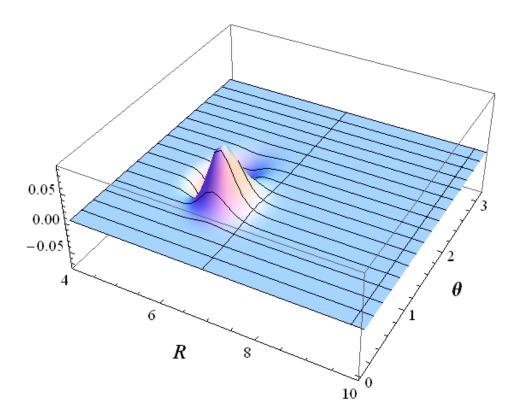
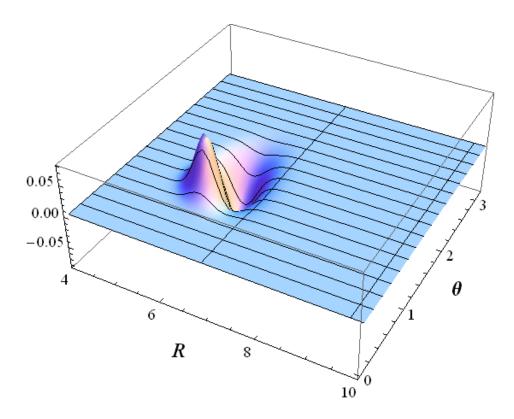
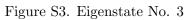


Figure S2. Eigenstate No. 2





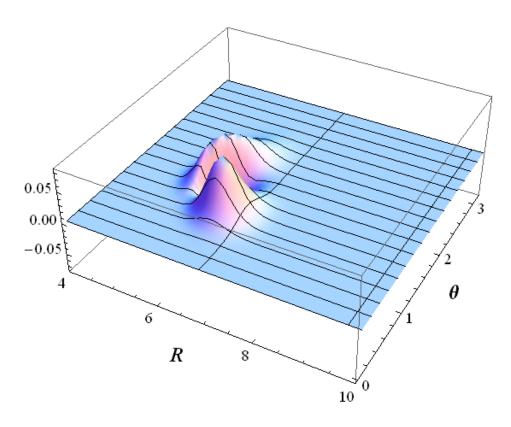
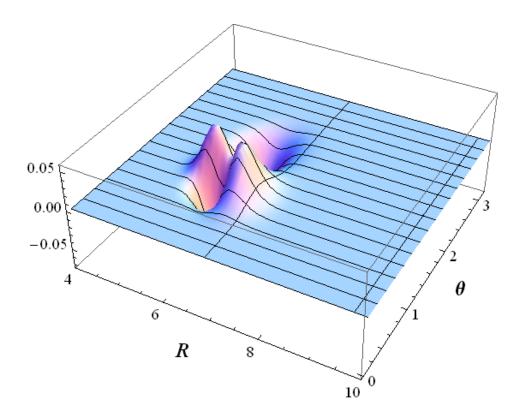
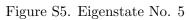


Figure S4. Eigenstate No. 4





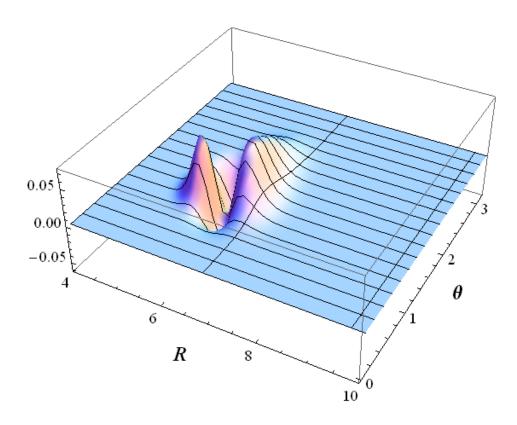


Figure S6. Eigenstate No. 6

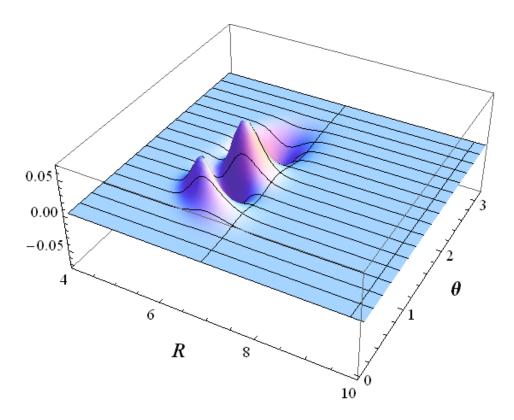


Figure S7. Eigenstate No. 7

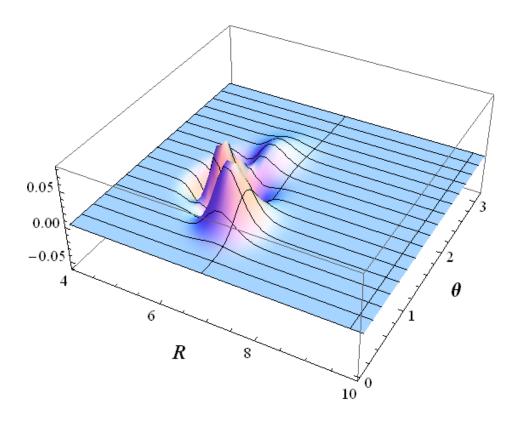
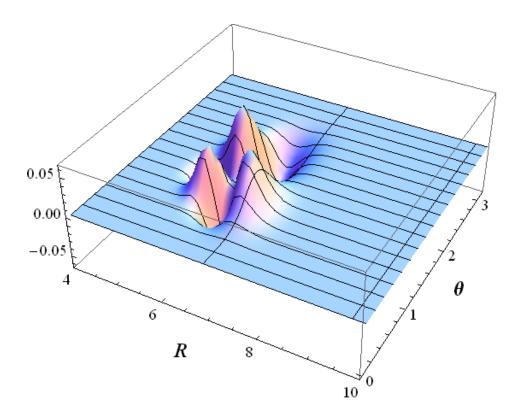
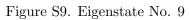


Figure S8. Eigenstate No. 8





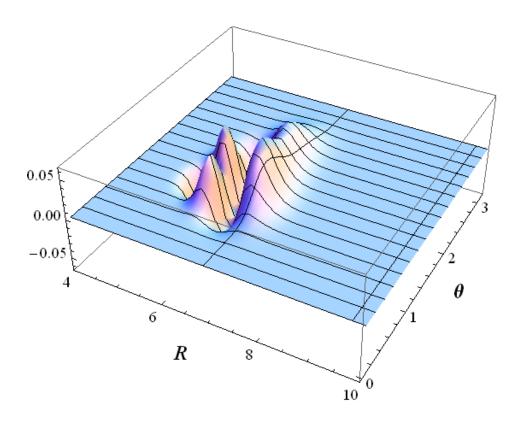


Figure S10. Eigenstate No. 10

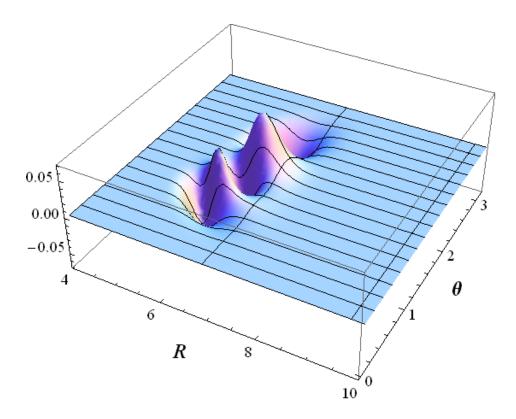


Figure S11. Eigenstate No. 11

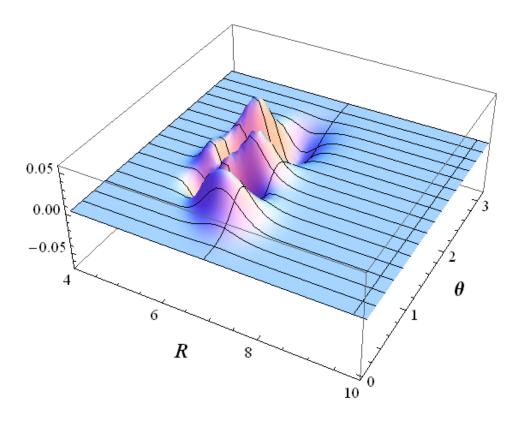


Figure S12. Eigenstate No.  $12\,$ 

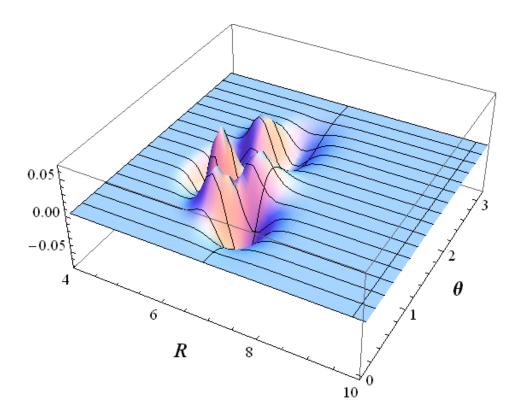


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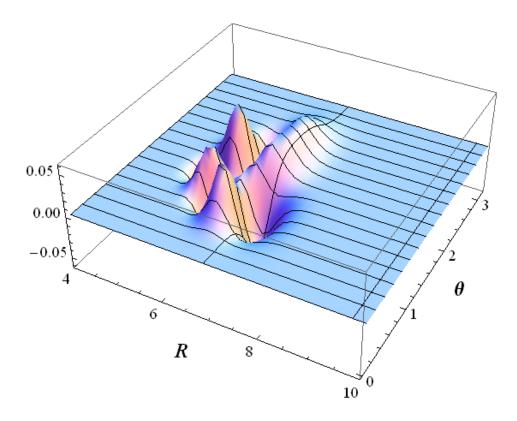


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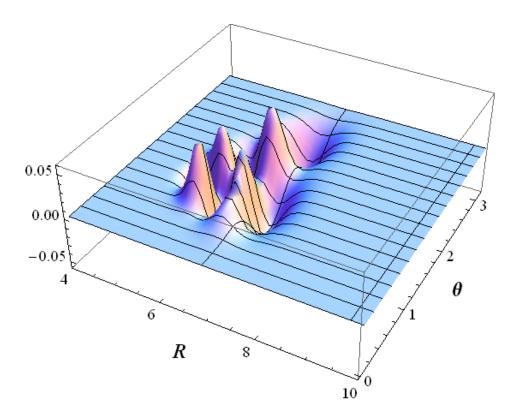


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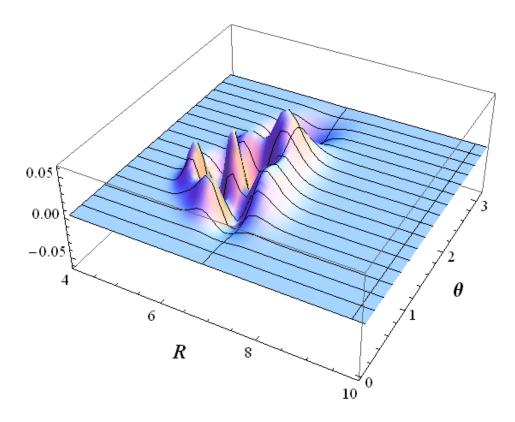


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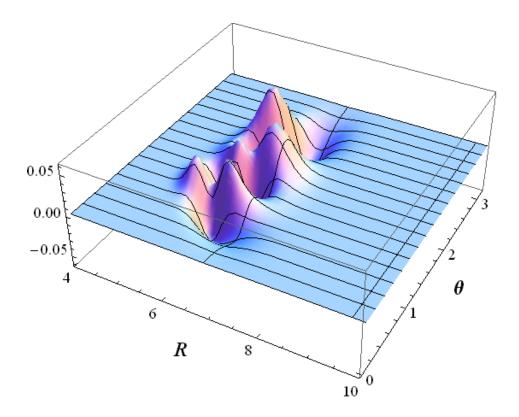


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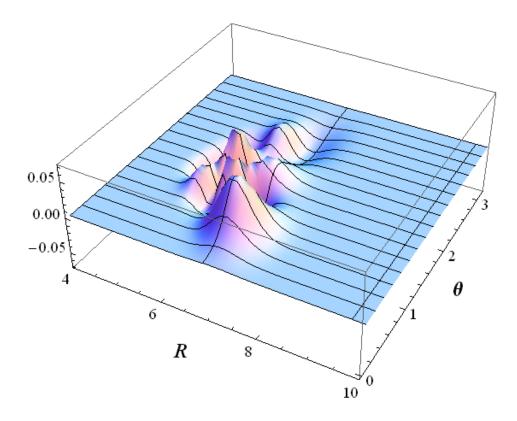


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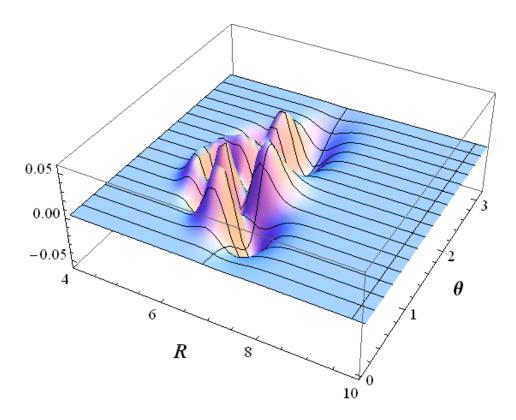


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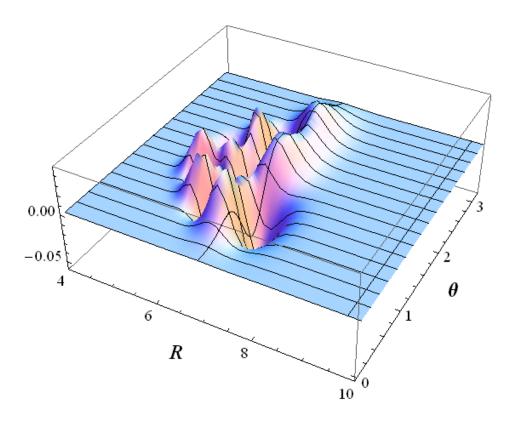


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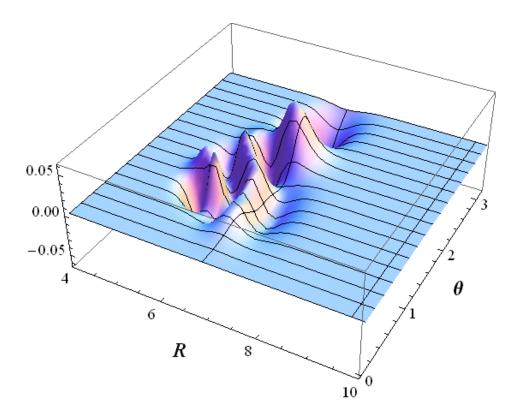


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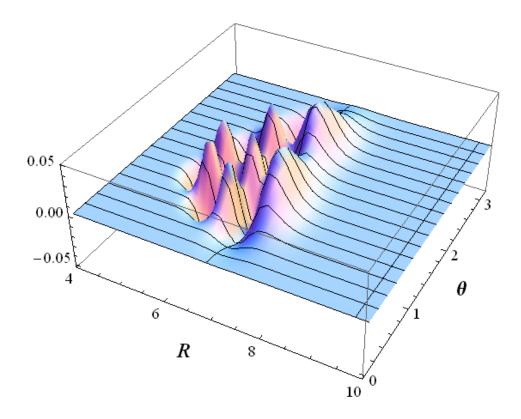


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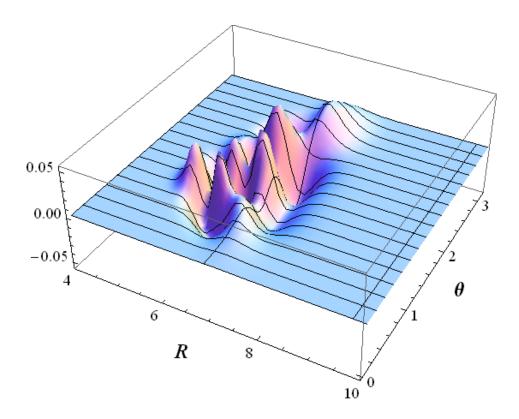


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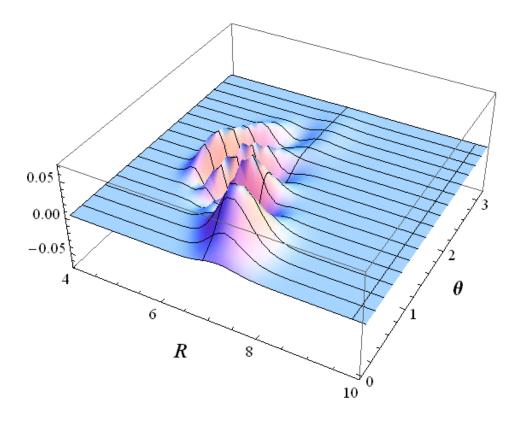


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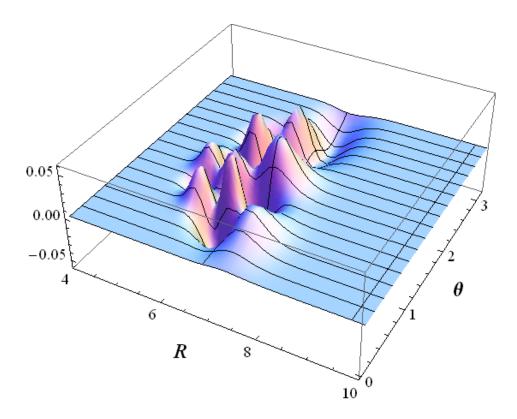


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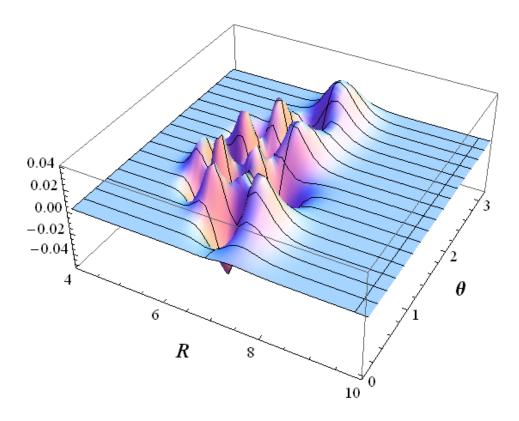


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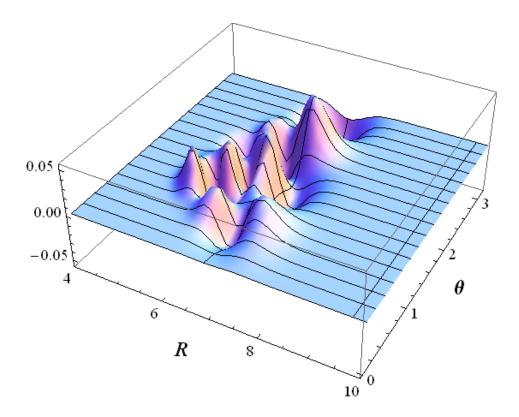


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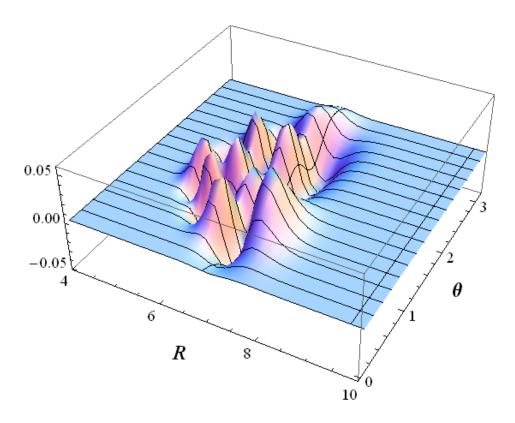


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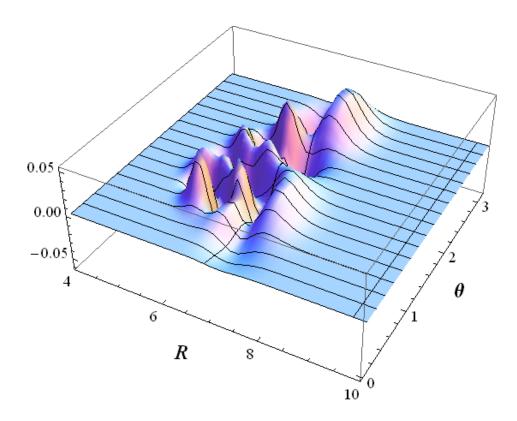


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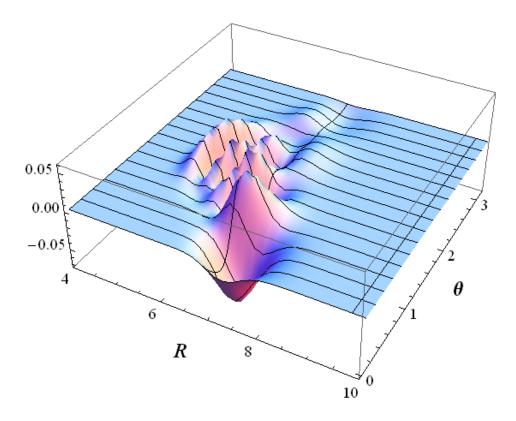


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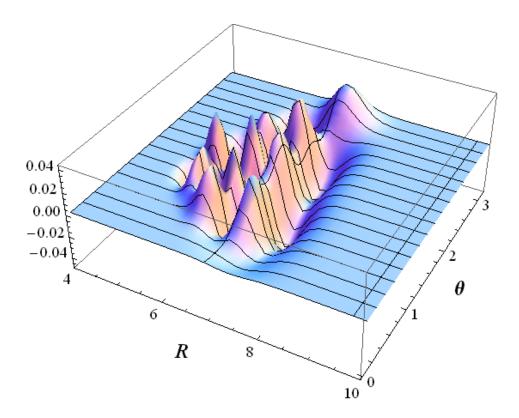


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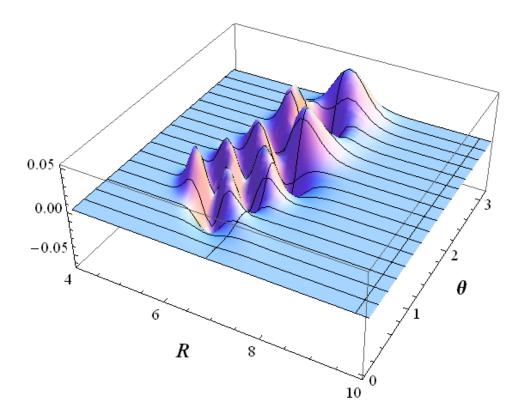


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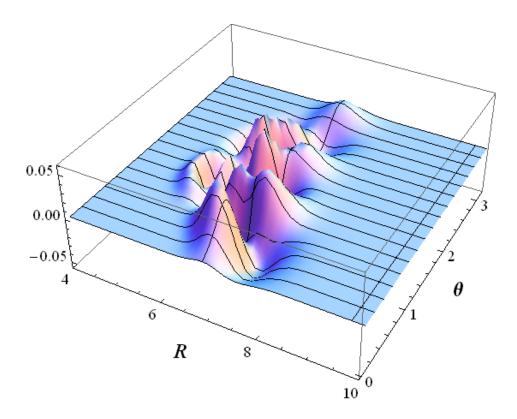


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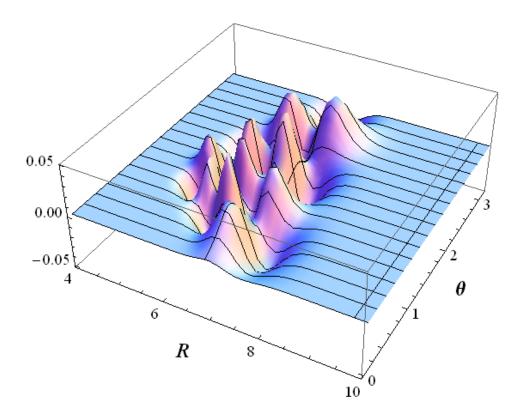


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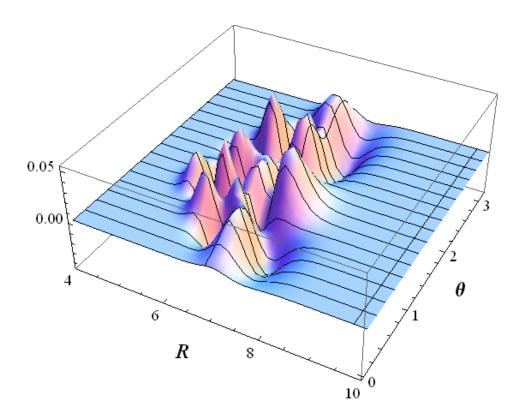


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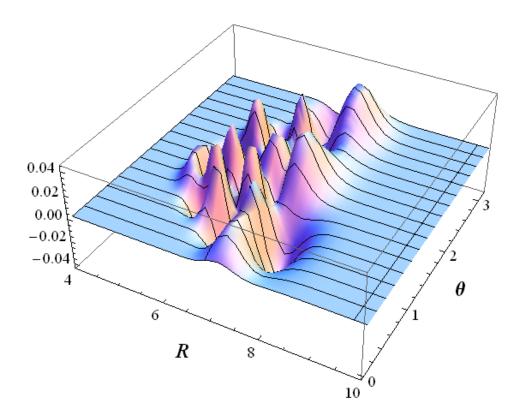


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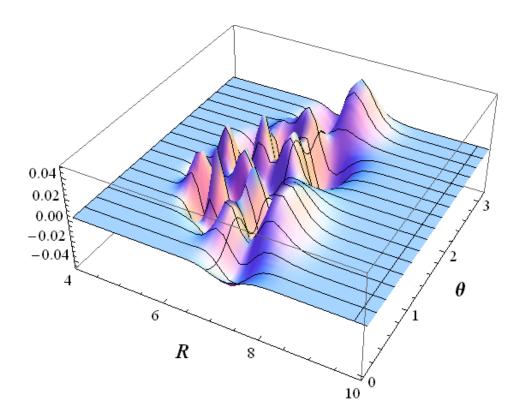


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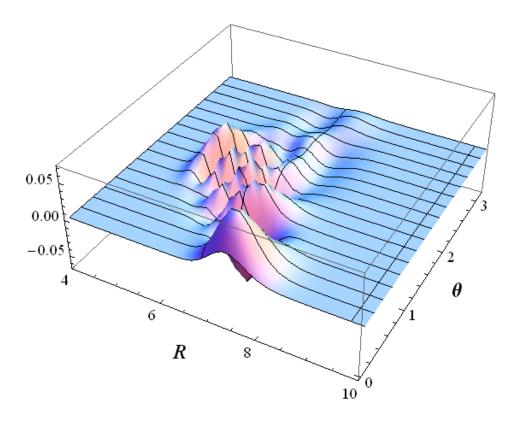


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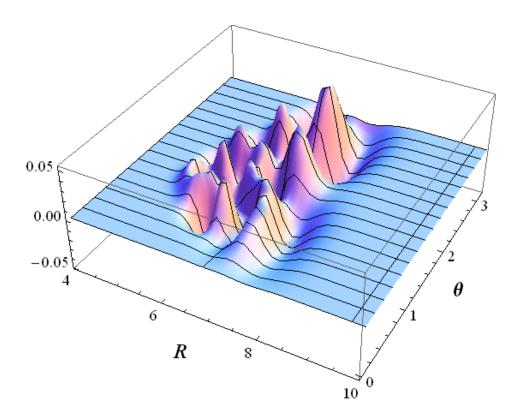


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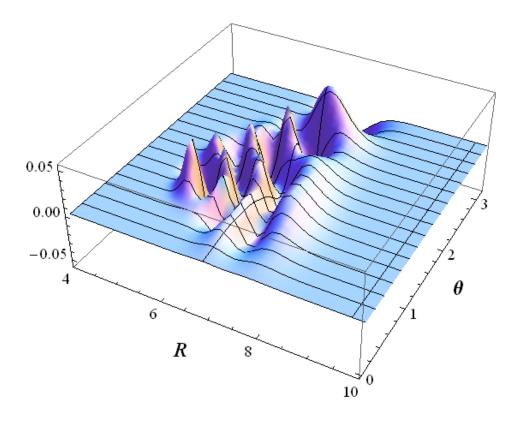


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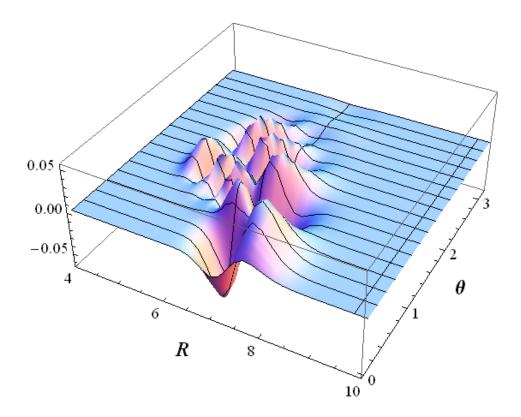


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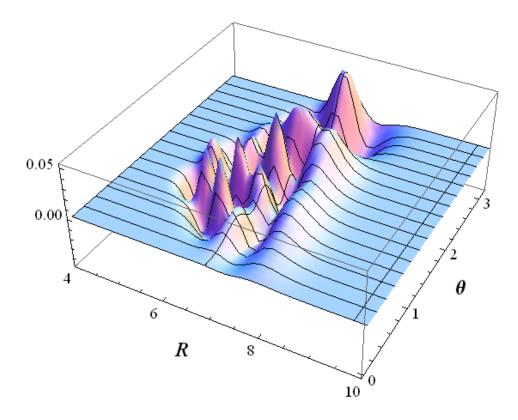


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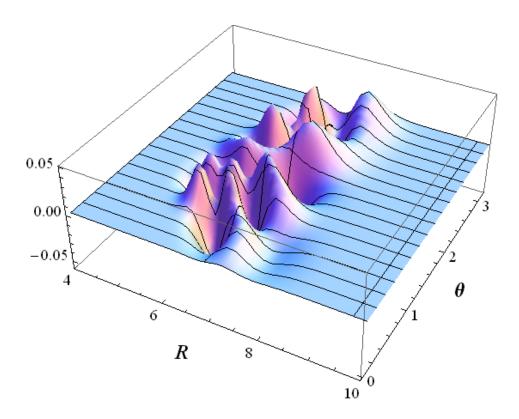


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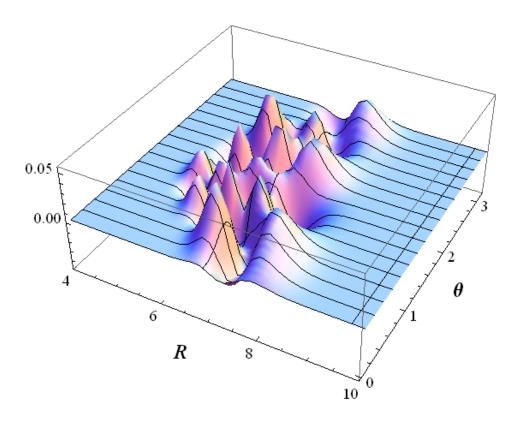


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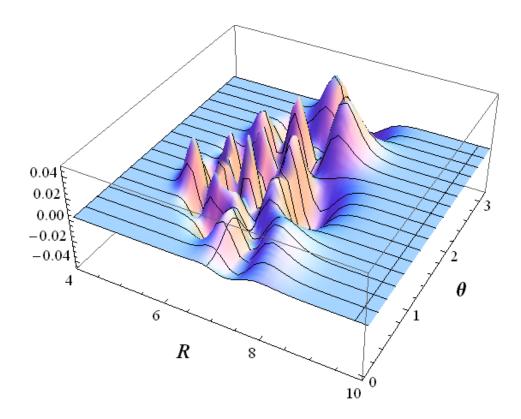


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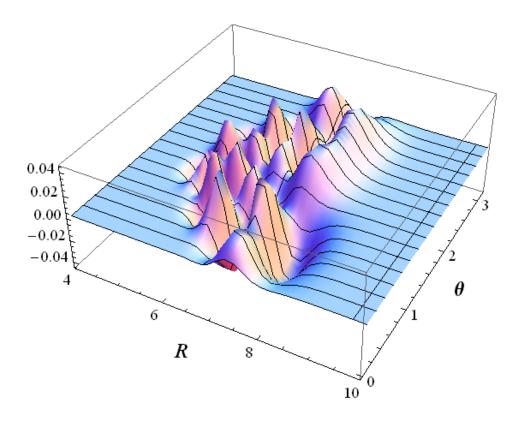


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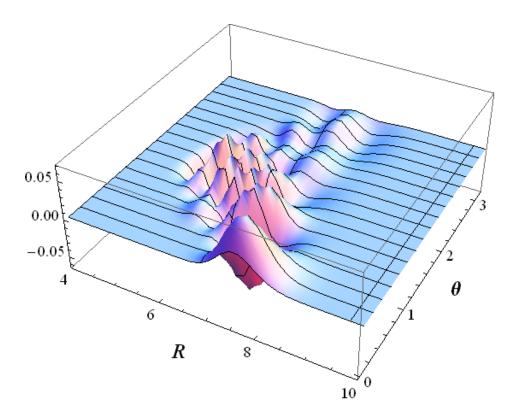


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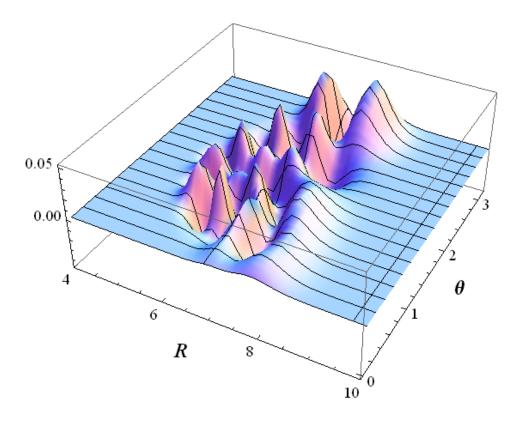


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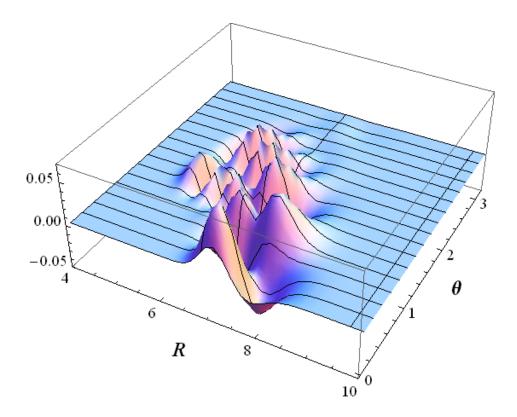


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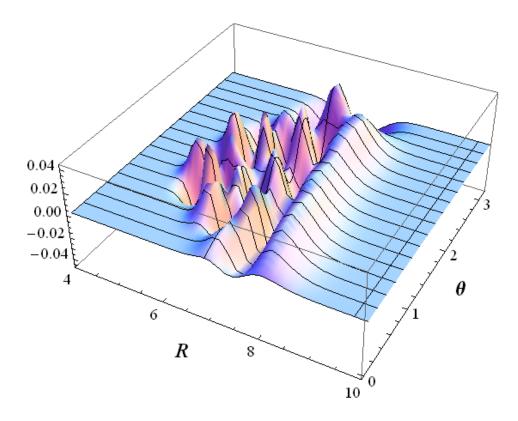
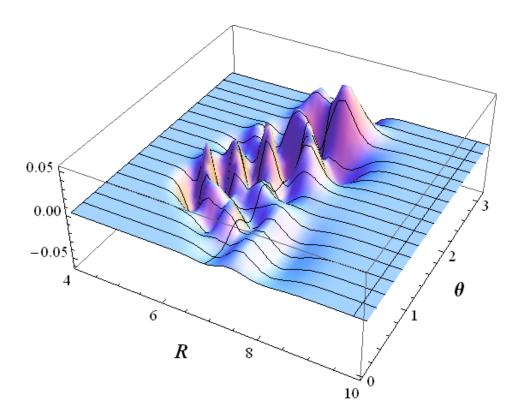
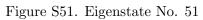


Figure S50. Eigenstate No. 50





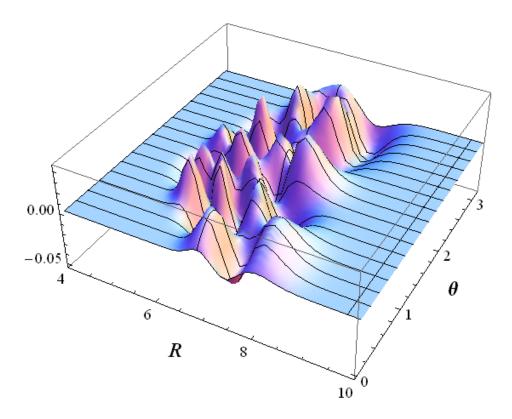


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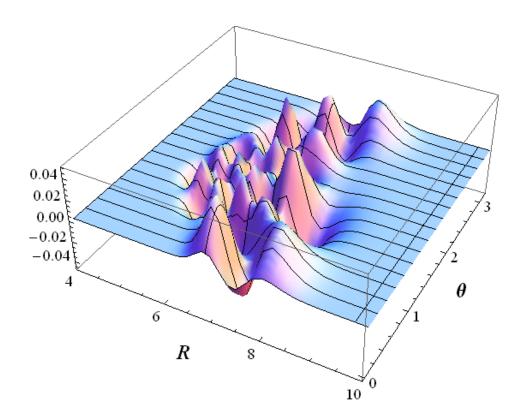


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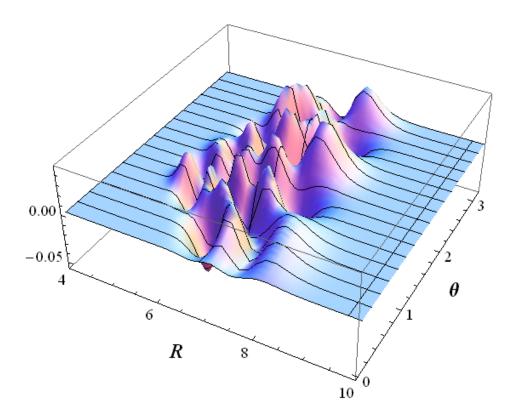


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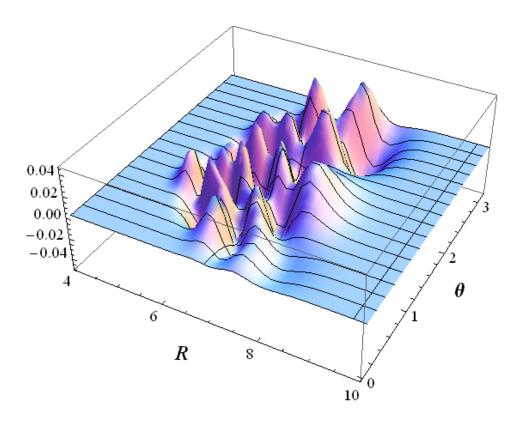


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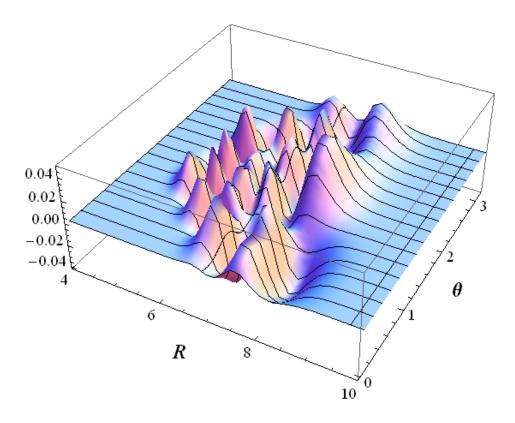


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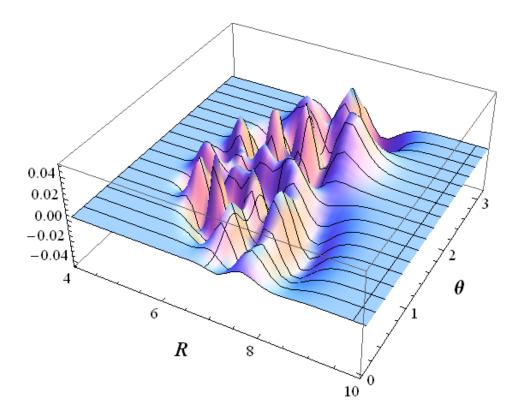


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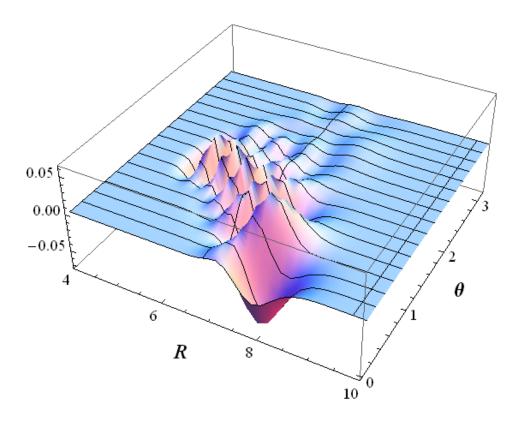


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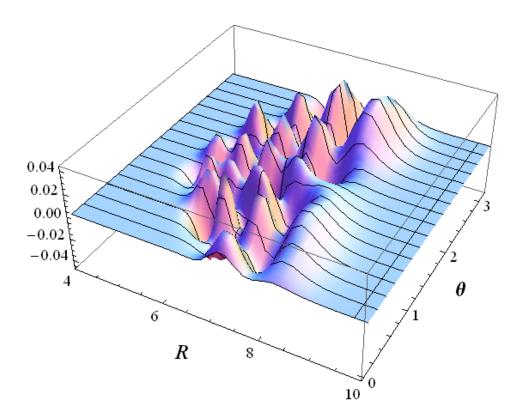


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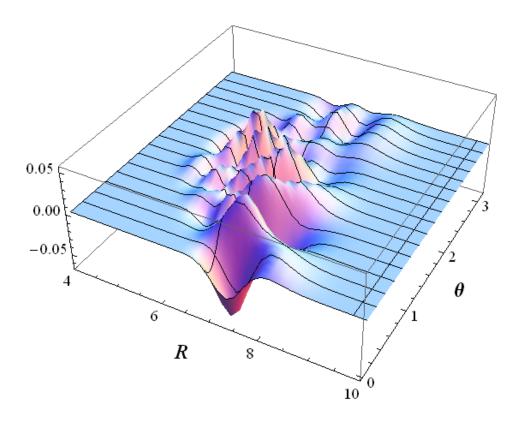


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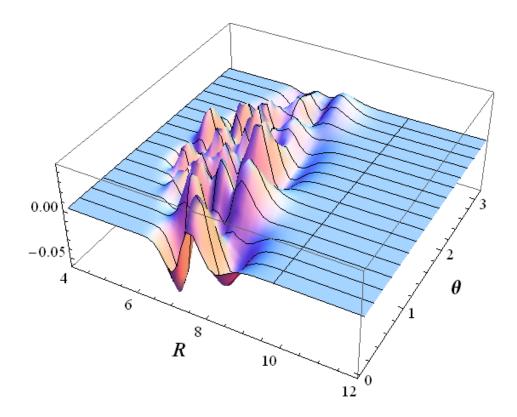


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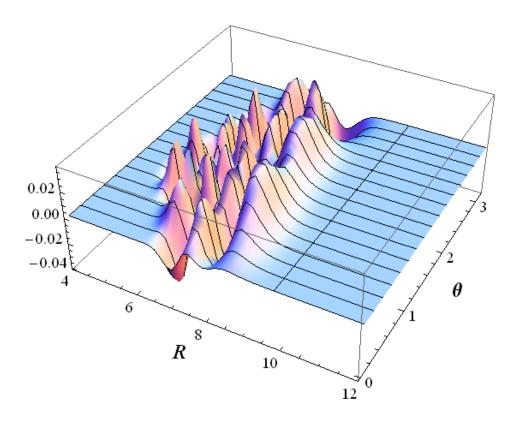


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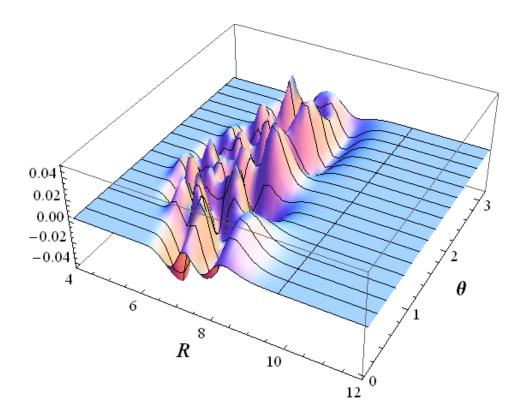


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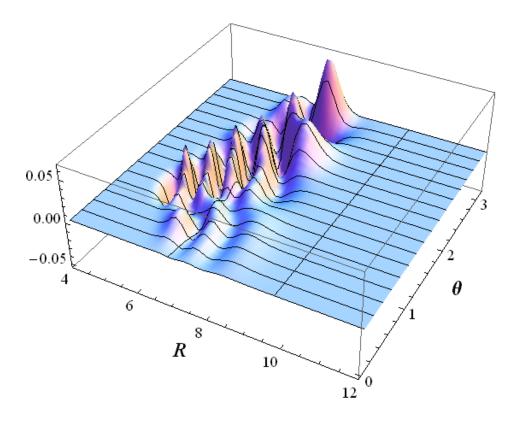


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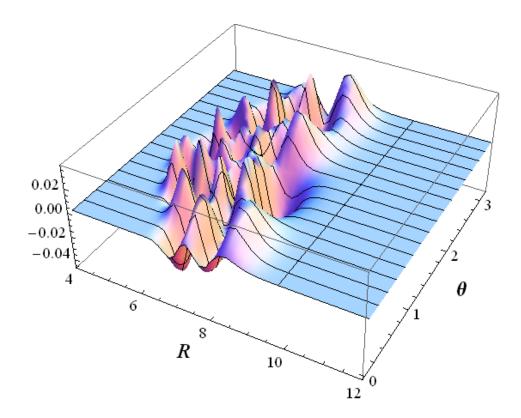


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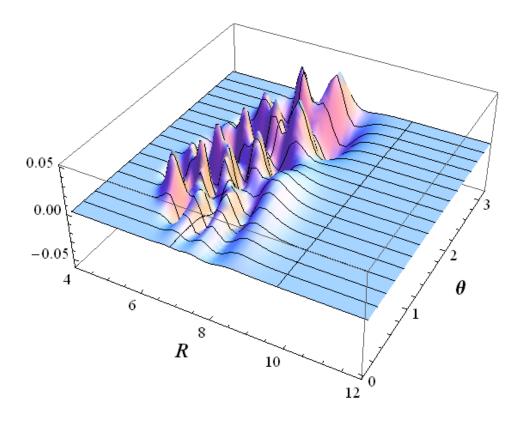


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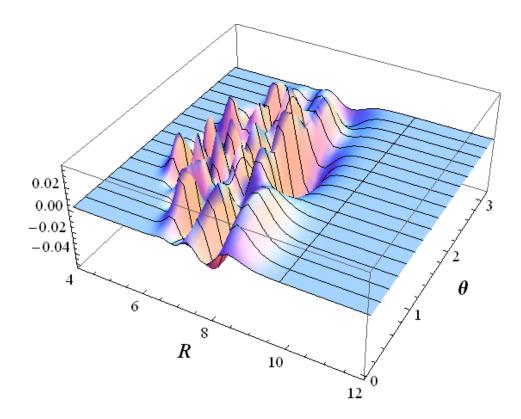


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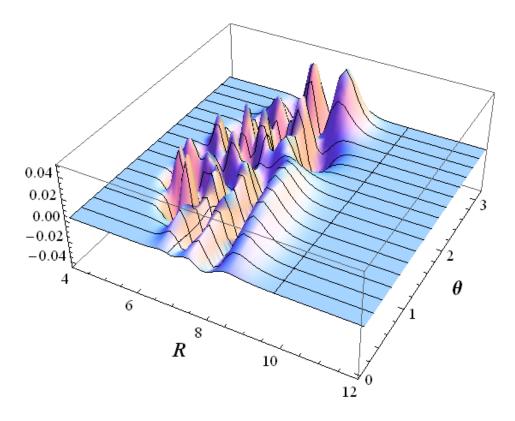


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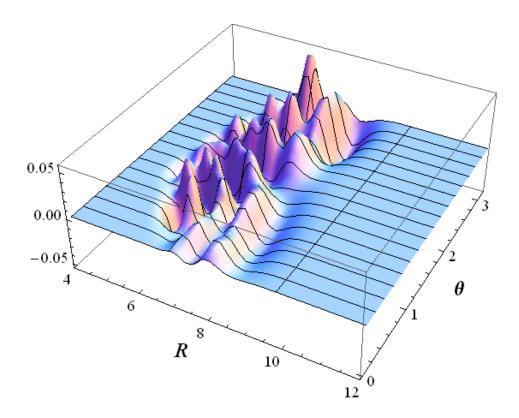


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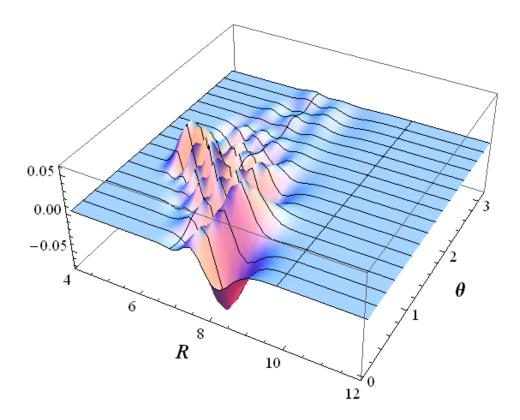


Figure S70. Eigenstate No. 70

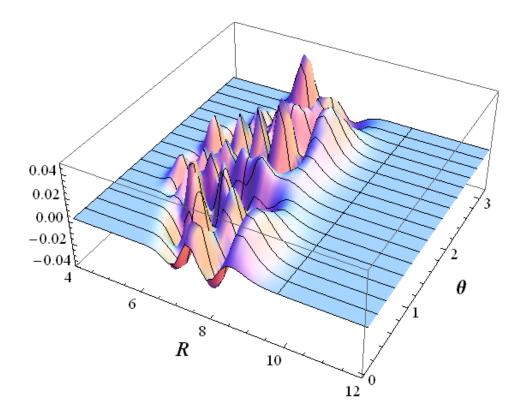


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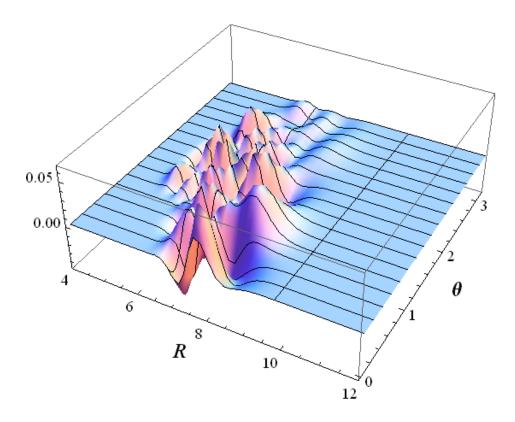


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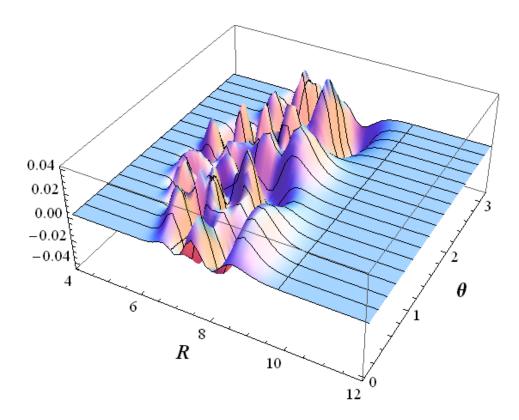


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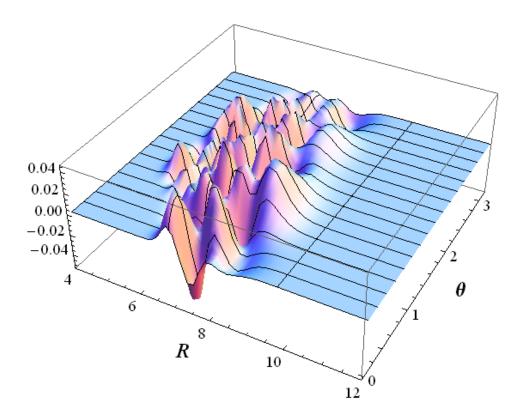


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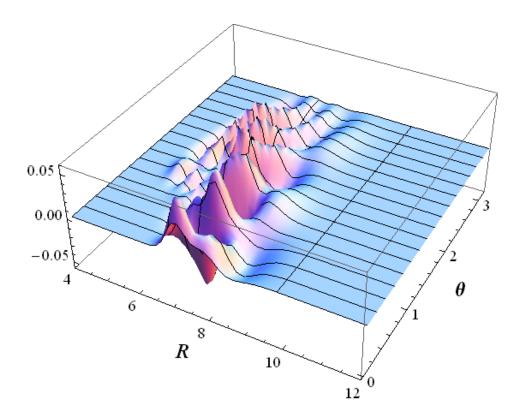


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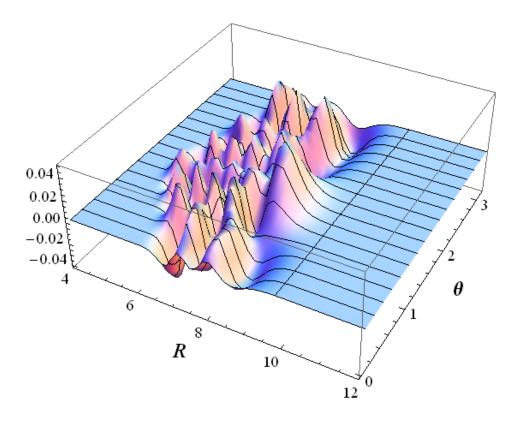


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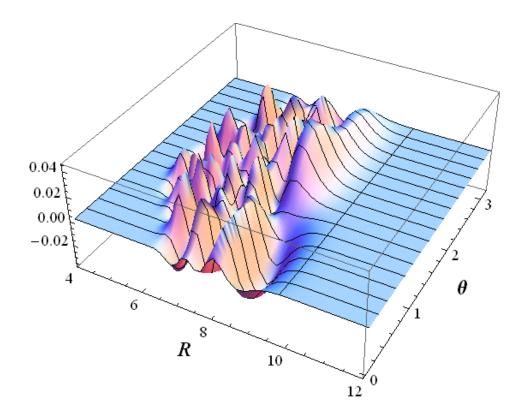


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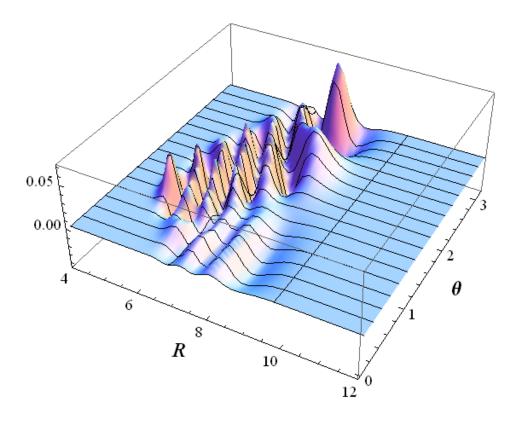


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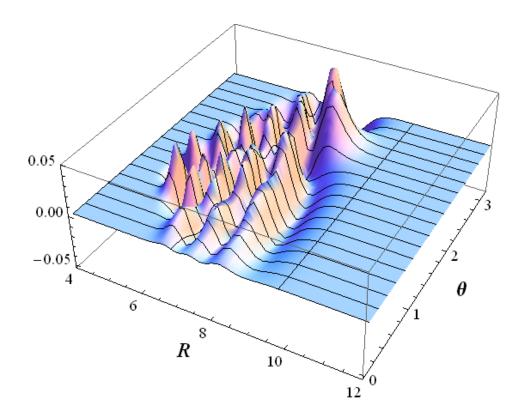


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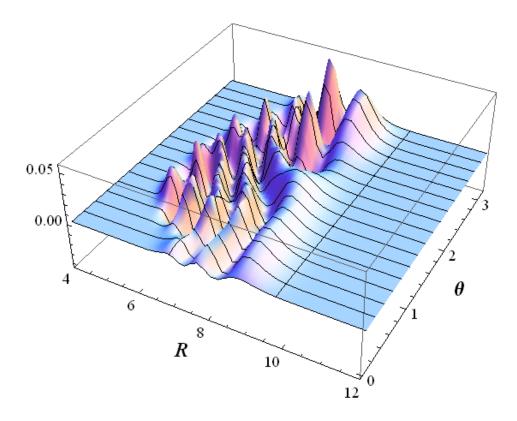


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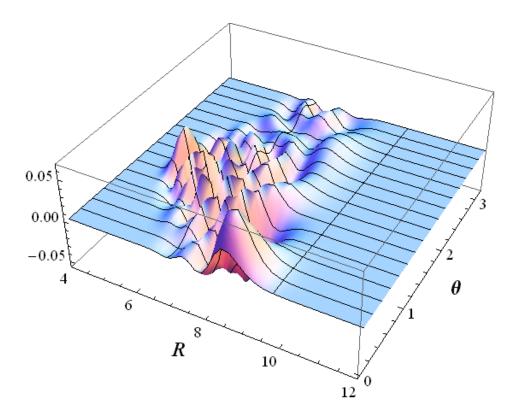


Figure S81. Eigenstate No. 81

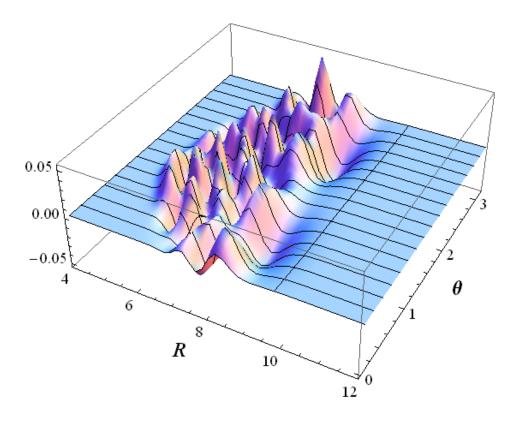


Figure S82. Eigenstate No. 82

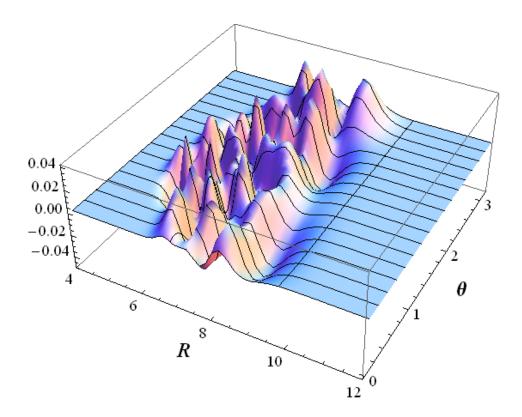


Figure S83. Eigenstate No. 83

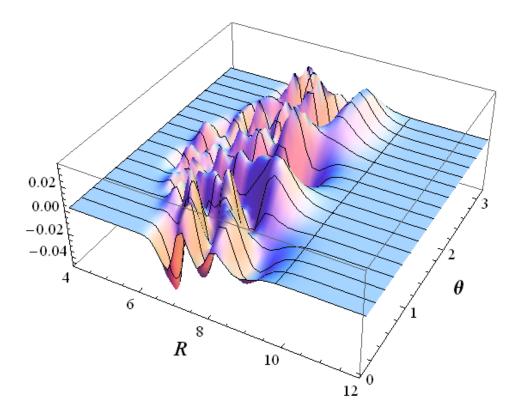


Figure S84. Eigenstate No. 84

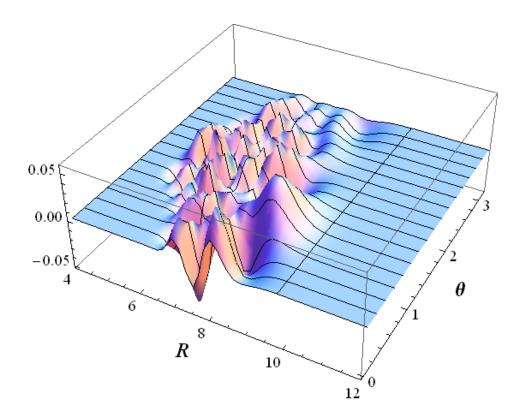


Figure S85. Eigenstate No. 85

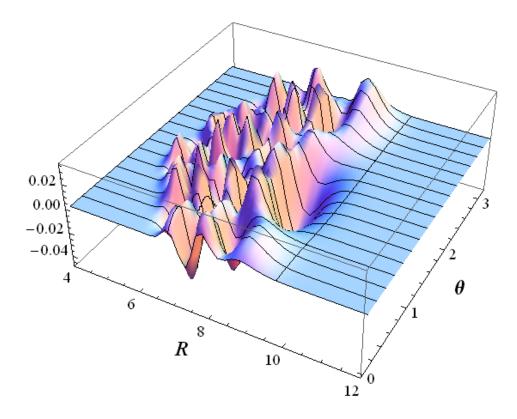


Figure S86. Eigenstate No. 86

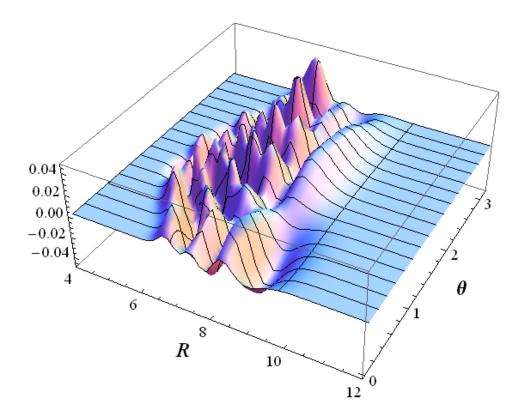


Figure S87. Eigenstate No. 87

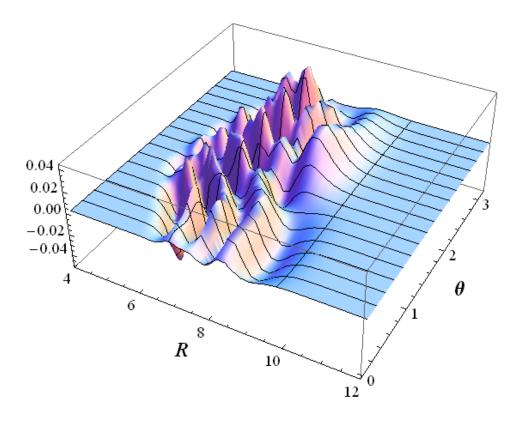


Figure S88. Eigenstate No. 88

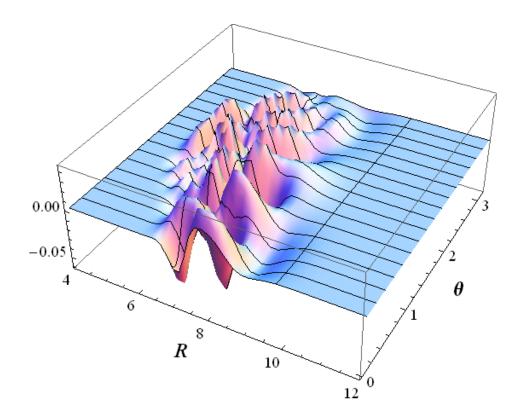


Figure S89. Eigenstate No. 89

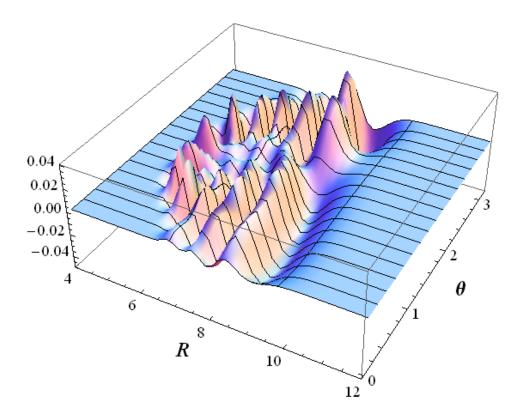


Figure S90. Eigenstate No. 90

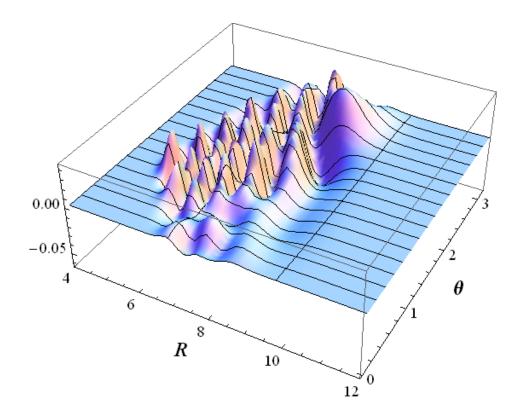


Figure S91. Eigenstate No. 91

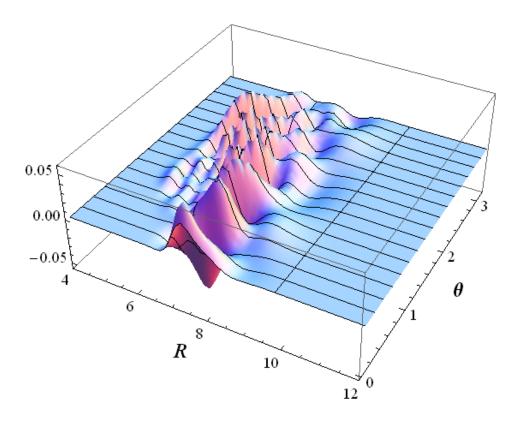


Figure S92. Eigenstate No. 92

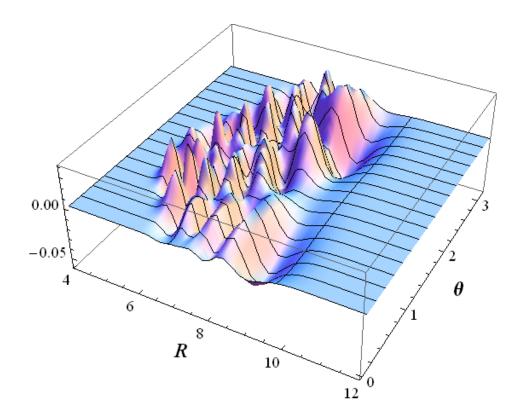


Figure S93. Eigenstate No. 93

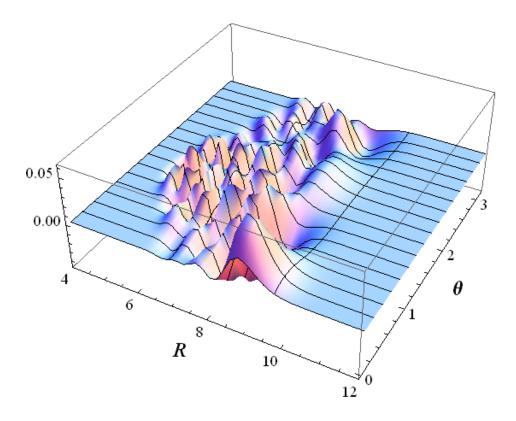


Figure S94. Eigenstate No. 94

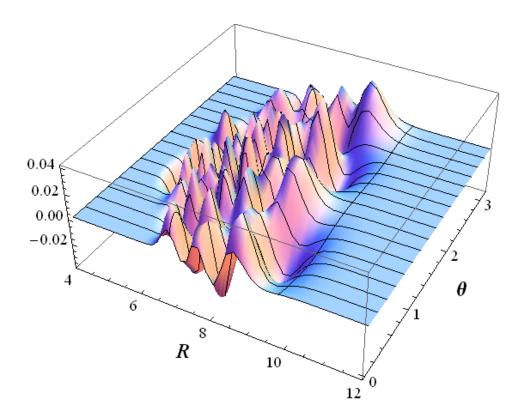


Figure S95. Eigenstate No. 95

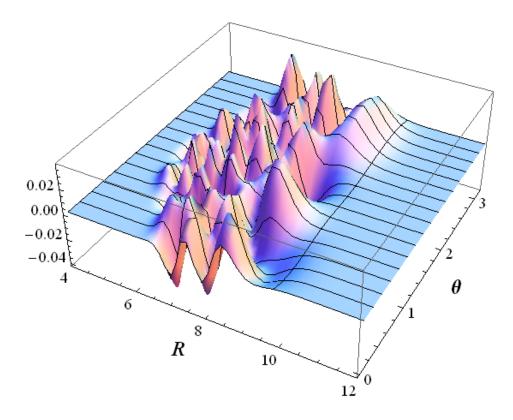


Figure S96. Eigenstate No. 96

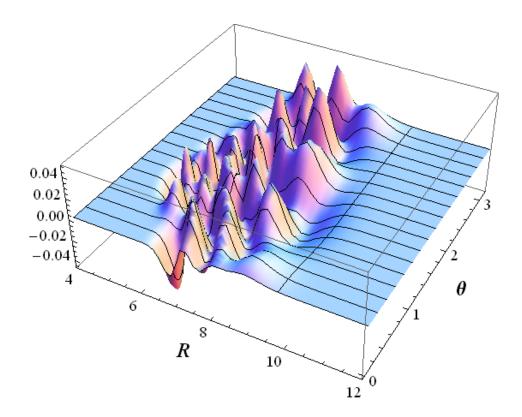


Figure S97. Eigenstate No. 97

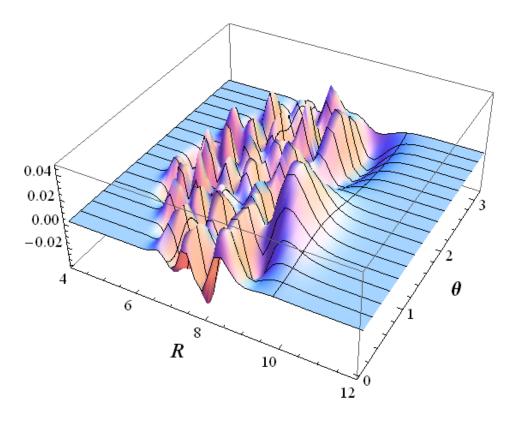


Figure S98. Eigenstate No. 98

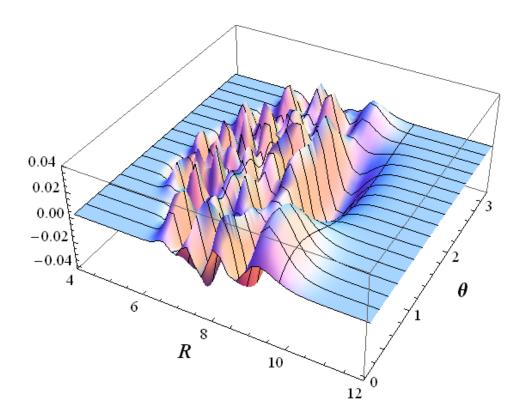


Figure S99. Eigenstate No. 99

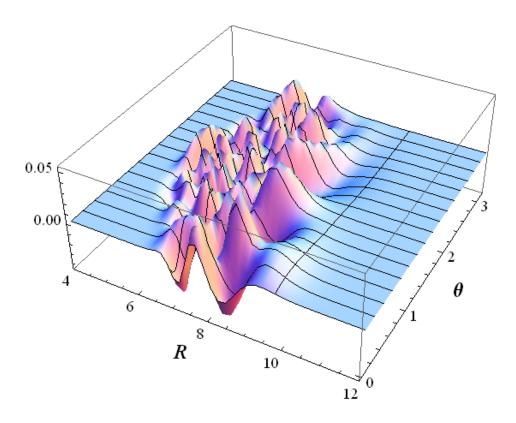


Figure S100. Eigenstate No. 100

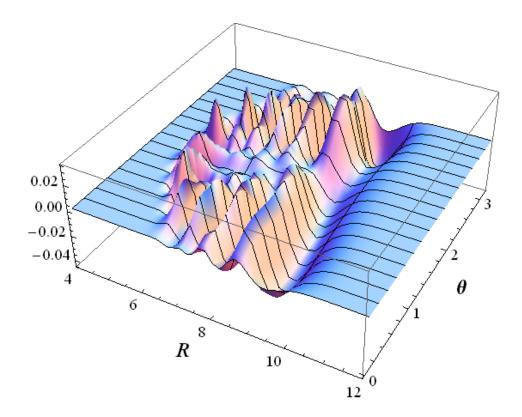


Figure S101. Eigenstate No. 101

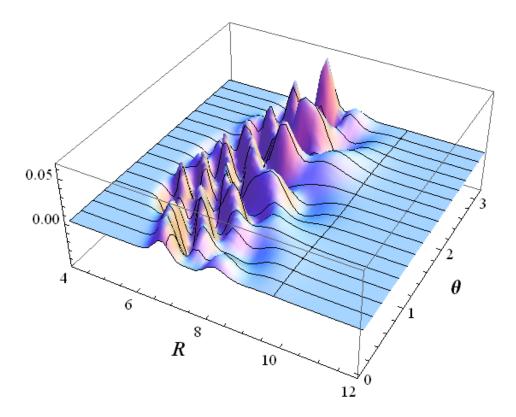


Figure S102. Eigenstate No. 102

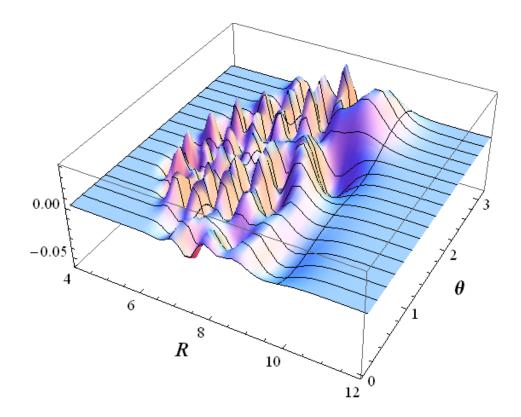


Figure S103. Eigenstate No. 103

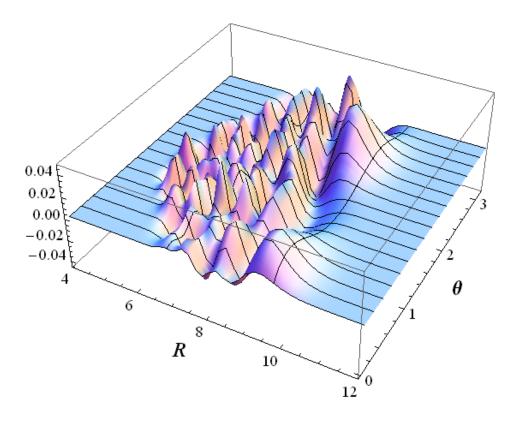


Figure S104. Eigenstate No. 104

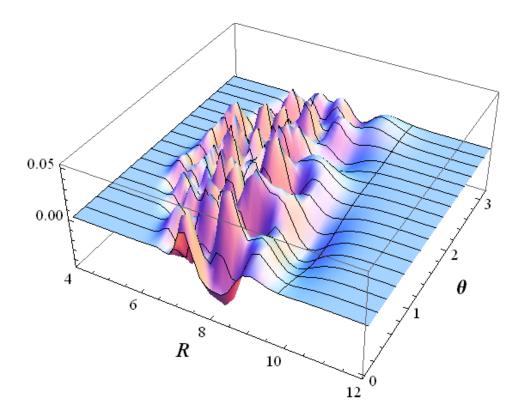


Figure S105. Eigenstate No. 105

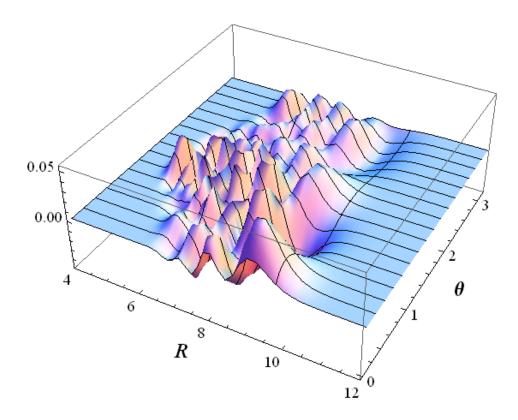


Figure S106. Eigenstate No. 106

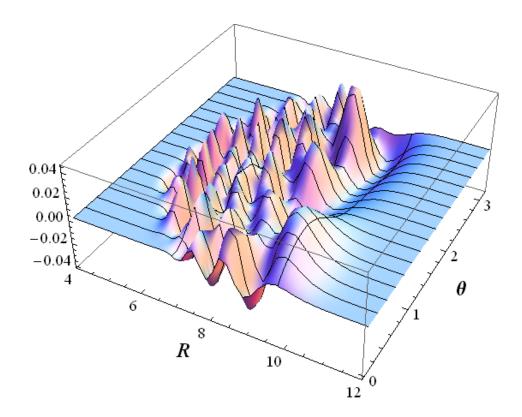


Figure S107. Eigenstate No. 107

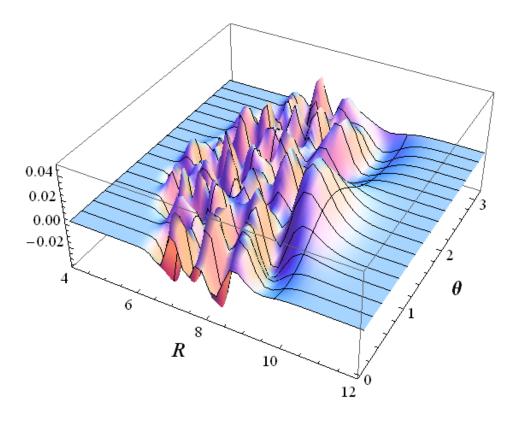


Figure S108. Eigenstate No. 108

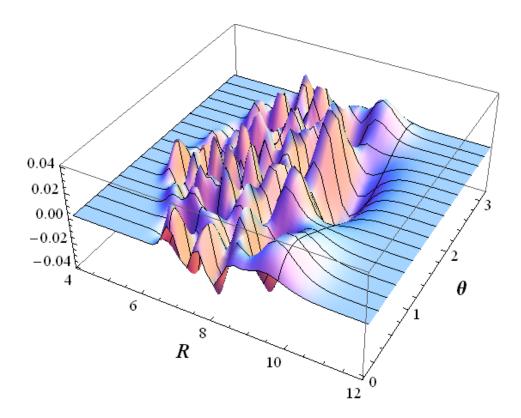


Figure S109. Eigenstate No. 109

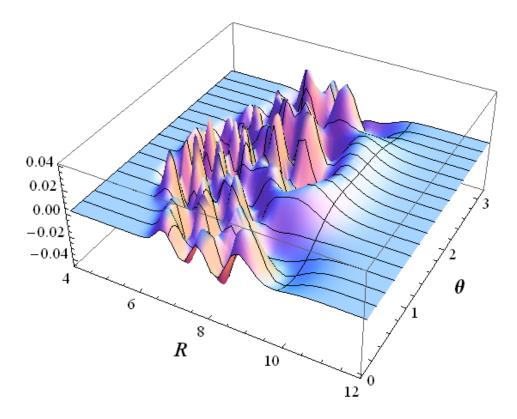


Figure S110. Eigenstate No. 110

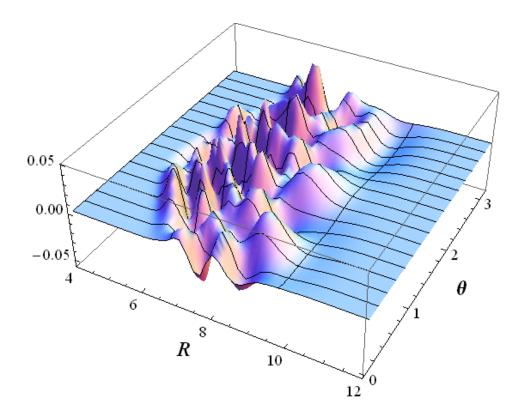


Figure S111. Eigenstate No. 111

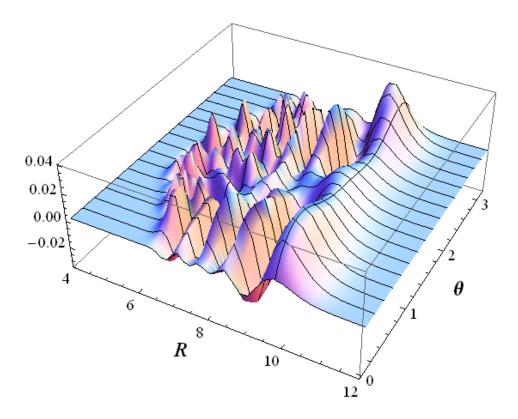


Figure S112. Eigenstate No. 112

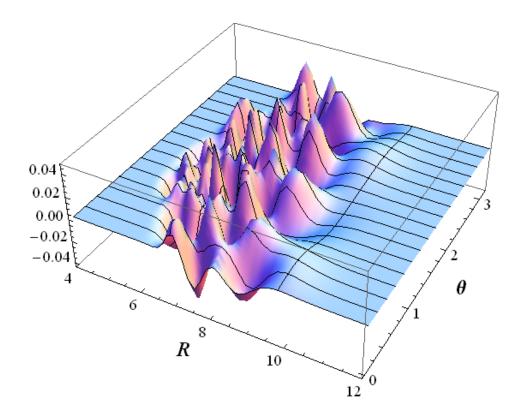


Figure S113. Eigenstate No. 113

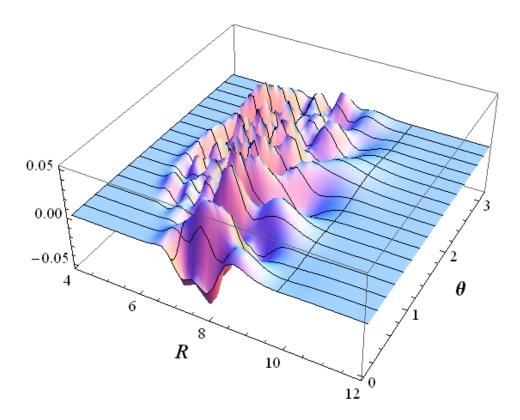


Figure S114. Eigenstate No. 114

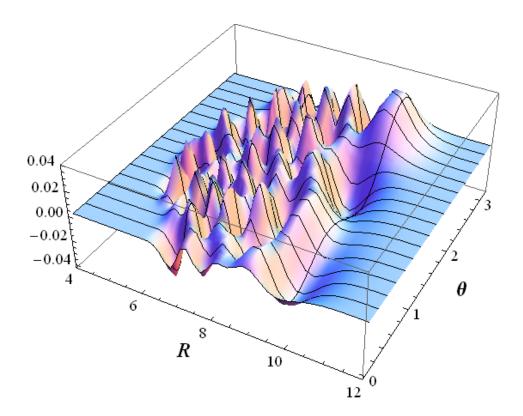


Figure S115. Eigenstate No. 115

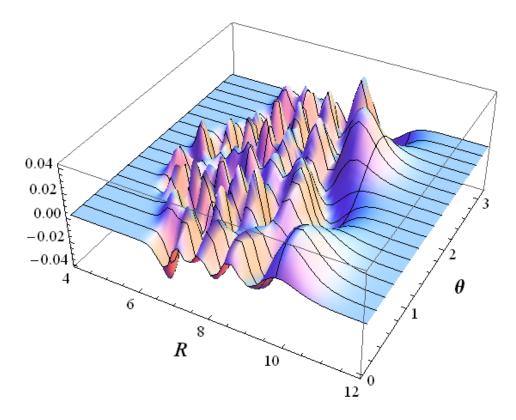


Figure S116. Eigenstate No. 116

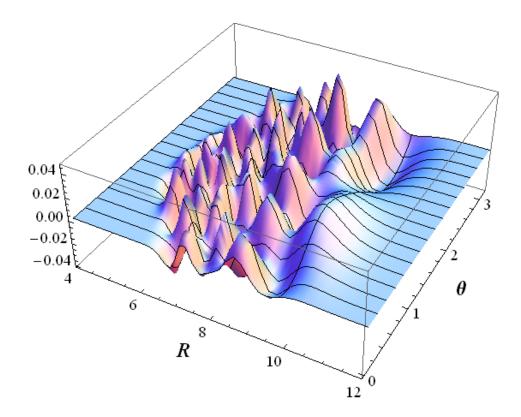


Figure S117. Eigenstate No. 117

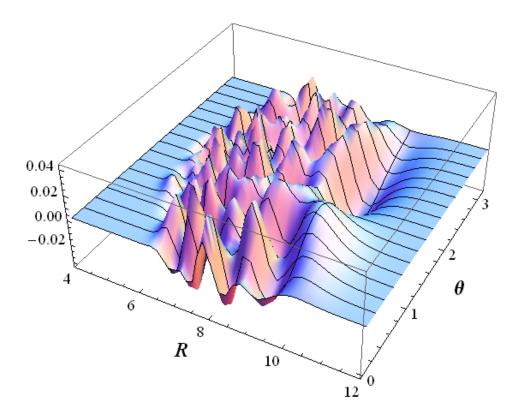


Figure S118. Eigenstate No. 118

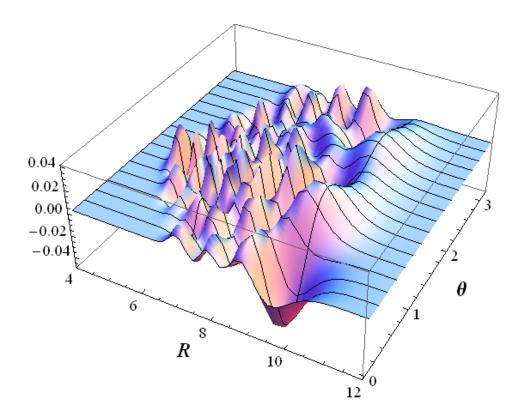


Figure S119. Eigenstate No. 119

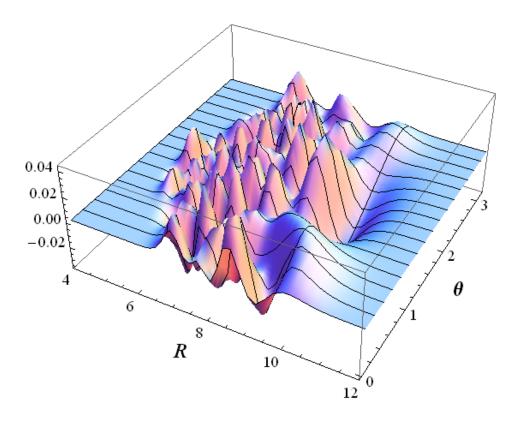


Figure S120. Eigenstate No. 120

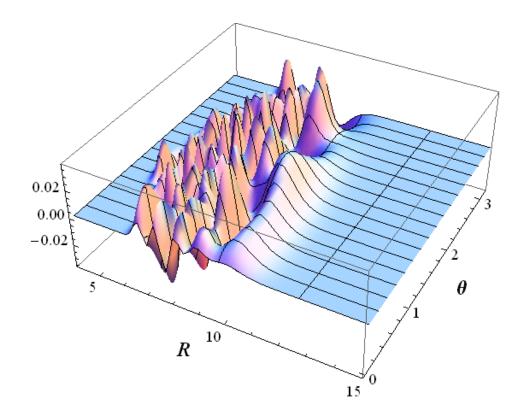


Figure S121. Eigenstate No. 121

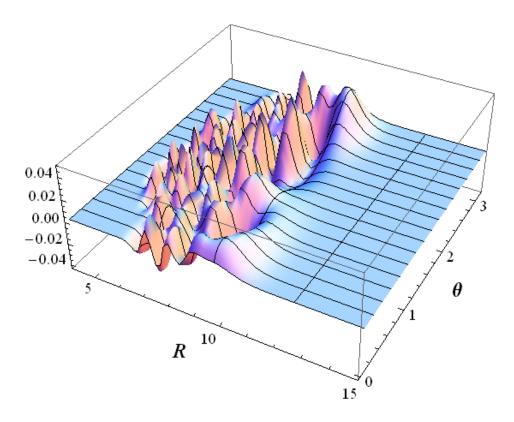


Figure S122. Eigenstate No. 122

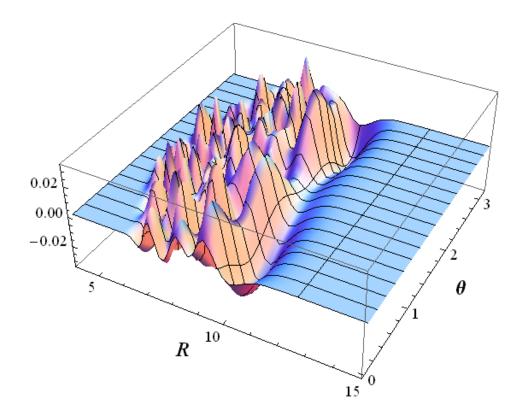


Figure S123. Eigenstate No. 123

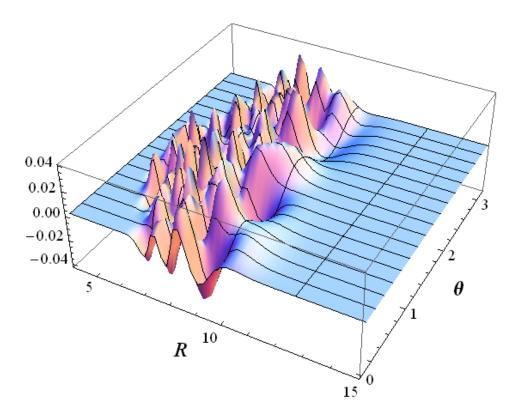


Figure S124. Eigenstate No. 124

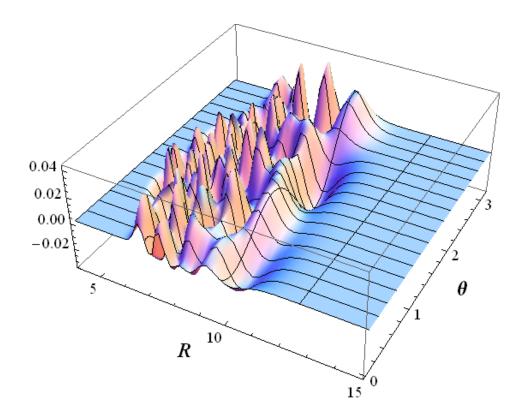


Figure S125. Eigenstate No. 125

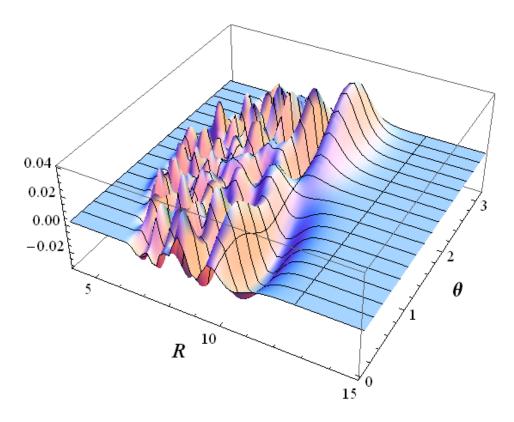


Figure S126. Eigenstate No. 126

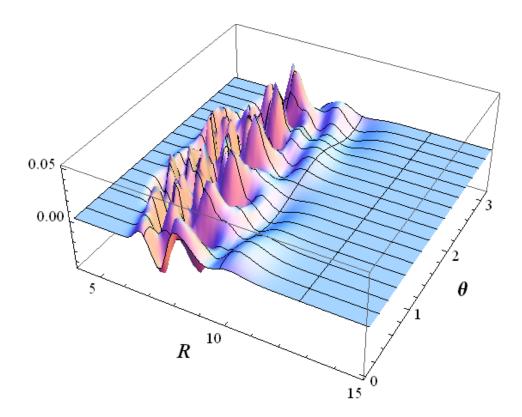


Figure S127. Eigenstate No. 127

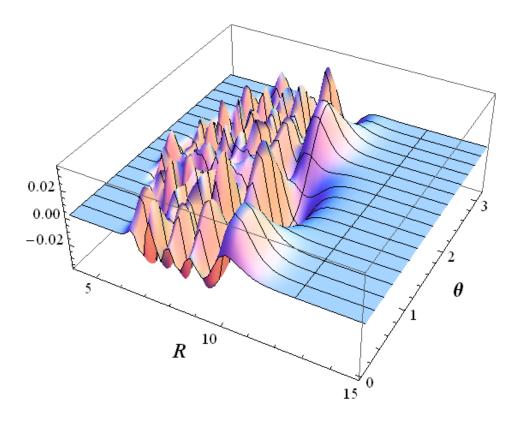


Figure S128. Eigenstate No. 128

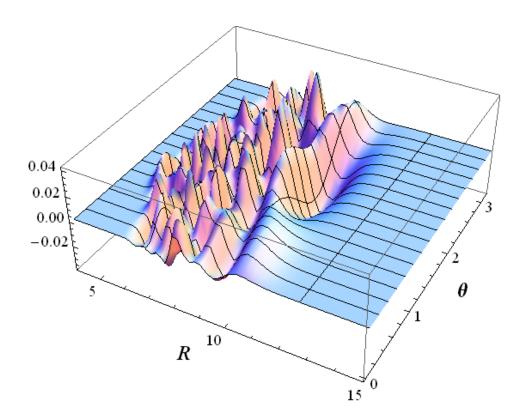


Figure S129. Eigenstate No. 129

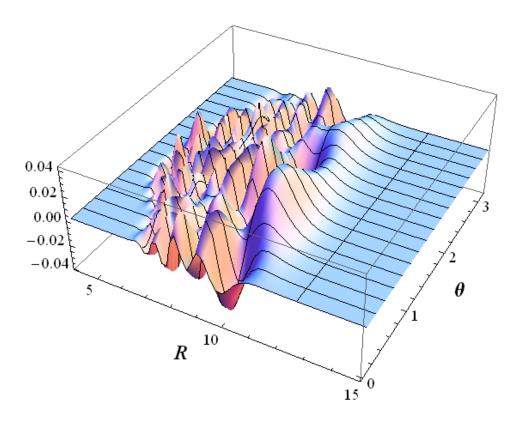


Figure S130. Eigenstate No. 130

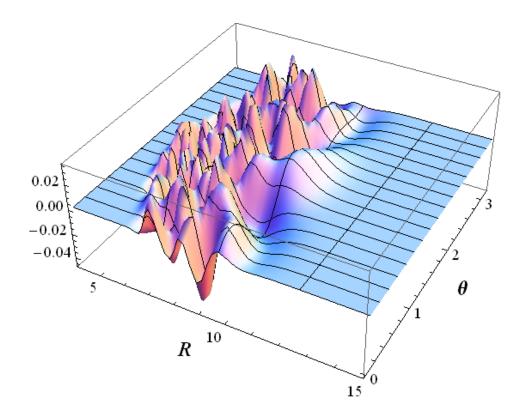


Figure S131. Eigenstate No. 131

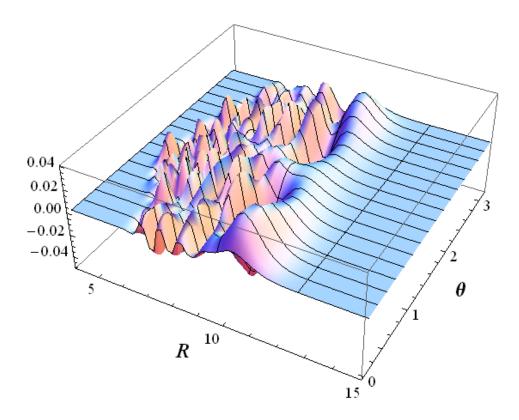


Figure S132. Eigenstate No. 132

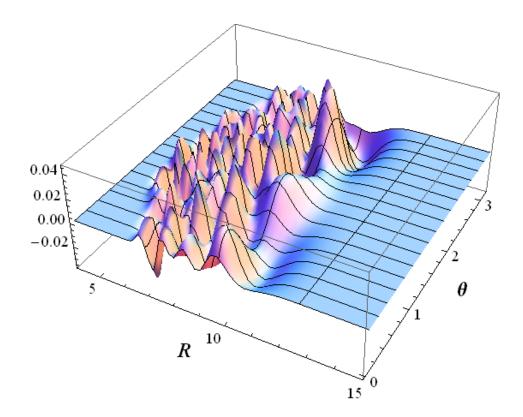


Figure S133. Eigenstate No. 133

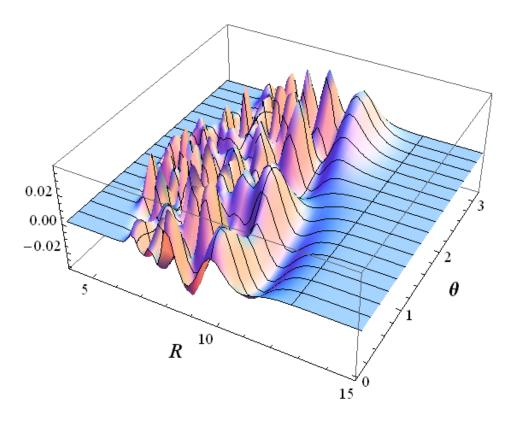


Figure S134. Eigenstate No. 134

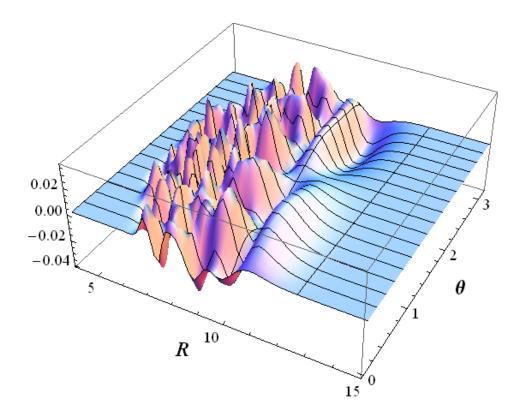


Figure S135. Eigenstate No. 135

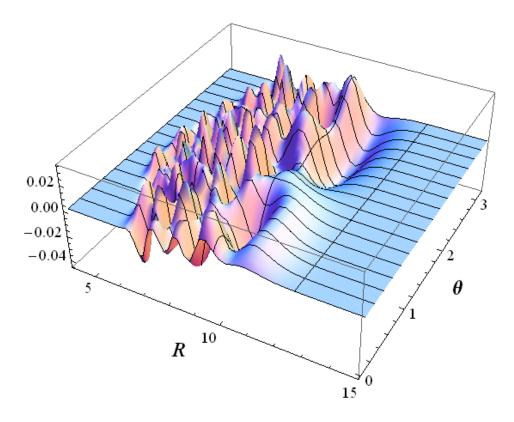


Figure S136. Eigenstate No. 136

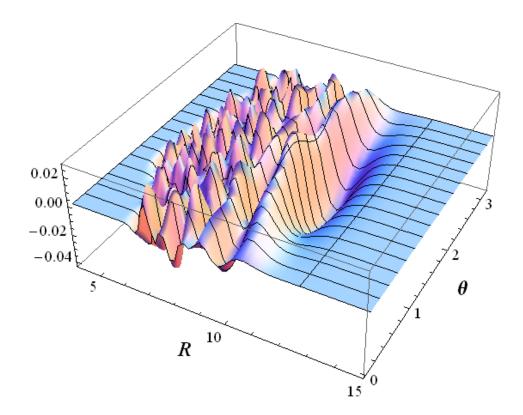


Figure S137. Eigenstate No. 137

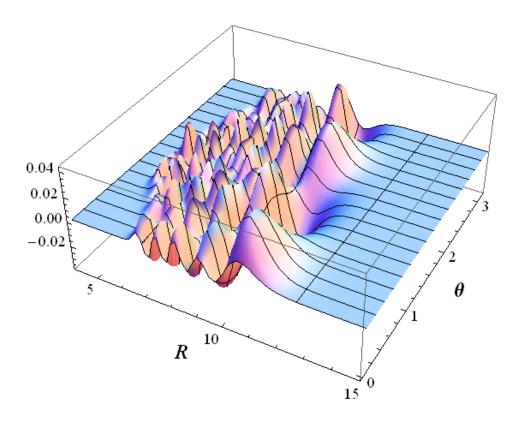


Figure S138. Eigenstate No. 138

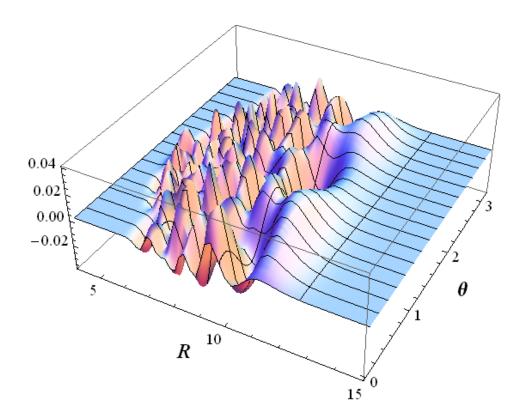


Figure S139. Eigenstate No. 139

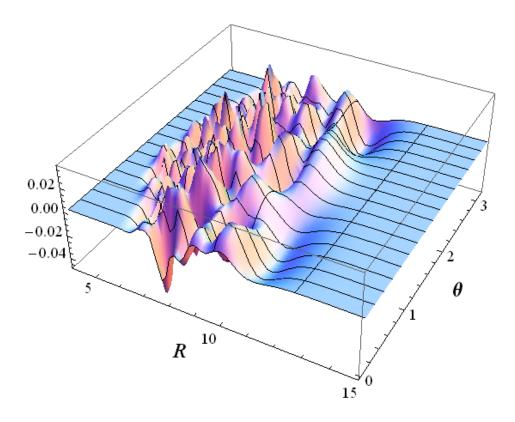


Figure S140. Eigenstate No. 140

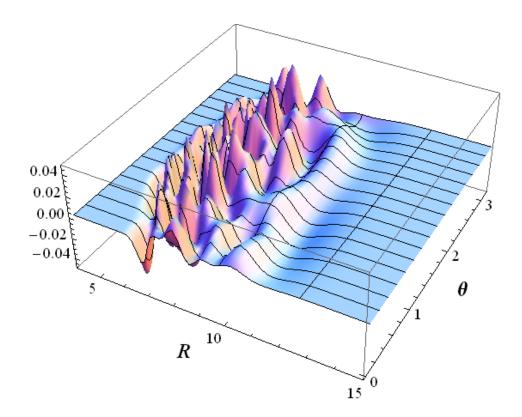


Figure S141. Eigenstate No. 141

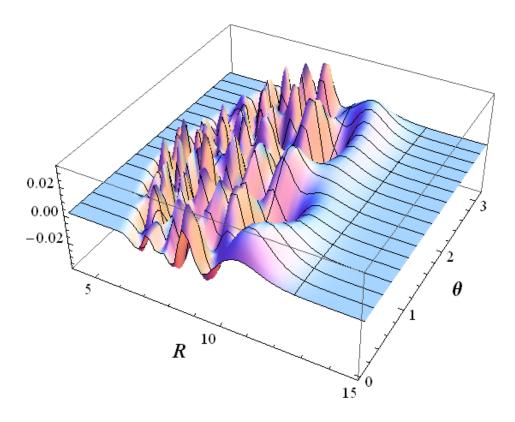


Figure S142. Eigenstate No. 142

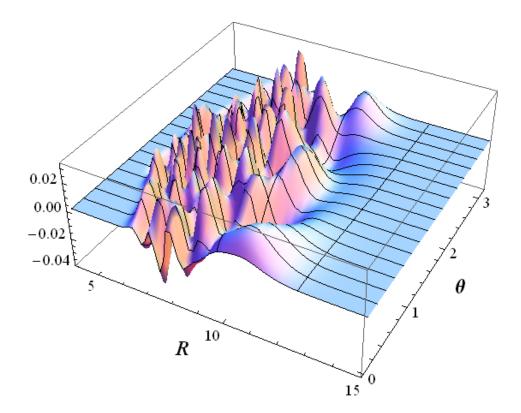


Figure S143. Eigenstate No. 143

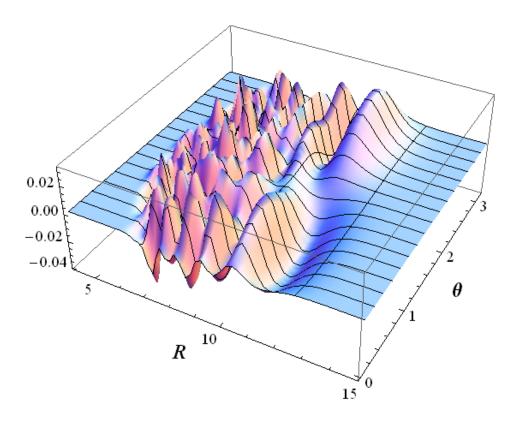


Figure S144. Eigenstate No. 144

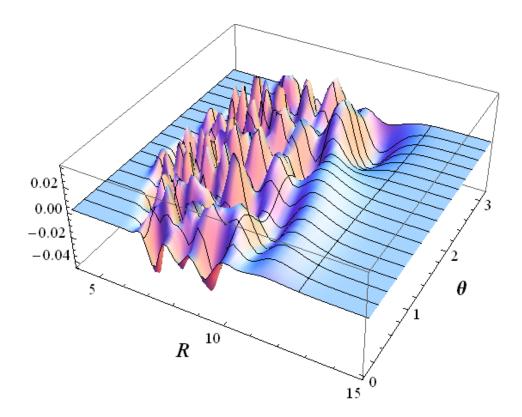


Figure S145. Eigenstate No. 145

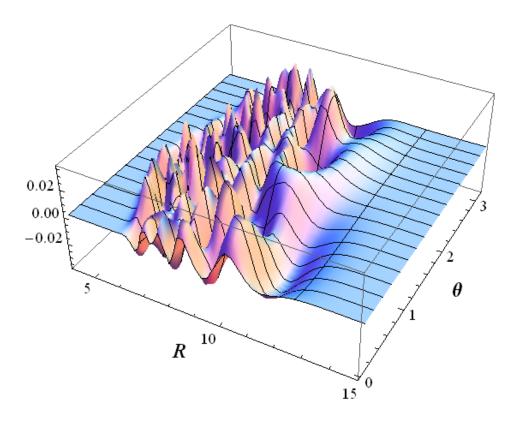


Figure S146. Eigenstate No. 146

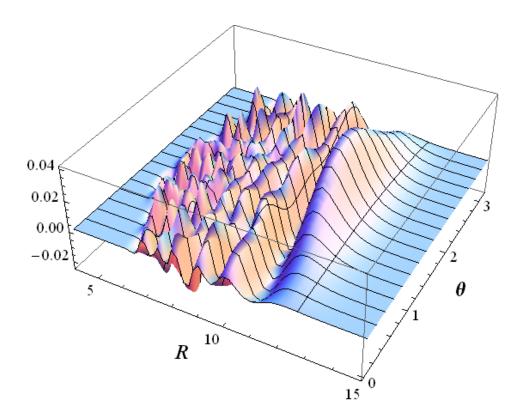


Figure S147. Eigenstate No. 147

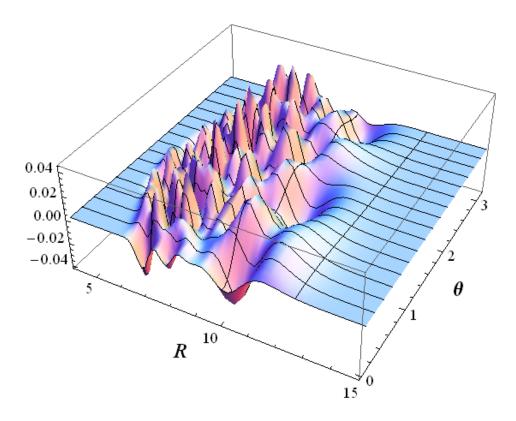


Figure S148. Eigenstate No. 148

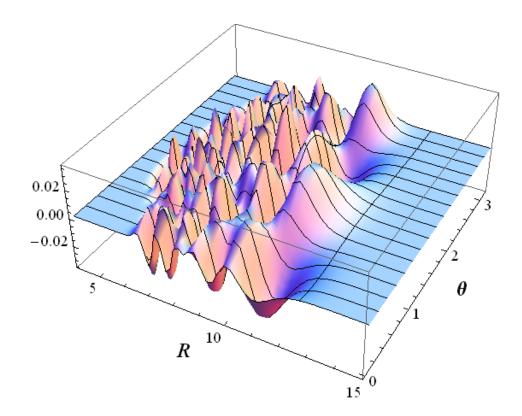


Figure S149. Eigenstate No. 149

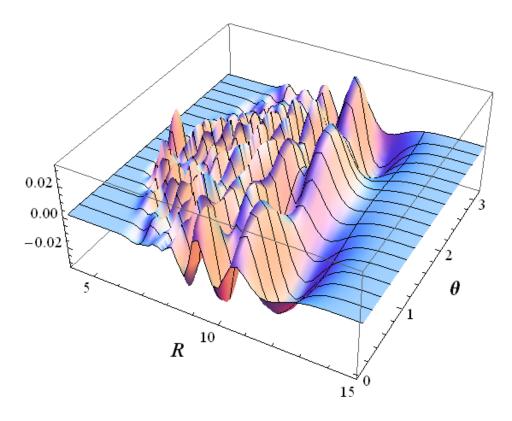


Figure S150. Eigenstate No. 150

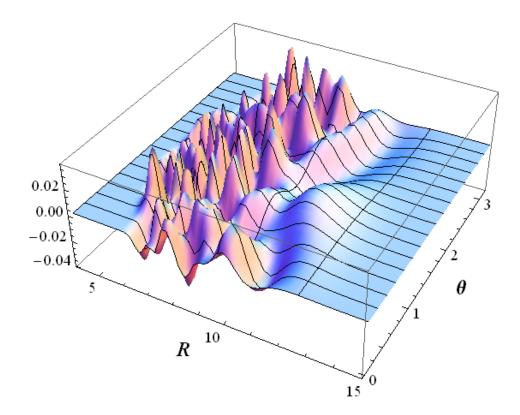


Figure S151. Eigenstate No. 151

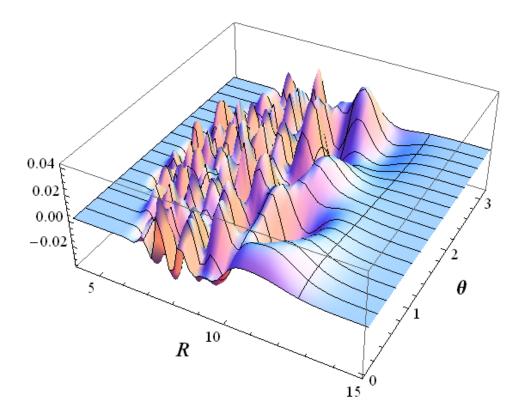


Figure S152. Eigenstate No. 152

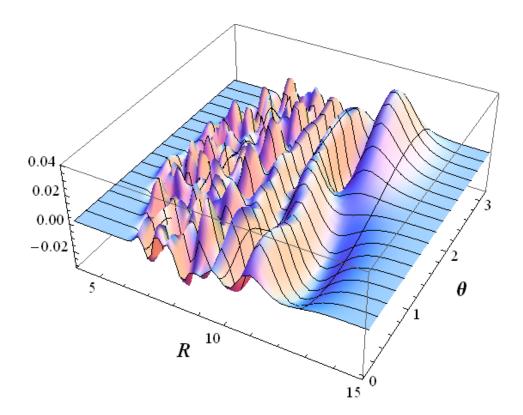


Figure S153. Eigenstate No. 153

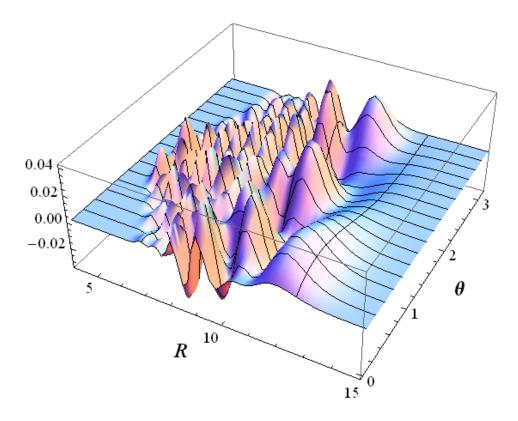


Figure S154. Eigenstate No. 154

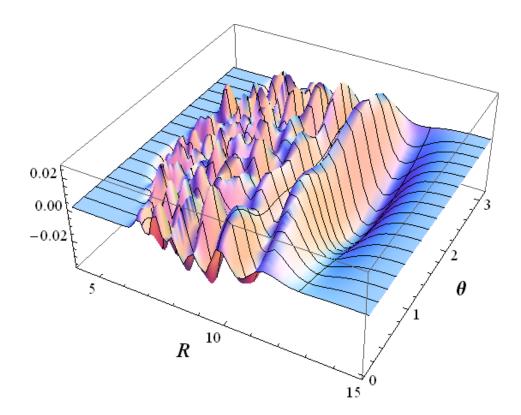


Figure S155. Eigenstate No. 155

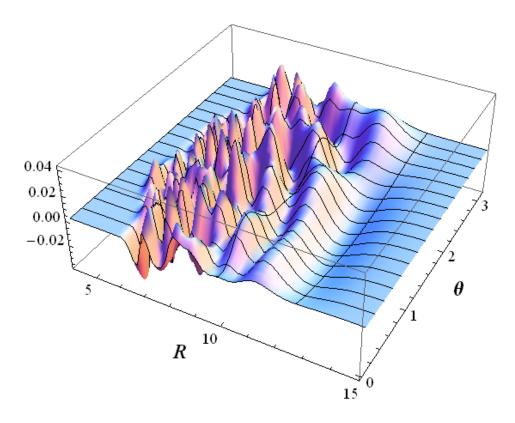


Figure S156. Eigenstate No. 156

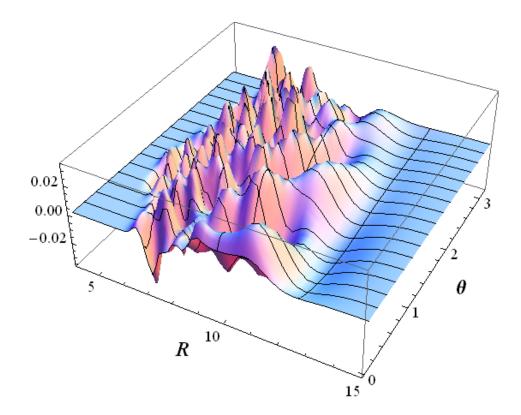


Figure S157. Eigenstate No. 157

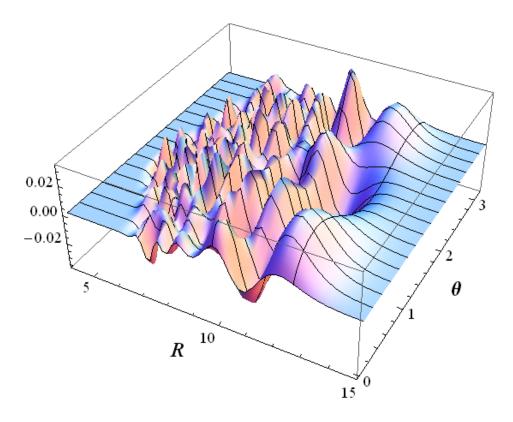


Figure S158. Eigenstate No. 158

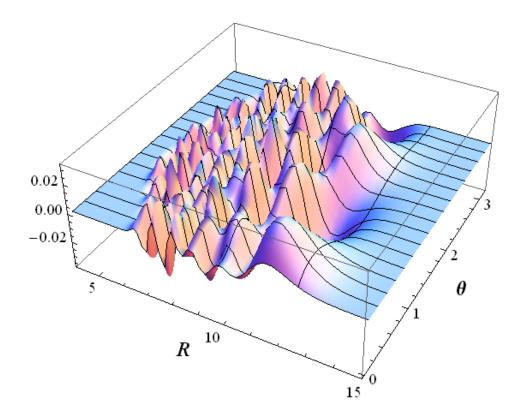


Figure S159. Eigenstate No. 159

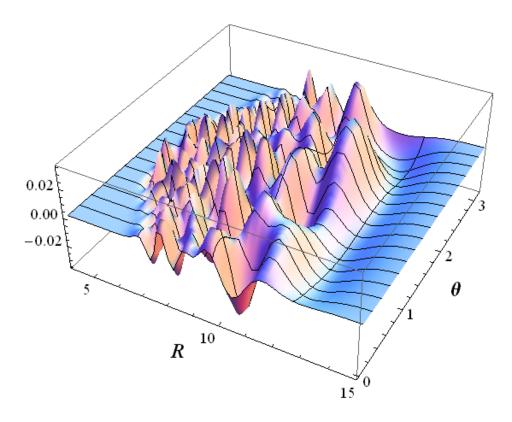


Figure S160. Eigenstate No. 160

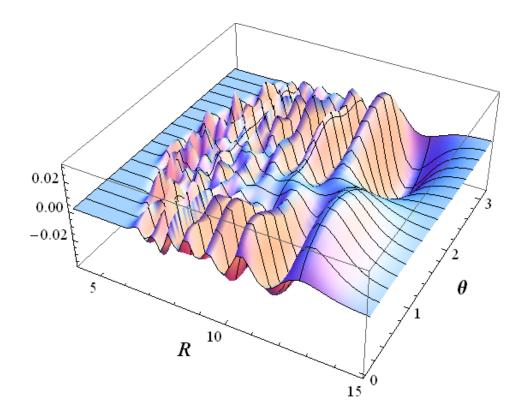


Figure S161. Eigenstate No. 161

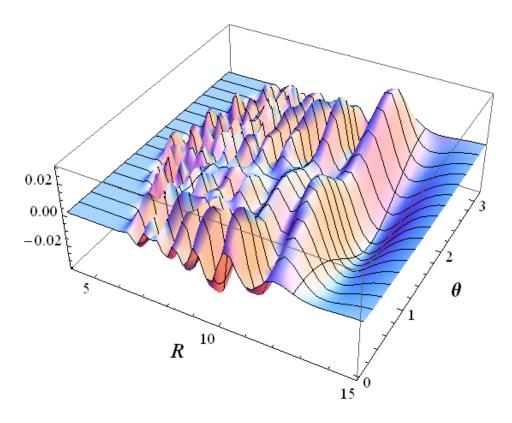


Figure S162. Eigenstate No. 162

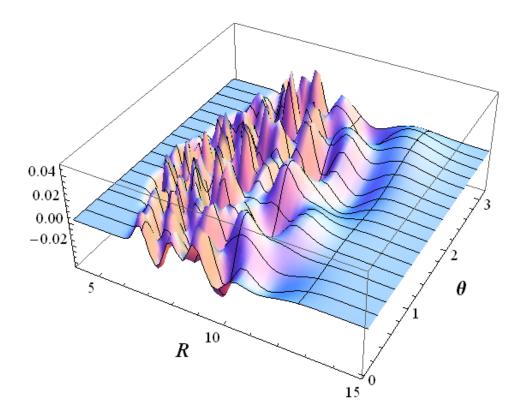


Figure S163. Eigenstate No. 163

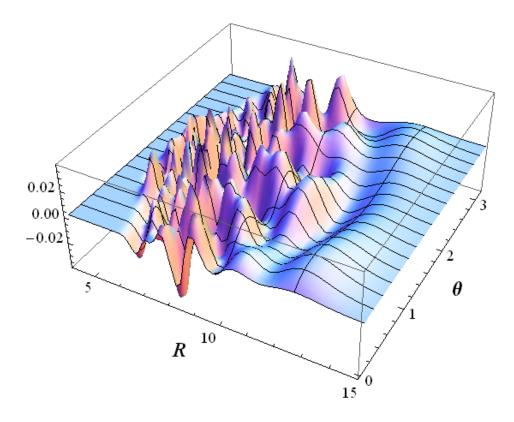


Figure S164. Eigenstate No. 164

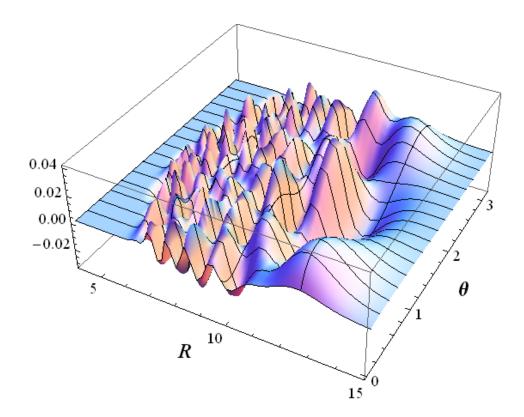


Figure S165. Eigenstate No. 165

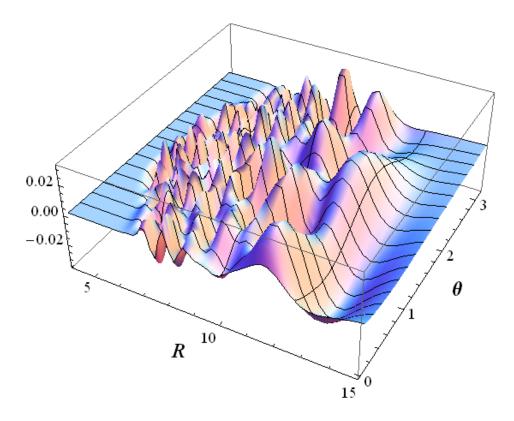


Figure S166. Eigenstate No. 166

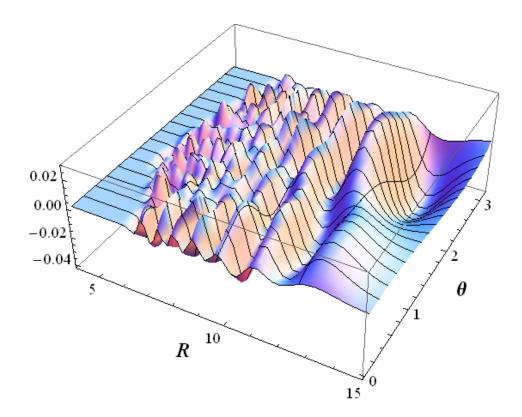


Figure S167. Eigenstate No. 167

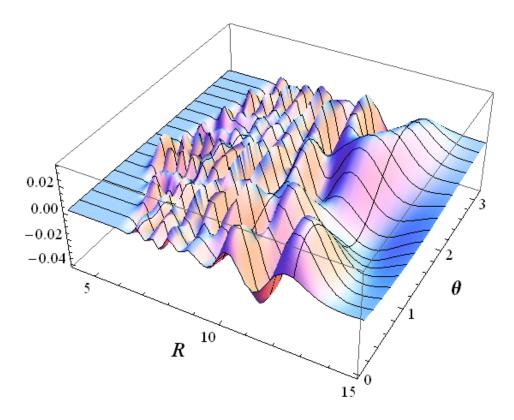


Figure S168. Eigenstate No. 168

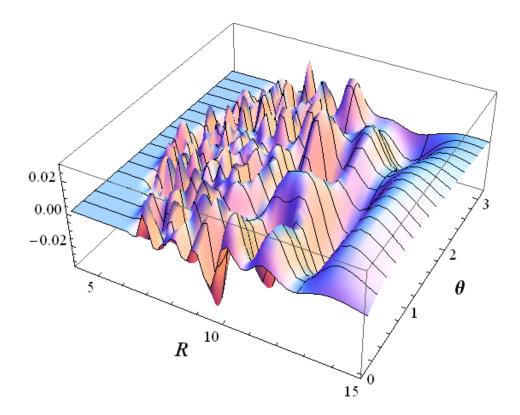


Figure S169. Eigenstate No. 169

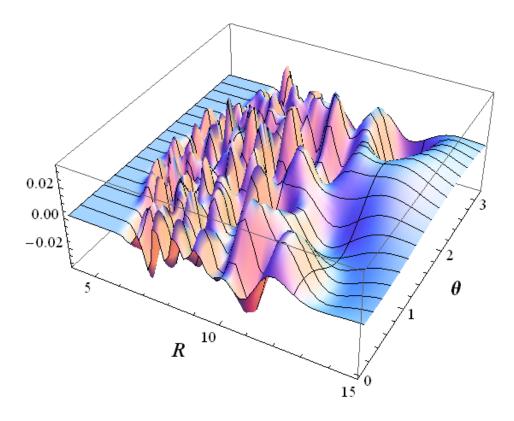


Figure S170. Eigenstate No. 170

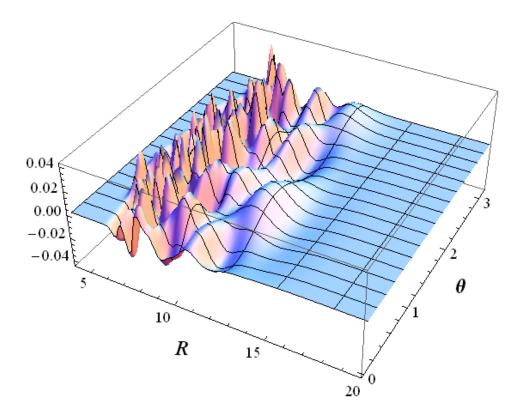


Figure S171. Eigenstate No. 171

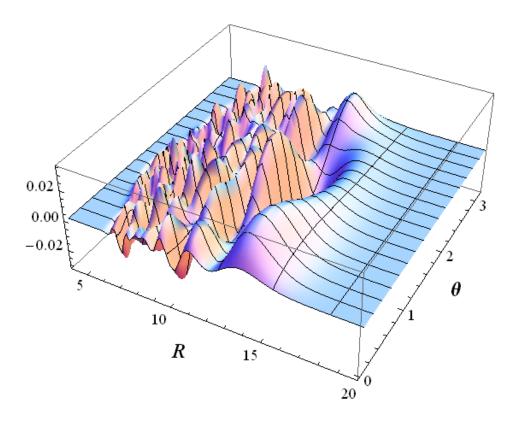


Figure S172. Eigenstate No. 172

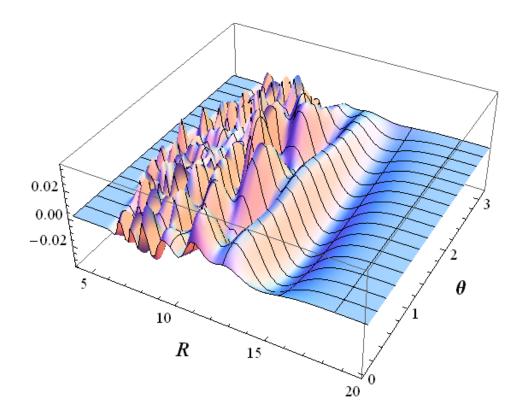


Figure S173. Eigenstate No. 173

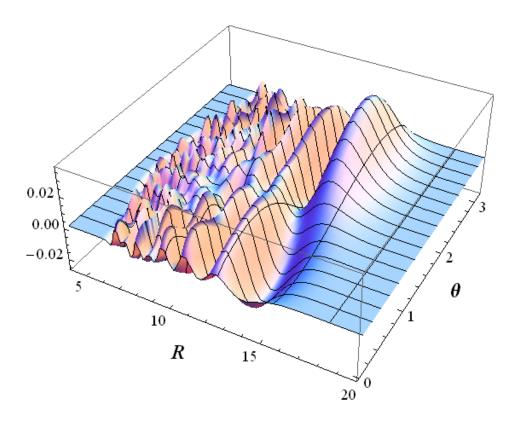


Figure S174. Eigenstate No. 174

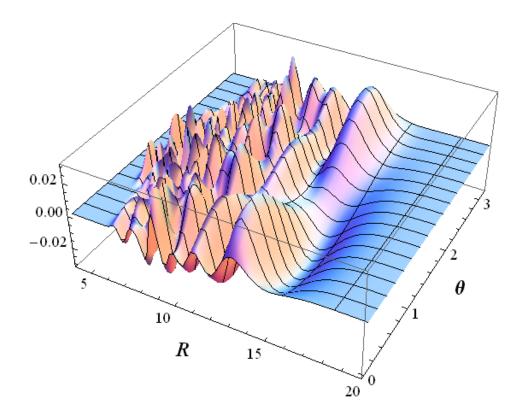


Figure S175. Eigenstate No. 175

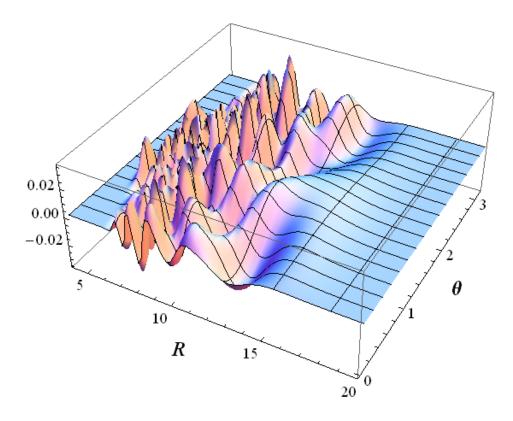


Figure S176. Eigenstate No. 176

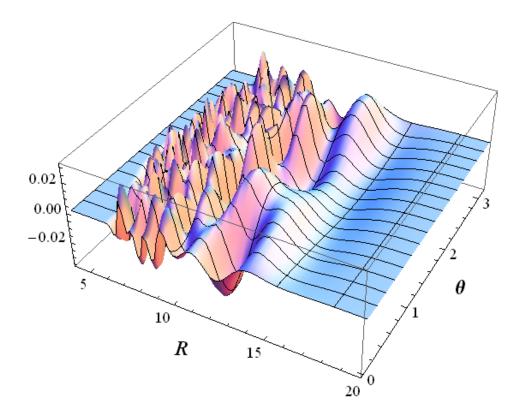


Figure S177. Eigenstate No. 177

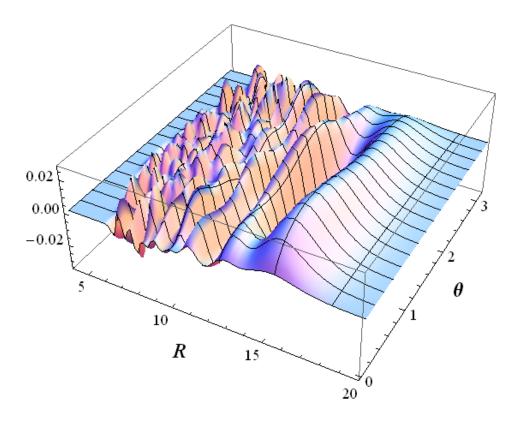


Figure S178. Eigenstate No. 178

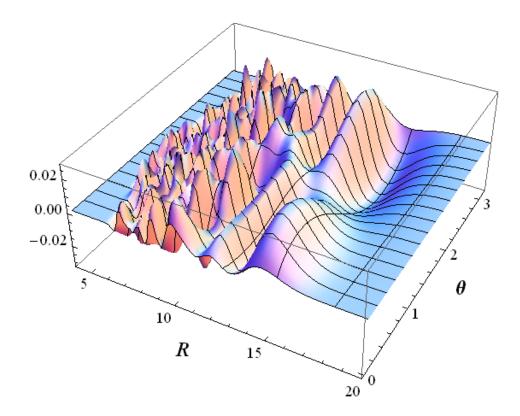


Figure S179. Eigenstate No. 179

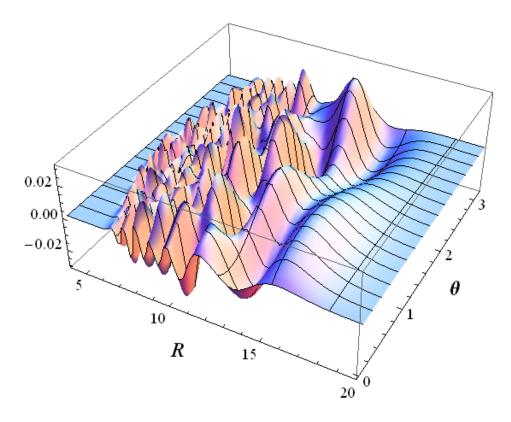


Figure S180. Eigenstate No. 180

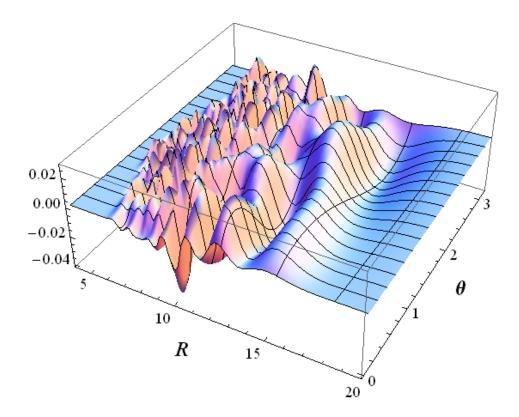


Figure S181. Eigenstate No. 181

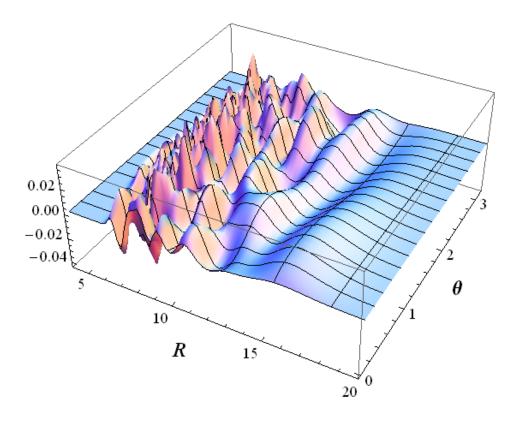


Figure S182. Eigenstate No. 182

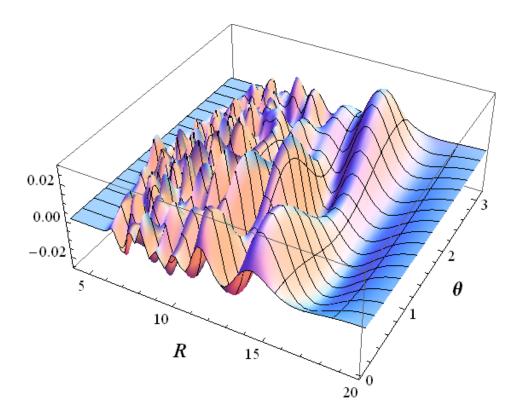


Figure S183. Eigenstate No. 183

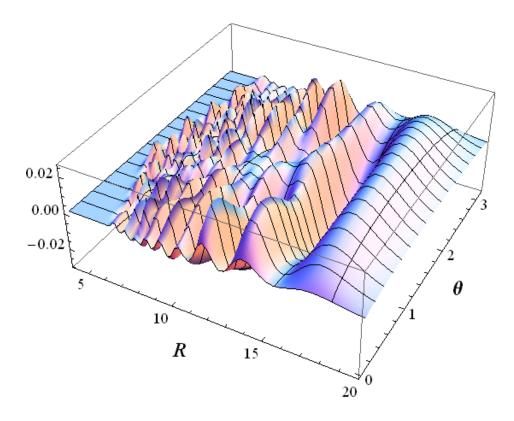


Figure S184. Eigenstate No. 184

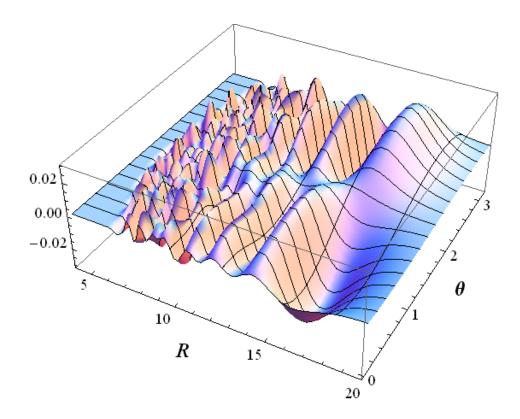


Figure S185. Eigenstate No. 185

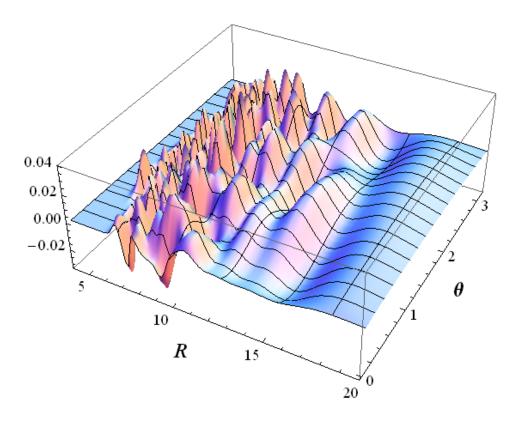


Figure S186. Eigenstate No. 186

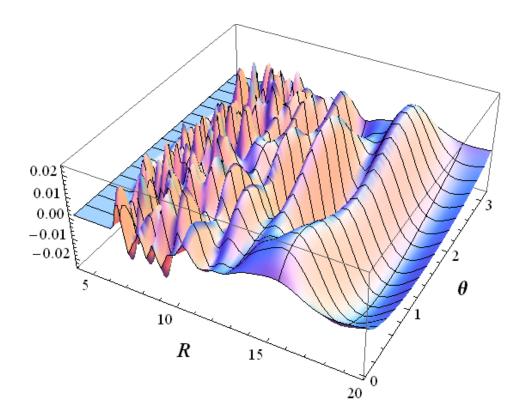


Figure S187. Eigenstate No. 187

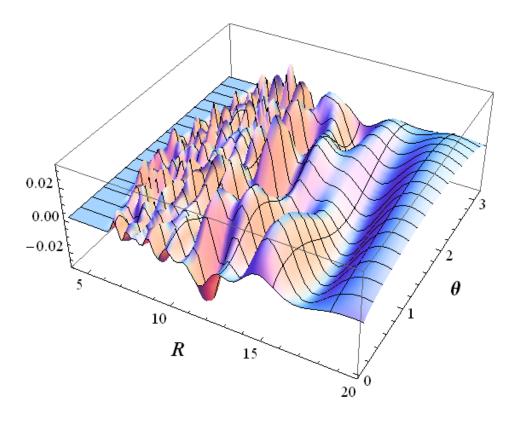


Figure S188. Eigenstate No. 188

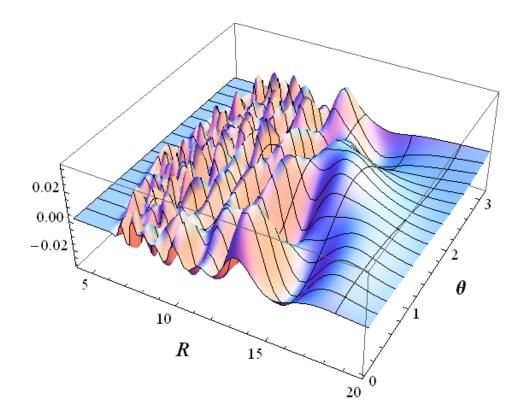


Figure S189. Eigenstate No. 189

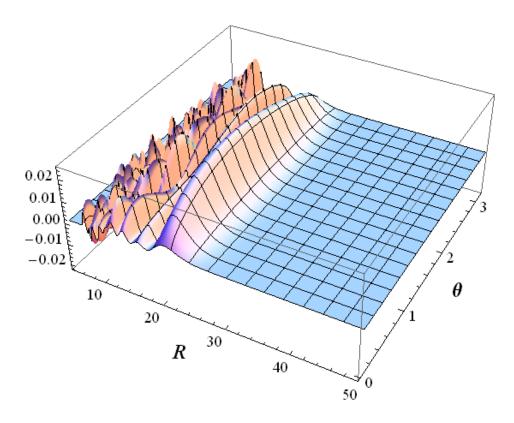


Figure S190. Eigenstate No. 190

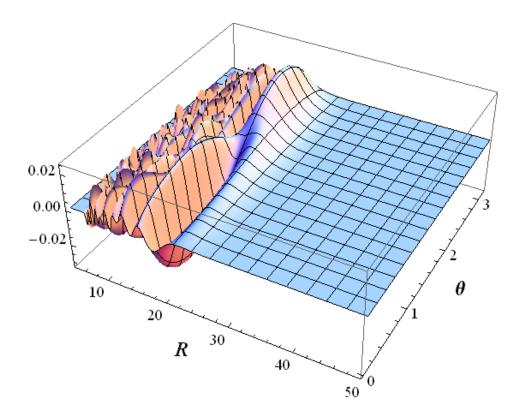


Figure S191. Eigenstate No. 191

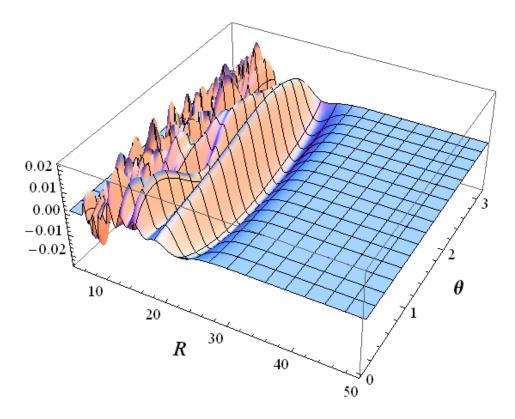


Figure S192. Eigenstate No. 192

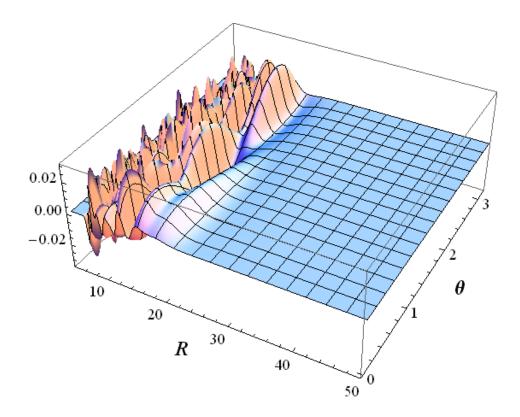


Figure S193. Eigenstate No. 193

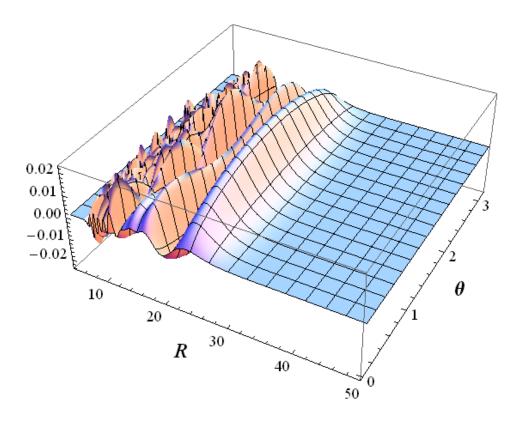


Figure S194. Eigenstate No. 194

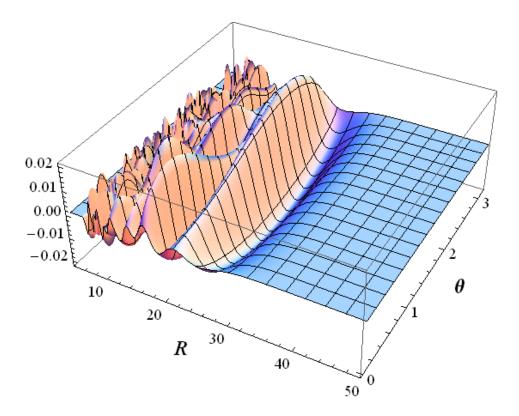


Figure S195. Eigenstate No. 195

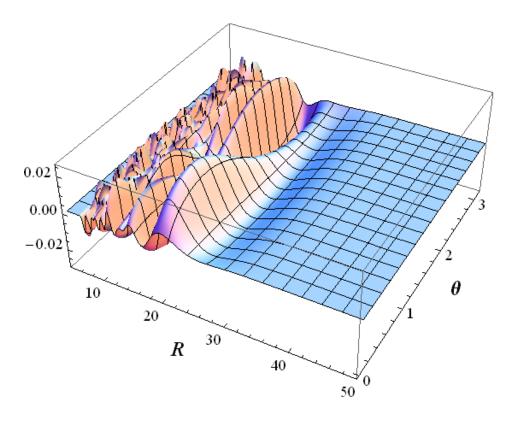


Figure S196. Eigenstate No. 196

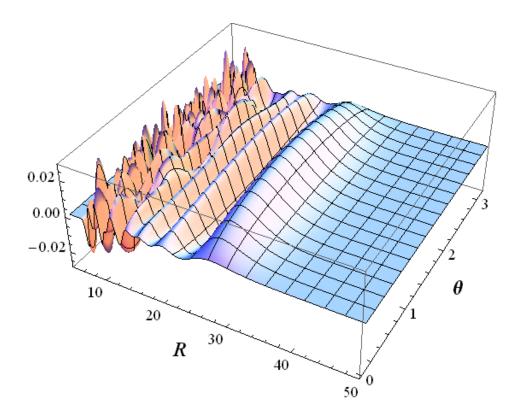


Figure S197. Eigenstate No. 197

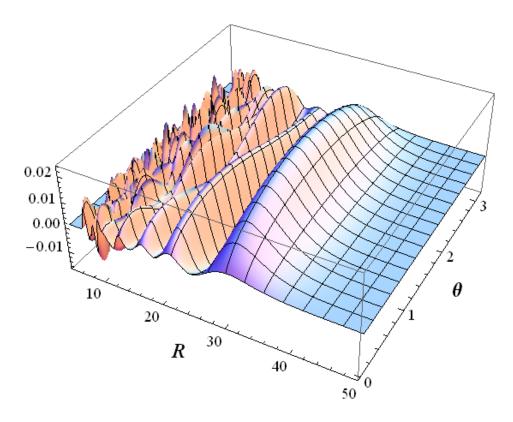


Figure S198. Eigenstate No. 198

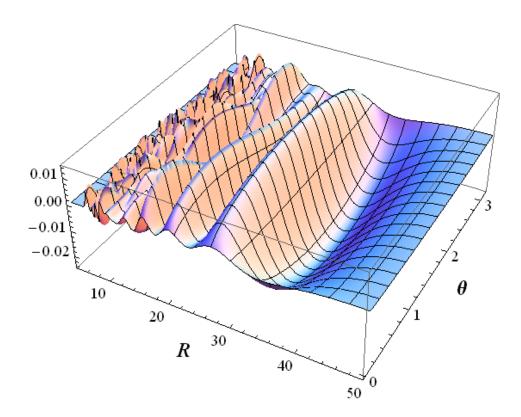


Figure S199. Eigenstate No. 199

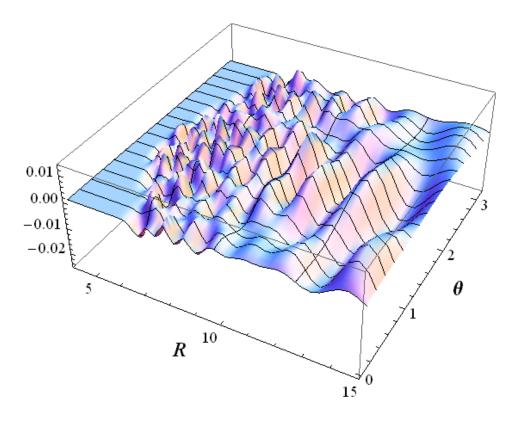


Figure S200. Eigenstate No. 200