www.ijonest.net

Interdisciplinary Fundamental Concepts in STEM: Solid State Physics and COVID-19 Pandemic Evolution

Michael Shur
Rensselaer Polytechnic Institute, USA

To cite this article:

Shur, M. (2023). Interdisciplinary Fundamental Concepts in STEM: Solid State Physics and COVID-19 Pandemic Evolution. *International Journal on Engineering, Science, and Technology (IJonEST), 5*(2), 119-127. https://doi.org/10.46328/ijonest.160

International Journal on Engineering, Science, and Technology
2023, Vol. 5, No. 2, 119-127 https://doi.org/10.46328/ijonest.160

Interdisciplinary Fundamental Concepts in STEM: Solid State Physics and COVID-19 Pandemic Evolution

Michael Shur

Article Info

Article History

Received:
15 January 2023
Accepted:
30 March 2023

Keywords

Pandemics
COVID-19
Pandemic evolution
Generalized Fermi-Dirac function

Abstract

The rapid development of computer-aided design tools, such as MATLAB or Octave, or Mathematica enabled students to solve many complicated problems focusing less on underlying STEM-related concepts that are interdisciplinary. Therefore, it is important to demonstrate how it could be done using specific examples that could be linked to different subjects or even to their everyday life experience. This paper reports on using the COVID-19 pandemic evolution model (Shur, 2022) in my class on the physics of advanced semiconductors devices. I use this model to show how the concepts, such as the Born-Oppenheimer approximation and Fermi-Dirac distribution function could be used in a completely different STEM field. In solid-state physics, the Born-Oppenheimer approximation is used to separate rapid electronic motion, relevant to the electronic states and much slower nuclei motion (since nuclei are thousands of times heavier than electrons). Likewise, the COVID-19 model uses a relatively fast pandemic evolution growth or decay constant, a slow function of time itself. In solid-state physics, the Fermi-Dirac distribution function describes the transition from the occupied electronic states to empty electron states with the temperature determining the transition interval. The COVID-19 model uses the generalized Fermi-distribution function to describe the mitigation measures that determine the transition from a high to a lower infection rate. A more accurate COVID-19 evolution model requires a generalized Fermi-Dirac function that accounts for a slow variation of the effect of the mitigation measures with time. In turn, this generalization could be used in solid-state physics to describe the electron temperature increase in the electric field.

Introduction

Computer-aided design tools, such as MATLAB, Octave, or Mathematica, have allowed students to solve complex problems without fully understanding the underlying interdisciplinary STEM concepts. To address this issue, it is important to provide specific examples that connect these concepts to different subjects or even to students' everyday experiences. In this paper, we report on the use of the COVID-19 pandemic evolution model (Shur (2022)) in a class on the physics of advanced semiconductor devices. This model is used to demonstrate how concepts from solid-state physics, such as the Born-Oppenheimer approximation and the Fermi-Dirac distribution function, can be applied to a completely different STEM field.

The Born-Oppenheimer approximation (Born and Oppenheimer (1927)) describes rapid electronic motion for frozen positions of nuclei. It introduces two-time scales; a rapid time scale relevant to the electronic motion and a slow time scale describing nuclei motion. This approximation holds because of much slower nuclear motion, due to the large difference in mass between electrons and nuclei. Similarly, the COVID-19 model (Shur(2021), (2022)) uses a fast pandemic evolution growth or decay constant that is itself a slow function of time. Another example of such a process is inflation. The inflation rate varies a little from day to day but changes significantly over periods on the order of a month or longer.

The Fermi-Dirac distribution function (Fermi (1926)) describes the transition from occupied to empty electronic states as a function of energy. The energy levels below the Fermi level energy are occupied, and the energy levels above the Fermi level energy are empty. The transition region, where the Fermi Dirac function changes from near unity to nearly zero is on the order of several (~6) thermal energies proportional to temperature. I explain in my class that such a function could be used to describe a gradual transition between any two states. For example, in the COVID-19 model, a Fermi-Dirac distribution function is used to describe the effect of mitigation measures on infection rates – from a higher rate before the mitigation measures are introduced to a lower infection rate after a transition period after the mitigation measures are introduced. It is important to demonstrate how the same mathematics could be used for describing completely different phenomena.

A more accurate COVID-19 evolution model (Shur(2023)) uses a generalized Fermi-Dirac function that accounts for the slow variation of mitigation measures over time. This generalization could also be applied in solid-state physics to describe the increase in electron temperature in an electric field more accurately (Shur(1969)).

The COVID-19 pandemic is a good case in point because of its huge impact on the health system (see Figures 1 and 2 illustrating the tragic consequences of the COVID-19 pandemic).

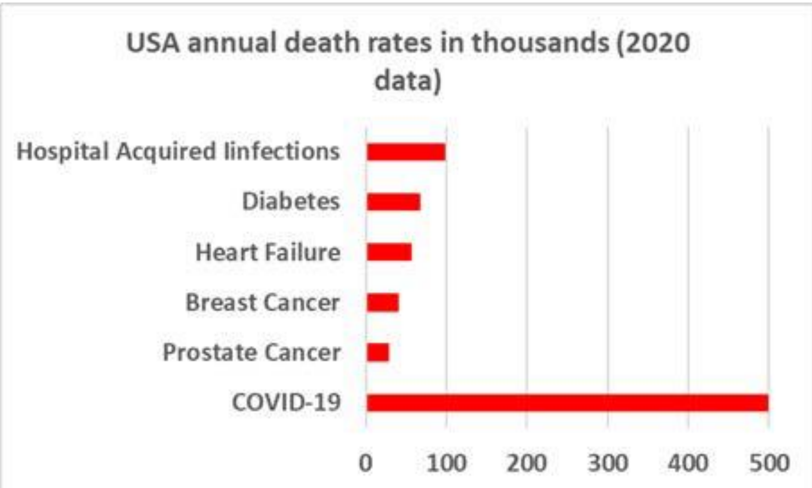


Figure 1. USA Annual Death Rates for Different Reasons. Data from https://www.ontherighttrack.com/news/the- healthcare-paradox Accessed 28 July 2022

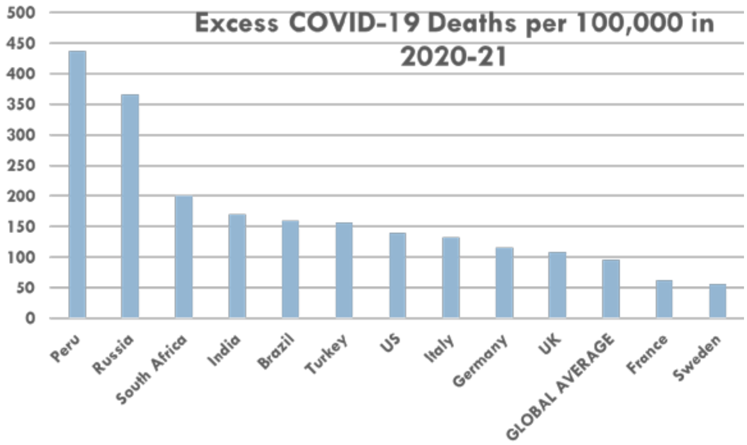


Figure 2. Excess COVID-19 Deaths in Different Countries. Data from; https://www.bbc.com/news/61333847, accessed 04/14/2023.

An example where such an approach of simulating the impact of mitigation measures could also be useful is Hospital Acquired Infections (HAI). Each year in U.S. hospitals there are an estimated 1.7 million healthcare-acquired infections (HAI) resulting in approximately 99,000 deaths (2018 data). The cost estimates for HAI range from $20 to $45 billion annually. It is approximately 1/6 of the US COVID-19 cost per year. An example of the mitigation measure for controlling Hai is using mattress pad disinfection in hospitals (see Shur (2010)).

Another similarity between the waves of the electron density that are considered in my class on advanced electronic devices and the COVID-19 pandemic evolution is that the pandemic came in waves that rose, crested, and dropped (see Figure 3). These waves vary from location to location (see Figure 4). The reason for these waves is the virus evolution. A virus is asexual and replicates making copies of itself. Making mistakes (mutations) during reproduction causes new strains to appear. Some strains are not competitive and die out, but some are more easily spread or more deadly. Another mechanism of virus evolution is recombination which occurs when a host cell is infected with two different variants at the same time exchanging one part of a virus for another (one example: overtaking of Delta by Omicron.).

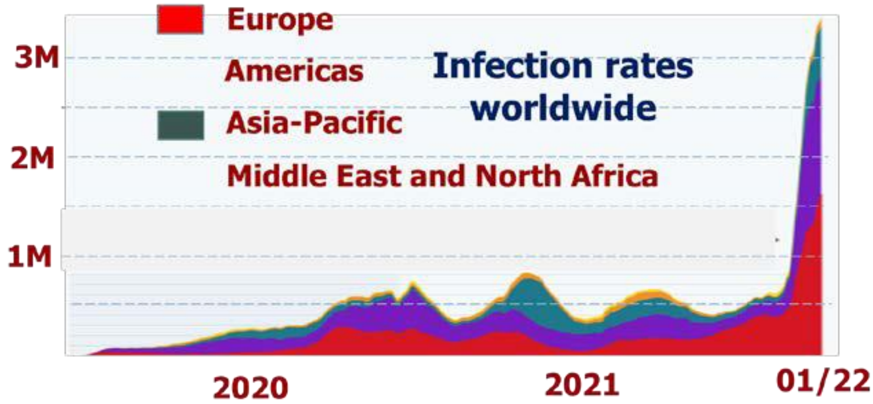


Figure 3. COVID-19 Infection Rates Worldwide. Data from https://www.statista.com/chart/22067/daily-new- cases-by-world-region/ Accessed 12 April 2022

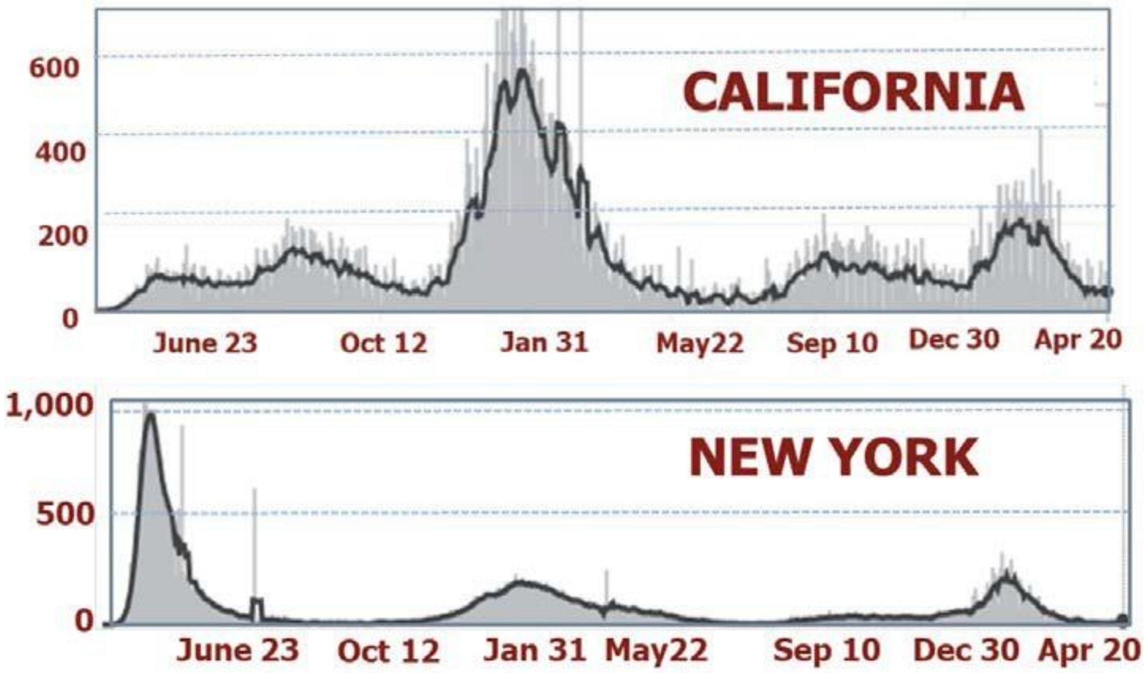


Figure 4. COVID-19 Evolution for New York State and California (from Shur(2023)). Data from https://www.google.com/search?q=covid+new+cases&rlz accessed 22 April 2022

Results and Discussion

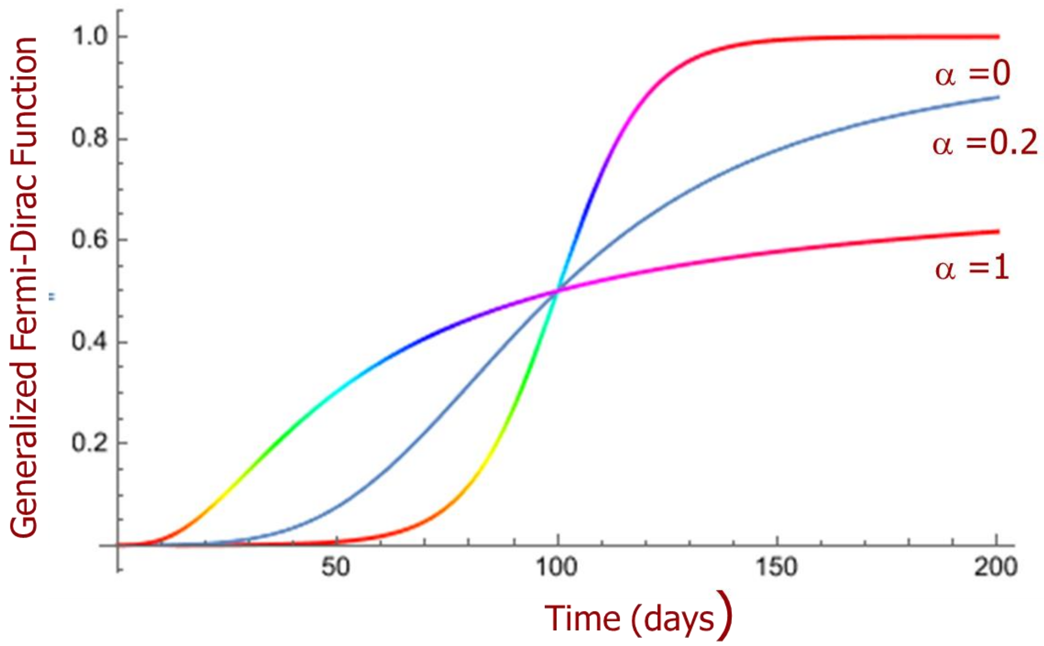
Physics-based transparent pandemic models needed to describe the complicated evolutions could use approximations similar to the Born-Oppenheimer approximation and transition functions similar to the Fermi-Dirac distribution function. The Fermi-Dirac distribution function describes the transition from the non-degenerate to degenerate distribution in semiconductors (see, for example, Shur (1996), page 91). The same function could describe any step-wise transition within a defined transition period. For pandemic processes, this function could describe changes associated with pandemic mitigation measures, such as mask requirements or vaccination:

$$f_{FDS} = \frac{1}{1 + \exp \dfrac{t_i - t}{\tau_i\left(t\right)}} \qquad (1)$$

Here f_{FDS} is the function describing event i (Fermi-Dirac Smoothed function -FDS), t_i is the moment of the transition, τ_i is the characteristic time constant determining how fast this transition takes place. In the generalized Fermi-Dirac distribution function (FDG) the time constant τ_i is a slow (compared to τ_i) function of time:

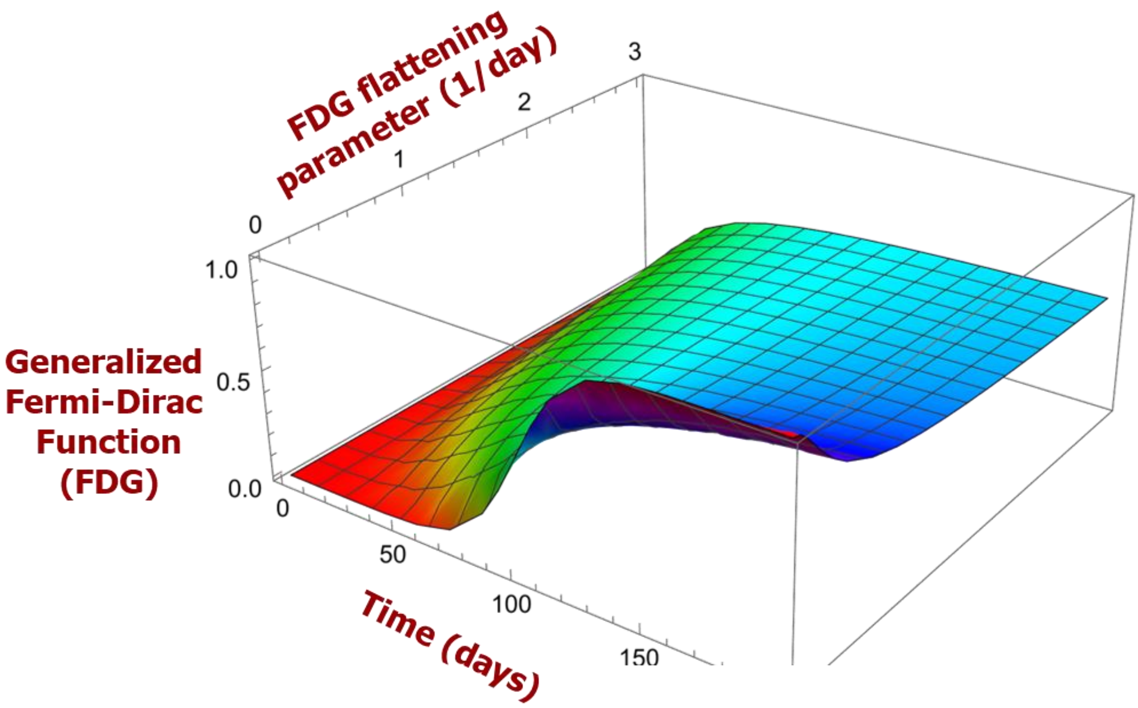
$$\tau_i\left(t\right) = \tau_{io} + \alpha_i t \qquad (2)$$

Figure 5a shows the generalized Fermi-Dirac function for t_i = 100 days, τ_i = 10 days, and different values parameter α_i. The effect of this parameter is clearer in Figure 5b.



(a)

Figure 5. Generalized Fermi-Dirac Distribution Function



(b)

Figure 5. Generalized Fermi-Dirac Distributions

The Pandemic Equation (Shur (2021), (2022), (2023)) accounts for asymmetric pandemic curves and multiple pandemic waves using. curve flattening parameter to account for the population adjustment to the infection and mitigation parameters to account for mitigation measures and new virus variants:

$$\Delta N_{\beta_1,\beta_2\cdots\beta_n}(t)=\Delta N_i(t,\alpha)\left(1-\frac{\beta_1}{1+\exp\left(\left(t-t_{\beta 1}\right)/\tau_{\beta 1}\right)}\right)\times \left(1-\frac{\beta_2}{1+\exp\left(\left(t-t_{\beta 2}\right)/\tau_{\beta 2}\right)}\right)\cdots\left(1-\frac{\beta_n}{1+\exp\left(\left(t-t_{\beta n}\right)/\tau_{\beta n}\right)}\right) \tag{3}$$

Here $\Delta N_{\beta_1,\beta_2\cdots\beta_n}(t)$ is the daily number of new infections,

$$\Delta N_i=\frac{N_t(t)\,f_o e^{t/\tau(t)}}{\left(1+f_o e^{t/\tau(t)}\right)^2\tau(t)} \tag{4}$$

describes the evolutions of the daily number of new infections in the period of time before the first mitigation event, f_o is the ratio of the initial infections to the total number of people in the infection pool. The time dependence of the initial characteristic constant of the pandemic evolution also includes the mitigation parameter a making it a slow function of time:

$$\tau(t)=\tau_o+\alpha t \tag{5}$$

Examples of mitigation and anti-mitigation measures include masks (see Figure 6), closing or opening the economy, vaccination, and new medications, such as Evusheld and Paxlovid.

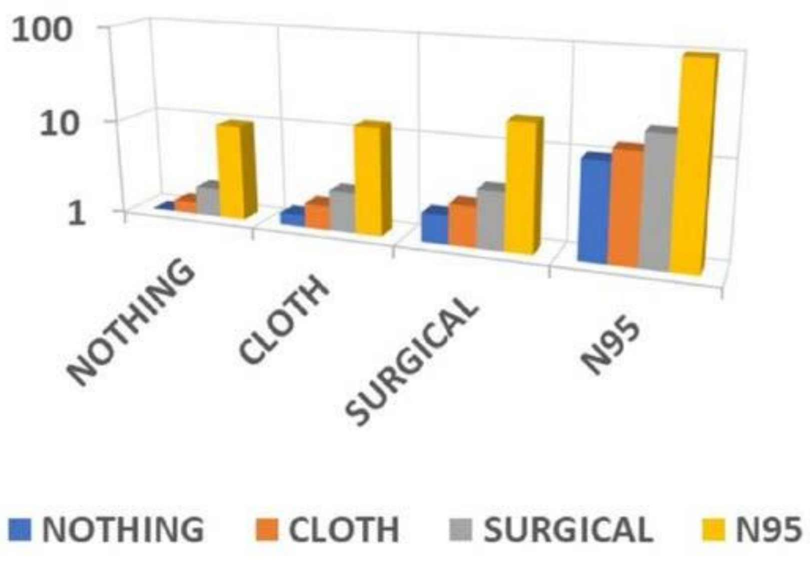


Figure 6. Masks as a Mitigation Measure: Relative Improvement in Protection Time compared to No Mask (from Shur(2022)).

Figure 7 illustrates the effect of the curve flattening parameter on the predicted pandemic evolution. As a challenge, I ask my students to suggest how the same generalization of the Fermi-Dirac distribution function could be used to describe non-equilibrium electron distribution with electrons having a higher directed energy and also a higher effective temperature.

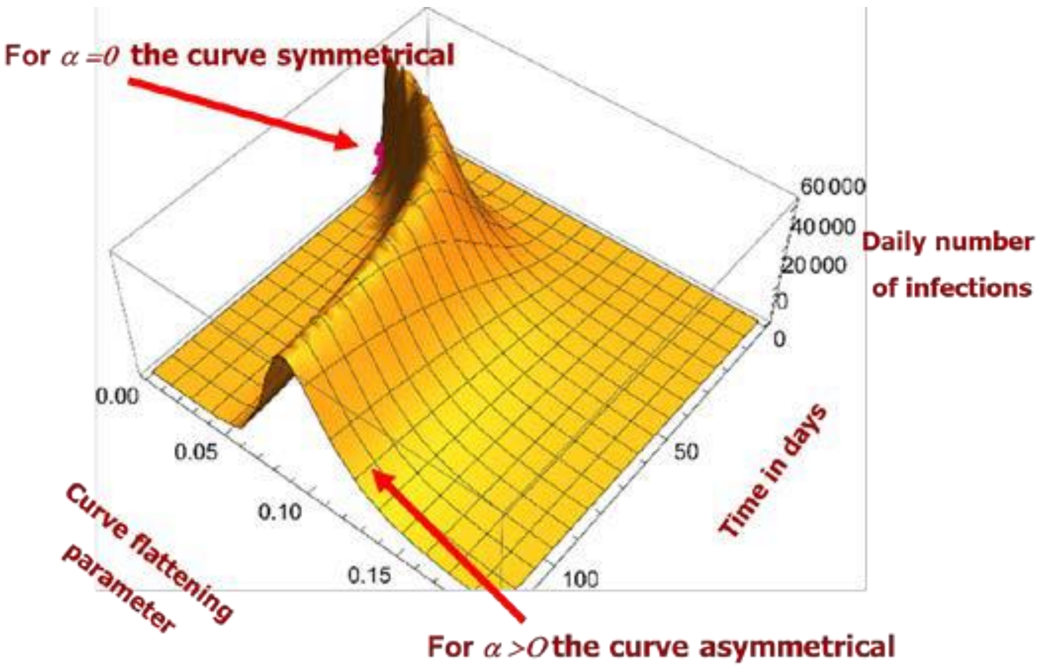


Figure 7. Effect of Flattening Parameter on COVID-19 Pandemic Model. (From Shur (2022)).

The crown result of the Pandemic Equation shown in Figure 8 also brings up interesting questions. How good is the agreement? How to see trends in a stochastic process? What is Uncertainty Quantification? Could techniques used in solid-state theory for quantifying Uncertainty (see, for example) be applied to modeling COVID-19 Pandemic (see Figure 9)? And, finally, could the approach accounting for space dependence of the pandemic infection (see Fig. 10) be used to describe spatially non-uniform electronic distributions?

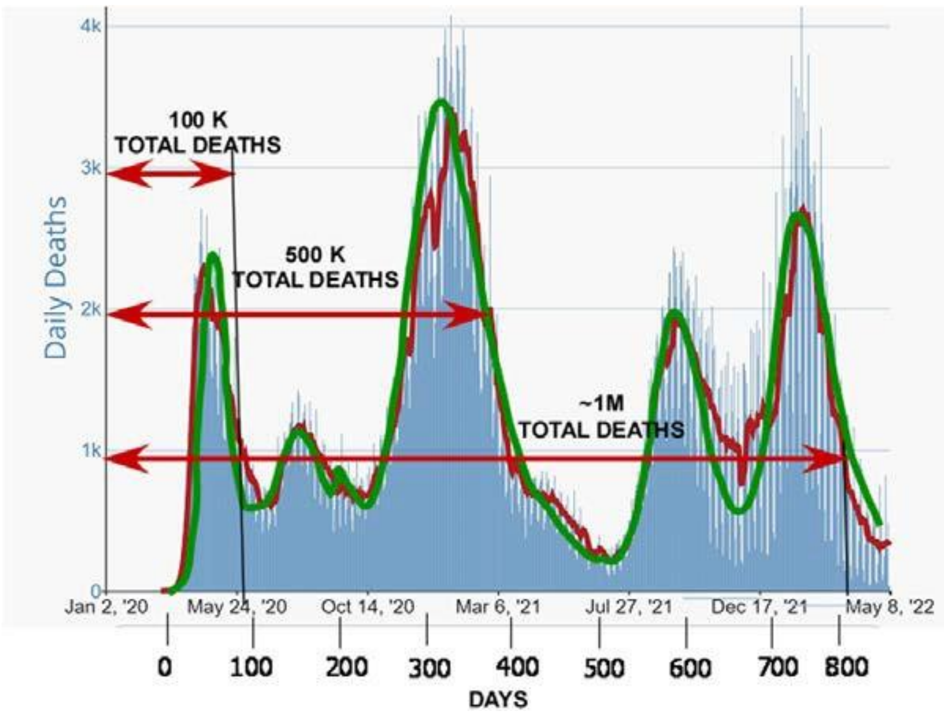


Figure 8. Comparison of Five COVID-19 Pandemic Waves described by Pandemic Equation with Daily COVID-19 Deaths in the USA (from Shur (2023)).

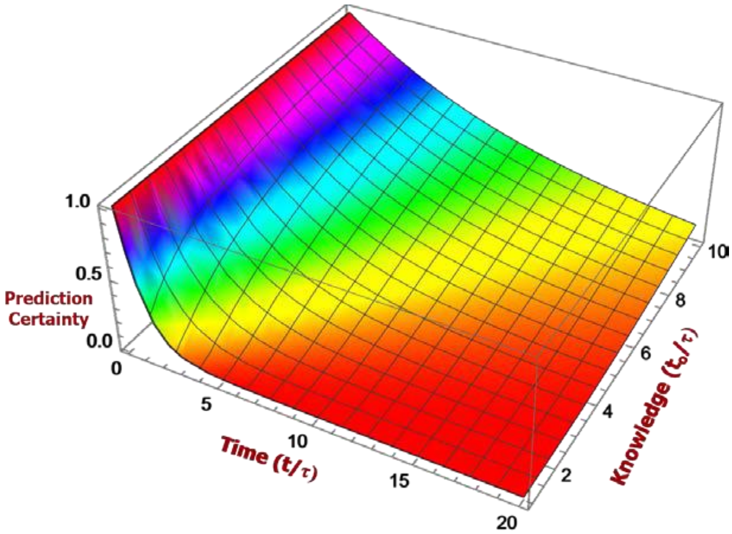
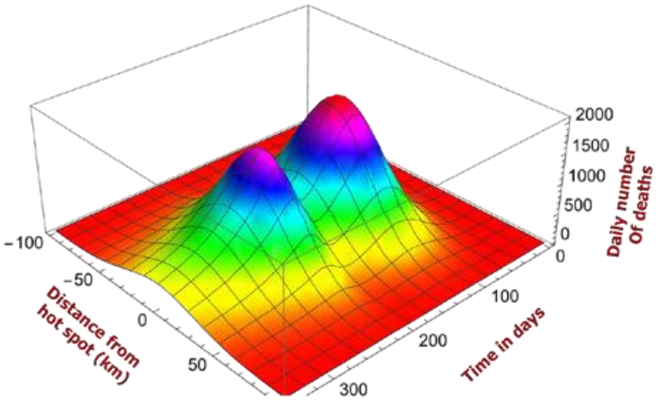
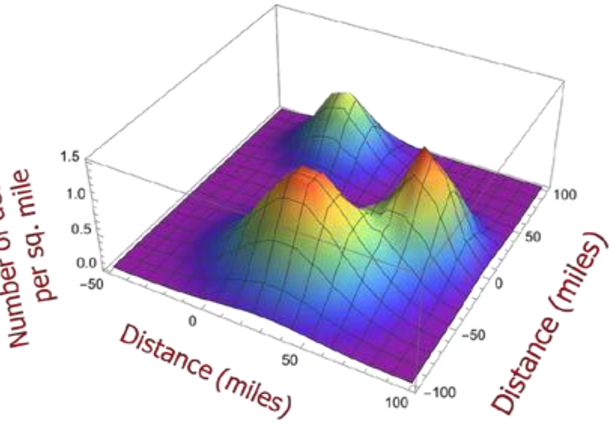


Figure 9. Prediction Certainty in the Extrapolation of the Pandemic Equation Solution.



(a)



(b)

Figure 10. Simulating Space-dependent Infection Rates with Two Hot Spots (a) and Three Hot Spots (b)

Conclusion

The Pandemic Equation is a modified rate equation with slowly varying parameters. It uses an approach similar to the adiabatic approximation (i.e., Born-Oppenheimer approximation) in the quantum theory of solids and uses the generalized Fermi-Dirac distribution function. The Pandemic Equation describes the pandemic evolution curves accounting for curve flattening and mitigation and antimotivation measures. Extracting the Pandemic Equation parameters from the well-advanced pandemic curves allows for reaching conclusions about the pandemic trends and enables the Pandemic Equation to predict the pandemic evolution globally and locally for time periods of the order of the pandemic time constant. The generalization of the Pandemic equation used to describe the spatial dependence of the infection rates and slow time-dependent variation of the infection rate characteristic time constant could, in turn, find applications in the solid-state theory.

References

Born, M., & Heisenberg, W. (1985). Zur quantentheorie der molekeln. *Original Scientific Papers Wissenschaftliche Originalarbeiten*, 216-246.

Dirac, P. A. M. (1926). On the theory of quantum mechanics. *Proceedings of the Royal Society of London. Series A, Containing Papers of a Mathematical and Physical Character, 112*(762), 661-677.

Fermi, E. (1926). *Sulla quantizzazione del gas perfetto monoatomico.* Rendiconti Lincei

Shur, M. S., (1969). The effect of the shift of the absorption edge by electric field in degenerate semiconductors. *Phys. Lett., 29A*(9), 490.

Shur, M. S., (1996). *Introduction to Electronic Devices.* John Wiley and Sons, Inc.

Shur, M. et al. (2020). *Ultraviolet gradient sterilization, disinfection, and storage system*. US Patent 10,576,174, March 3, 2020

Shur. M. (2021). Pandemic Equation for Describing and Predicting COVID-19 Evolution. *Journal of Healthcare Informatics Research, 5*(2), 168-180. DOI: 10.1007/s41666-020-00084-2.

Shur. M. (2022). Pandemic Equation and Pandemic Evolution. *Academia Letters*, Article 4762. https://doi.org/10.20935/

Shur, M. (2023). Pandemic Equation and Waves of COVID-19 Evolution, Springer Nature - Book Series: Transactions on Computational Science & Computational Intelligence. In *Advances in Data Science and Information Engineering, Proceedings from ICDATA 2022 and IKE 2022*.

He Y., Chilleri J., O'Leary S., Shur M., Kirby R.M. (2019). Sensitivity Analysis for an Electron Transport System: Application to the Case of Wurtzite Gallium Nitride. *Journal of Computational Electronics, 19*(59). D

Author Information

Michael Shur

https://orcid.org/0000-0003-0976-6232

Rensselaer Polytechnic Institute

110 8-th Street, Troy, NY 12180

USA

Contact e-mail: *shurm@rpi.edu*