

Comment on “Hot gases: The transition from the line spectra to thermal radiation,” by M. Vollmer [Am. J. Phys. 73 (3), 215–223 (2005)]

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I call attention to several errors in a recent article by Vollmer¹ that invalidate his explanation for how the line spectrum of atoms is transformed into the continuous spectrum of thermal radiation. Following Einstein’s 1916 derivation² of Planck’s black-body formula, the transformation of this line spectrum to thermal radiation at discrete frequencies associated with these transitions has been discussed often, particularly in the astronomy literature.³ But the question of how discrete atomic transitions can give rise to black-body radiation that is continuous in frequency has been ignored. To fill this gap, I present here a novel derivation of this transformation in a model of a hot gas of atoms with only two energy levels.

Vollmer’s arguments are based on Einstein’s original model of stationary atoms,² but with only two energy levels corresponding to an excited state and a ground state, which are in thermal equilibrium with the emitted and absorbed photons.⁵ Such a model cannot give rise to a thermal spectrum which is continuous for a finite range of frequencies because, apart from a line width due to the finite lifetime of the excited state, the photons are essentially monochromatic with a frequency ν_0 . This frequency is determined by the well-known Bohr-Einstein relation $h\nu_0 = \epsilon$, where ϵ is the energy difference between the two atomic levels and h is Planck’s constant. Vollmer ignored this fundamental relation in his derivation of the Planck black-body formula, and misapplied Einstein’s detailed balance condition. Instead of setting $N_2/N_1 = \exp(-h\nu_0/kT)$ for the ratio of the population of the excited and ground state atomic levels at a temperature T , he incorrectly set $N_2/N_1 = \exp(-h\nu/kT)$ for arbitrary values of $\nu \neq \nu_0$ [see Eqs. (11), (15), and (16) in Ref. 1]. Then, he attributed the source of the continuous thermal spectrum to the finite width of the excited level⁶ but, as I will show, this attribution is not correct.

Vollmer also argued that the Doppler width in the frequency of photons emitted by the randomly moving atoms in a hot gas can be neglected in the calculation of the thermal spectrum.⁷ I will show, however, that in a simplified model of two level atoms, it is precisely the Doppler shift that gives rise, for an optically thick gas of such atoms, to a thermal spectrum which is continuous over a range of frequencies.

The necessary and sufficient conditions for the energy distribution of thermal radiation to be a continuous function of frequency in any given frequency range is the occurrence of radiative processes in thermal equilibrium that emit and ab-

sorb photons in this frequency range. It is counter intuitive that the energy density of photons that are emitted and absorbed by various radiative process, which may also differ greatly in intensity and in the rate of transitions, should lead at thermal equilibrium to a universal energy density distribution. But this universality, which was first formulated in 1859 by Kirchhoff on general thermodynamic grounds, is the essence of Einstein’s detailed balance derivation of the black-body distribution first obtained in 1900 by Planck.

We illustrate how this universality comes about by considering a hot gas of two level atoms in thermal equilibrium. When an atom in the excited state moving with velocity \vec{v}_e emits a photon with frequency ν , then by conservation of momentum, the velocity in the ground state is changed to

$$\vec{v}_g = \vec{v}_e - \frac{h\nu}{mc} \vec{n}, \tag{1}$$

where m is the mass of the atom, c is the speed of light, and \vec{n} is a unit vector along the direction of the emitted photon. Correspondingly, by conservation of energy

$$h\nu = \epsilon + \frac{1}{2}m(v_e^2 - v_g^2). \tag{2}$$

We substitute for v_g^2 in Eq. (2) the result obtained from Eq. (1) and obtain for $v/c \ll 1$

$$\nu = \nu_0 \left(1 + \frac{v_n}{c} \right), \tag{3}$$

where $\nu_0 = \epsilon/h$, and v_n is the component of \vec{v}_e along \vec{n} . Equation (3) is the nonrelativistic Doppler change in frequency of a photon emitted by a moving atom,⁸ which is obtained by neglecting a small term of order ϵ/mc^2 due to the small loss in photon energy given to the atom as recoil kinetic energy. Hence, the Maxwell–Boltzmann distribution for the excited atoms with velocity component v_n yields a Gaussian probability distribution for the emission of photons with frequency ν centered at $\nu = \nu_0$,

$$P(\nu) = \frac{1}{\sqrt{2\pi}\Delta} e^{-(\nu - \nu_0)^2/2\Delta^2}, \tag{4}$$

where $\Delta = \nu_0 \sqrt{kT/mc^2}$ is the Doppler width of the radiation.

If photons of a given frequency ν are in thermal equilibrium with the atoms, the absorption of these photons by atoms in the ground state must be taken into account. Follow-

ing Einstein's derivation,² the radiation energy density ρ is determined by the detailed balance condition between the emission and absorption of photons,

$$(A + B\rho)N_e = B\rho N_g, \quad (5)$$

where A is the Einstein coefficient for spontaneous emission, B is the corresponding coefficient for stimulated emission and absorption of photons, and $A/B = 8\pi h\nu^3/c^3$. Here N_g and N_e are the populations of atoms in the ground and excited states respectively, given by the canonical density distribution

$$N_e = C \exp\left(-\left(\epsilon + \frac{1}{2}m v_e^2\right)/kT\right) \quad (6)$$

and

$$N_g = C \exp\left(-\frac{1}{2}m v_g^2/kT\right), \quad (7)$$

where C is a normalization constant. The range of random atomic velocities is determined by the momentum and energy conservation given in Eqs. (1) and (2) for a given frequency ν of the photon. We solve Eq. (5) for the energy density ρ and obtain

$$\rho = \frac{8\pi h\nu^3}{c^3} \frac{1}{(N_g/N_e - 1)}, \quad (8)$$

where by Eqs. (6) and (7) we have

$$\frac{N_g}{N_e} = \exp\left(\left(\epsilon + \frac{1}{2}m(v_e^2 - v_g^2)\right)/kT\right). \quad (9)$$

If we apply the conservation of energy relation, Eq. (2), and substitute the resulting expression into Eq. (8), we obtain the Planck black-body distribution for the radiation energy density

$$\rho = \frac{8\pi}{c^3} \frac{\nu^3}{(\exp(h\nu/kT) - 1)}, \quad (10)$$

for a continuous range of frequencies ν .⁴

This frequency range is restricted by the conservation of momentum and energy in the emission and absorption of photons by the atoms, Eqs. (1) and (2). We have shown that photons of frequency $\nu \neq \nu_0$ are emitted by excited atoms moving with a component of velocity $v_n = c(\nu/\nu_0 - 1)$ along the direction of the propagation of this photon. But according to the Maxwell-Boltzmann distribution, the number of such atoms decreases exponentially as a function of $(\nu - \nu_0)^2/2\Delta^2$, where $\Delta = \nu_0\sqrt{kT/mc^2}$ [see Eq. (4)]. Because the mean free path $\ell(\nu)$ for absorption of photons with frequency ν is inversely proportional to the density of these atoms, the photons for an optically thick gas cloud with linear dimension D are no longer in thermal equilibrium when $\ell(\nu)$ is larger than D . According to Eq. (4), this occurs when

$$|\nu - \nu_0| > \Delta\sqrt{\ln(D/\ell(\nu_0))}, \quad (11)$$

which gives the range of frequencies for which continuous thermal radiation occurs in this idealized model of a hot gas cloud.

The model of stationary atoms discussed originally by Einstein^{2,5} and treated by Vollmer,¹ corresponds to $m \rightarrow \infty$ for which $\Delta \rightarrow 0$; in this limit the thermal radiation is essentially monochromatic with frequency $\nu = \nu_0$.

For an optically thin gas, $D < l(\nu_0)$, the probability for the absorption of photons can be neglected, and the Maxwell-Boltzmann distribution for the random velocities of excited atoms gives rise to the Doppler broadening of the line width. If we include the Lorentzian line shape factor for the natural line width of the radiation,

$$\frac{\gamma/\pi}{(\nu - \nu')^2 + (\gamma)^2}, \quad (12)$$

where γ is half the line width at half maximum, the final line shape is given by the Voigt form factor⁹

$$F(\nu) = \int d\nu' \frac{\gamma/\pi}{[(\nu - \nu')^2 + \gamma^2]} \frac{1}{\sqrt{2\pi}\Delta} e^{-(\nu' - \nu_0)^2/2\Delta^2}. \quad (13)$$

This result differs from the corresponding limit in Eq. (17) of Ref. 1, where the important effect of the Doppler shift has been neglected.

Thermal photons due to additional atomic transitions with different energy level separations, different masses, and different total number of atoms lead to the same universal Planck black-body radiation energy distribution, even if the range of photon frequency for the separate processes overlap. Moreover, due to the finite lifetime of the excited levels of atoms, the energy conservation relation Eq. (2) is not strictly maintained, and photons can also be emitted and absorbed with frequencies confined by the Lorentzian line shape, Eq. (12), in the rest frame of the atoms. These photons also contribute to the thermal spectrum ρ without modifying it.

The universality and continuity in the frequency of thermal radiation is due to the fact that induced emission and absorption of photons in radiative processes is independent of the nature of its sources, provided that these sources emit photons in the frequency range under consideration. However, a derivation of the thermal spectrum by Einstein's detailed balance method requires processes that conserve energy and momentum. Photons in the wings of the Lorentz line width are due to the finite lifetime of the excited state, which implies an uncertainty of the energy of this state. Therefore, although these photons contribute to the thermal spectrum, the transitions associated with these photons cannot be included in the detailed balance equation as has been proposed in Ref. 1. Our treatment answers the question of the nature of the radiation spectrum in an ideal model of a hot gas consisting of atoms with only two levels for which the only source of photons is the transition between the excited and the ground state of the atom.

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¹M. Vollmer, "Hot gases: The transition from line spectra to thermal radiation," *Am. J. Phys.* **73**, 215–223 (2005).

²A. Einstein, "Zur Quantum Theorie der Strahlung," *Phys. Z.* **18**, 121–128 (1917). First printed in *Mitteilungender Physikalischen Gesellschaft Zurich*. No. 18, 1916. Translated into English in Van der Waerden, *Sources of Quantum Mechanics* (North-Holland, Amsterdam, 1967), pp. 63–77.

³The first treatment of this transformation in a thermal gas of two level atoms was given by E. A. Milne, "Thermodynamics of the stars," *Handbuch der Astrophysik* **3**, Part 1, 159–164 (1930). This article is reprinted in *Selected Papers on the Transfer of Radiation*, edited by D. H. Menzel (Dover, New York, 1966), pp. 173–178. Milne's derivation has been reproduced, almost unchanged, in several astrophysics textbooks that discuss radiative transfer. See, for example, S. Chandrasekhar, *An Introduction to the Study of Stellar Structure* (Dover, New York, 1958), pp. 205–207; D. Mihalas, *Stellar Atmospheres* (Freeman, San Francisco, 1978), pp. 336–339; A. Peraiah, *An Introduction to Radiative Transfer* (Cambridge University Press, Cambridge, 2002), pp. 15–16. In all these treatments the effect of the Doppler shift on the radiation frequency due to the random motions of the atoms in a hot gas has been included only for its effect on the line width, although as we show here, it is this shift that can also give rise to thermal radiation continuous in the frequency of the radiation.

⁴In our derivation of Planck's black-body formula we required both conservation of energy and momentum in the emission and absorption of photons. In his original derivation Einstein applied only the conservation of energy, "for we have only formulated our hypothesis on emission and absorption of radiation for the case of stationary molecules." Subsequently, he showed by a very elaborate calculation of the momentum transfer of radiation to the atoms that the mean thermal energy of the atoms satisfies the equipartition theorem, assuming that the elementary

process transmits an amount of momentum $h\nu/c$. He concluded that if a radiation bundle has the effect that a molecule struck by it absorbs or emits a quantity of energy $h\nu$ in the radiation, then a momentum $h\nu/c$ is always transferred to the molecule (Ref. 2). Our derivation demonstrates the relevance of this momentum transfer to the formation of a thermal spectrum in hot gases.

⁵M. Nauenberg, "The evolution of radiation towards thermal equilibrium: A soluble model which illustrates the foundations of statistical mechanics," *Am. J. Phys.* **72**, 313–323 (2004). In this paper I assumed that the atoms are fixed, but the extension to randomly moving atoms in a thermal gas is straightforward along the lines indicated here.

⁶After obtaining Eq. (11), Vollmer writes: "Note we assumed discrete energy levels and transitions between them. But suddenly the result, Eq. (11), is interpreted as a continuous spectrum. Where do all the possible transitions arise? The answer is simple: each atom or molecule possesses at least one resonance frequency for absorption. An absorption line extends over the entire spectrum because it has a finite width, that is, each atom or molecule can absorb radiation at every wavelength, although with different cross sections..." Ref. 1, p. 218.

⁷Vollmer writes: "The justification for the assumption that the Doppler width or collisional width is not important [to explain the formation of the continuous spectrum] comes from a numerical estimate of the Doppler width and the effects of pressure broadening," Ref. 1, p. 216.

⁸E. Fermi, "Quantum theory of radiation," *Rev. Mod. Phys.* **4**, 87–132 (1932).

⁹R. Loudon, *The Quantum Theory of Light* (Oxford University Press, New York, 2000), p. 67.

Reply to "Comment on 'Hot gases: The transition from line spectra to thermal radiation,'" by M. Vollmer [*Am. J. Phys.* **73** (3), 215–223 (2005)]

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Nauenberg¹ has pointed out some problems with my article.² Although I agree with parts of his criticism, I cannot follow all of his arguments.

I agree that my approach of using a simple two-level system was oversimplified and that a proper application of Einstein's derivation is not possible if only a two-level system with well-defined energies is assumed. However, I do not agree with Nauenberg¹ that my explanation of how a line spectrum is transformed to the continuous spectrum of thermal radiation is invalidated.

My intent was to provide a simple radiation transfer model to explain how line spectra are transformed into continuous spectra of blackbody radiation. To follow the apparently simplest approach, I used a pure two-level system with the simplest line shape, a Lorentzian, usually related to the natural line width of the transition between two energy levels. I agree that this choice led to an oversimplification of the theory with an incorrect use of Einstein's argument of thermal equilibrium and detailed balance.

Although this oversimplification led to an error in my simple model, all my other arguments would hold if a correct system instead of a simple two-level system is chosen. For example, any extension to more than two energy levels will allow the use of Einstein's argument of detailed balance (detailed balance in a three-level system was discussed, for example, by Lewis³). Similarly, any mechanism that can lead to

thermal equilibrium such as collisions, leading to the Doppler width as mentioned by Nauenberg¹ will do.

The main thrust of my paper, how continuous blackbody radiation is formed from a line spectrum for a system of atoms in thermal equilibrium is beyond the specific use of a certain energy level system and is hence not invalidated as stated by Nauenberg.¹ The reasoning of my paper just needs a line shape factor for absorption and emission processes in the simple radiation transfer model [Ref. 2, Eq. (14)]. The argument then uses the concept of optical depth to explain how the line shape of the radiation changes as a function of optical thickness of the gas. It also illustrates a simple way of estimating emissivities of gases and explaining the broadening of spectral lines in gases due to self-absorption.

From the spectroscopy of gases, there are three well-known and prominent examples of line shapes, the Lorentz profile of the natural line width, the pure Gaussian profile (approximating the Doppler profile), and the Voigt profile, which could correctly describe the Doppler broadened profile. I chose the Lorentzian (and incorrectly related it to a two-level system) because it is a good approximation to the Voigt profile in the far wings. If we used a more complex system such as a three-level system in thermal equilibrium, a Lorentzian would still be a reasonable choice.

We should keep the following arguments in mind. For a very precise model, the Doppler shift must be included.

However, my intent was not to state that the Doppler shift can be neglected. Instead I argued that the Doppler width is not important (in the context of my simple model) because it is small compared to the width of a thermal spectrum. I agree that a Voigt profile should be used when being very precise. Nauenberg correctly states that his result with the Voigt profile differs from my result with the Lorentzian. However, I stated (Ref. 2, p. 216) that the line shape of a Voigt profile is close to a Gaussian near the center and close to a Lorentzian in the far wings, which are both reasonable approximations.

I want to mention some other ideas that resulted from some discussions with a colleague. When considering far wing phenomena of atoms with two energy levels, the relevant processes could be referred to as Rayleigh scattering (lower frequencies) and Thomson scattering (higher frequencies). Does the argument of detailed balance hold for such scattering processes?

In the simplest description, Rayleigh and Thomson (and also Raman) scattering can be thought of as being due to a three-level system process (see Ref. 3) with the transition

from the ground state to an intermediate virtual state and then the transition from the intermediate state to the final state. If the ground state and the final state refer to my assumed two-level system, the whole process, which would be due to a three-level process with a virtual level, would allow one to use detailed balance arguments and correctly extending the simple approach of my paper.²

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I thank M. Nauenberg for pointing out the problem and presenting a solution for the ideal case of two-level atoms, which cannot be properly treated by my simple model. In this respect his comment provides a very useful complement to my paper.

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¹M. Nauenberg, *Am. J. Phys.* **75**, 947–949 (2007).

²M. Vollmer, “Hot gases: The transition from line spectra to thermal radiation,” *Am. J. Phys.* **73**, 215–223 (2005).

³H. R. Lewis, “Einstein’s derivation of Planck’s radiation law,” *Am. J. Phys.* **41**, 38–44 (1973).

Dispersion of non-Gaussian free particle wave packets

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In discussions of free particle wave packets, authors of quantum mechanics textbooks choose the Gaussian form. Some authors do so without explanation.¹ Others state the reason for their choice is that this particular wave packet can be nicely analyzed in closed form.² Apart from mathematical convenience, why do we choose the Gaussian wave packet? Yes, the Fourier transform of the Gaussian wave function is also Gaussian. Also, the Gaussian wave packet gives rise to the minimum uncertainty product at time $t=0$. These features are pedagogically useful. But is there something more to the Gaussian wave packet?

In this note, we show that the probability density of any non-Gaussian wave packet becomes approximately Gaussian as it disperses.³ We graphically illustrate this process by considering the example of a rectangular wave packet.

We start with the standard treatment of time dependent wave functions using propagators (Green’s functions).⁴ In this approach, we write the wave function as

$$\psi(x,t) = \int_{-\infty}^{\infty} K(x,x';t,0)\psi(x',0) dx', \quad (1)$$

where the propagator $K(x,x';t,0)$ is given by

$$K(x,x';t,0) = \sum_n \psi_n^*(x')\psi_n(x)e^{-i\omega_n t}. \quad (2)$$

The sum is over the complete set of stationary states and $\omega_n = E_n/\hbar$.

It is difficult to obtain explicit expressions of $K(x,x';t,0)$ in general. For a free particle, a simple, well-known form of $K(x,x';t,0)$ is given by⁴

$$\begin{aligned} K(x,x';t,0) &= \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ik(x-x')} e^{-i\hbar k^2 t/2m} dk \\ &= \sqrt{\frac{m}{i2\pi\hbar t}} e^{im(x-x')^2/2\hbar t}. \end{aligned} \quad (3)$$

Let us consider a simple, albeit artificial example of the rectangular wave packet:

$$\psi(x,0) = \begin{cases} \frac{1}{\sqrt{a}} e^{ik_0 x}, & |x| < a/2, \\ 0, & |x| > a/2. \end{cases} \quad (4)$$

Our focus is the dispersion of a wave packet. For this reason, it does not matter whether the center of the wave packet is moving. We set $k_0=0$ so that the packet is at rest. If we substitute the right-hand side of Eq. (3) and Eq. (4) into Eq. (1), we obtain⁵

$$\begin{aligned} \psi(x,t) &= \frac{(-1)^{3/4}}{2\sqrt{ia}} \left\{ \operatorname{erfi} \left[(-1)^{1/4} \sqrt{\frac{m}{2\hbar t}} \left(x - \frac{a}{2} \right) \right] \right. \\ &\quad \left. - \operatorname{erfi} \left[(-1)^{1/4} \sqrt{\frac{m}{2\hbar t}} \left(x + \frac{a}{2} \right) \right] \right\}, \end{aligned} \quad (5)$$

where $\operatorname{erfi}(x)$ is the imaginary error function,⁶ and Eq. (5) is valid for $t > 0$.

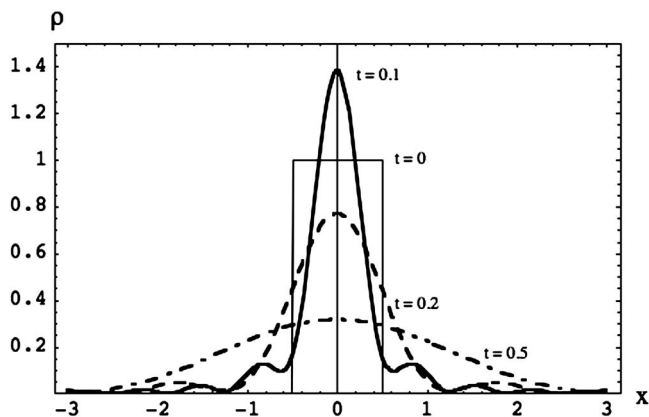


Fig. 1. Probability density of the rectangular wave packet at time $t=0$ (thin solid line), $t=0.1$ (thick solid line), $t=0.2$ (dashed line), and $t=0.5$ (dot-dashed line).

Figure 1 shows the probability density of the rectangular wave packet at time $t=0$ (thin solid line), $t=0.1$ (thick solid line), $t=0.2$ (dashed line), and $t=0.5$ (dot-dashed line). In these plots, the parameters are $a=1$, $m=1$, and $\hbar=1$.

Let us understand what is happening to the rectangular wave packet. The wave packet is composed of an infinite number of plane waves. At time $t=0$ these plane waves interfere to form a rectangular shape. As time elapses, the component plane waves travel, both to the right ($k>0$) and left ($k<0$), at different phase velocities $\hbar k/2m$. Thus the pattern of the interference of these plane waves gradually changes, resulting in the dispersion of the wave packet. At time $t=0.1$, we see that the rectangle begins to break up. At this time, the maximum height of the wave packet exceeds the height of the rectangle because the body of the packet is squeezed, but the total probability must remain equal to unity. At time $t=0.2$, we see two secondary maxima, one on the right and the other on the left of the central maximum. The central body of the wave packet is formed as a result of the interference of very slow moving plane waves with very small wave numbers k . By time $t=0.5$, all of the higher order maxima with very small maximum heights are out of sight, and we see the main body of the wave packet that appears Gaussian.

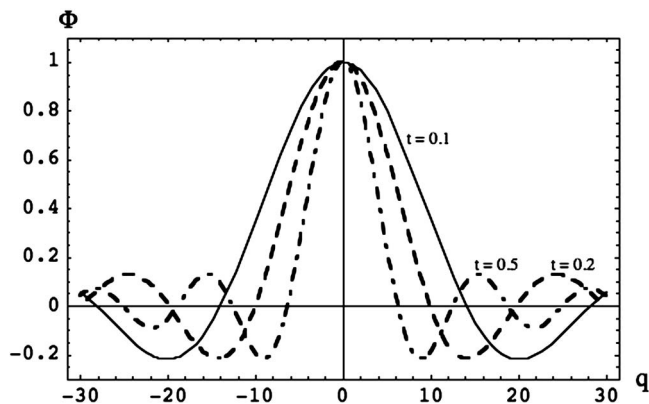
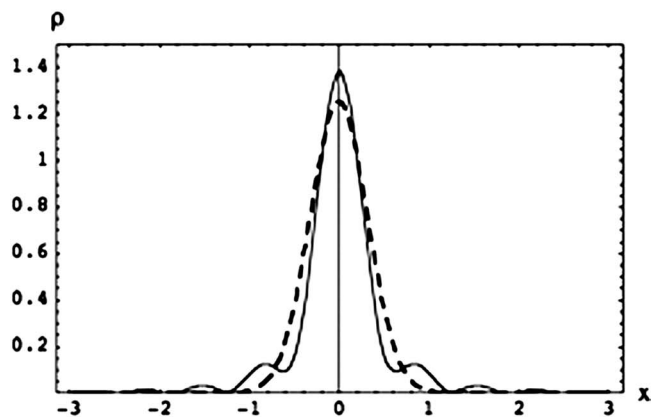
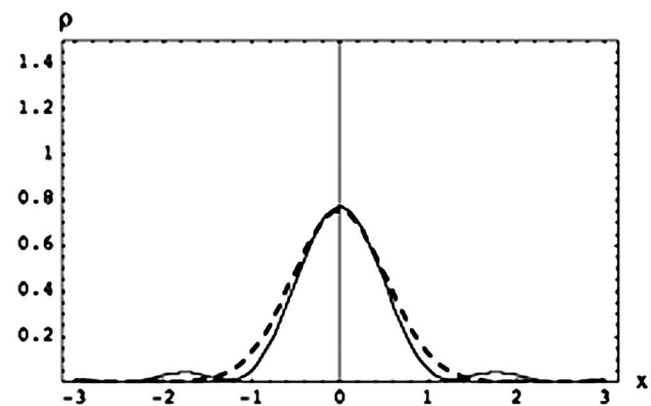


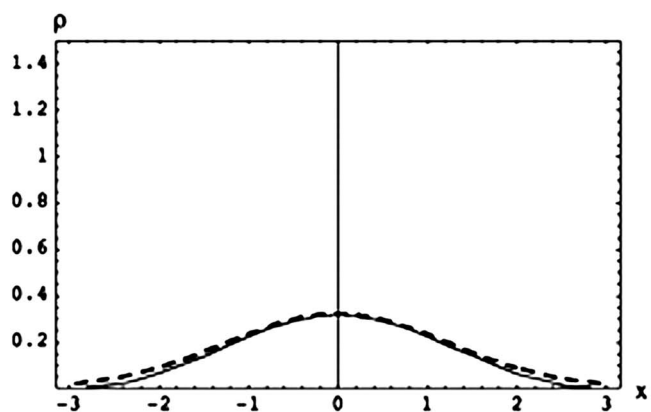
Fig. 2. Plot of Φ for the initial rectangular wave packet as a function of q at times $t=0.1$ (solid line), $t=0.2$ (dashed line), and $t=0.5$ (dot-dashed line).



(a) $t=0.1$



(b) $t=0.2$



(c) $t=0.5$

Fig. 3. Comparison between the exact probability density plots (solid lines) and the approximate plots (dashed lines) at time (a) $t=0.1$, (b) $t=0.2$, and (c) $t=0.5$. The initial wave packet is rectangular.

We now show the Gaussian approximation of a wave packet as the wave packet disperses. To examine the dispersion of a wave packet of initial shape $\psi(x,0)$, we substitute the right-hand side of Eq. (3) into Eq. (1) and change the order of the integration variables. Then $\psi(x,t)$ can be written as an integral over the wave numbers k :

$$\psi(x,t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \Phi(k) e^{ikx - i\hbar k^2 t/2m} dk, \quad (6)$$

where

$$\Phi(k) = \int_{-\infty}^{\infty} \psi(x',0) e^{-ikx'} dx'. \quad (7)$$

The wave packet in Eq. (6) is the sum of the component plane waves.

We next change the integration variable in Eq. (6) to illustrate the role that time plays in the process of dispersion. Let

$$q = \sqrt{\frac{m}{2\hbar t}} k. \quad (8)$$

Then Eqs. (6) and (7) become

$$\psi(x,t) = \frac{1}{2\pi} \sqrt{\frac{2\hbar t}{m}} \int_{-\infty}^{\infty} \Phi(q,t) \exp \left[i \sqrt{\frac{2\hbar t}{m}} qx - i \left(\frac{\hbar t}{m} \right)^2 q^2 \right] dq, \quad (9)$$

and

$$\Phi(q,t) = \int_{-\infty}^{\infty} \psi(x',0) \exp \left(-i \sqrt{\frac{2\hbar t}{m}} qx' \right) dx'. \quad (10)$$

For the rectangular wave packet of initial shape given in Eq. (4), $\Phi(q,t)$ is given by

$$\Phi(q,t) = \sqrt{a} \frac{\sin(\sqrt{\hbar t/2ma} q)}{\sqrt{\hbar t/2ma}}. \quad (11)$$

Figure 2 shows a plot of Φ as a function of q at times $t = 0.1$ (solid line), $t = 0.2$ (dashed line), and $t = 0.5$ (dot-dashed line). We see that the central part of Φ becomes squeezed as time elapses. This behavior suggests that the dominant contribution to the integral in Eq. (9) comes from small values of q . Thus, we may approximate the integral by small values of q , and the small q approximation improves as time elapses. This observation is consistent with our intuitive explanation of Fig. 1, in that small q means small k , which implies a small phase velocity. The main contribution to the Gaussian-like central body of the wave packet is the result of the interference of the slow moving component plane waves.

To perform the approximation in the integral of Eq. (9), we first rewrite $\Phi(q,t)$ as

$$\Phi(q,t) = e^{\ln[\Phi(q,t)]}, \quad (12)$$

and Taylor expand $\ln[\Phi(q,t)]$ to second order in q . (There is no need to approximate the other exponential factor in the integrand because it contains only terms in q and q^2 .)

$$\ln[\Phi(q,t)] \approx \ln[\Phi(0,t)] + \left[\frac{\partial}{\partial q} \ln(\Phi) \right]_{q=0} q + \frac{1}{2} \left[\frac{\partial^2}{\partial q^2} \ln(\Phi) \right]_{q=0} q^2. \quad (13)$$

We calculate the coefficient for each order of q and obtain

$$\ln[\Phi(q,t)] \approx \ln(\beta_0) - i \sqrt{\frac{2\hbar t}{m}} \gamma_1 q - \frac{\hbar t}{m} \gamma_2 q^2, \quad (14)$$

where

$$\gamma_1 = \frac{\beta_1}{\beta_0}, \quad \gamma_2 = \frac{\beta_2}{\beta_0} - \left(\frac{\beta_1}{\beta_0} \right)^2, \quad (15)$$

and

$$\beta_n = \int_{-\infty}^{\infty} x^n \psi(x,0) dx, \quad (16)$$

with $n=0,1,2$. By substituting Eqs. (12) and (14) into Eq. (9), and integrating over q , we obtain the normalized wave function

$$\psi(x,t) \approx \left(\frac{\gamma_2}{\pi} \right)^{1/4} \frac{1}{\sqrt{\gamma_2 + i\hbar t/m}} \exp \left[-\frac{(x - \gamma_1)^2}{2(\gamma_2 + i\hbar t/m)} \right]. \quad (17)$$

The probability density is given by

$$\rho(x,t) \approx \sqrt{\frac{\gamma_2}{\pi}} \frac{1}{\sqrt{\gamma_2^2 + (\hbar t/m)^2}} \exp \left[-\frac{\gamma_2(x - \gamma_1)^2}{\gamma_2^2 + (\hbar t/m)^2} \right]. \quad (18)$$

Thus, we see that the probability density becomes approximately Gaussian after the wave packet disperses.

For the initially rectangular wave packet, Fig. 3 shows the comparison between the exact probability density plots (solid lines), generated from Eq. (5), and the approximate ones (dashed lines), generated by Eq. (18) at time $t=0.1$, $t=0.2$, and $t=0.5$. We see that the small q approximation made improves as time elapses.

We showed that a free particle wave packet of any shape becomes approximately Gaussian after a period of time. The approximation we made in Eqs. (6)–(18) is similar to that employed in the proof of the central limit theorem.⁷ What we have shown in this note may be viewed as a quantum mechanical version of the central limit theorem.

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¹See, for example, A. Goswami, *Quantum Mechanics* (Brown, Dubuque, IA, 1997), p. 29.

²See, for example, R. W. Robinett, *Quantum Mechanics* (Oxford U. P., New York, 1997), p. 57.

³For previous articles on the dispersion of wave packets see, for example, H. M. Bradford, "Propagation and spreading of a pulse or wave packet," *Am. J. Phys.* **44**, 1058–1063 (1976); B. R. Holstein and A. R. Swift, "Spreading wave packets—a cautionary note," *Am. J. Phys.* **40**, 829–832 (1972); G. W. Ford and R. F. O'Connell, "Wave packet spreading: Temperature and squeezing effects with applications to quantum measurement and decoherence," *Am. J. Phys.* **70**, 319–324 (2002).

⁴For a good discussion of the propagator see, for example, E. Merzbacher, *Quantum Mechanics* (Wiley, New York, 1998), pp. 348–354.

⁵The computations were performed by Mathematica. The triangular wave packet can be treated similarly. The triangle quickly becomes Gaussian

without the multiple maxima. In this case, the exact expression of $\psi(x,t)$ is too lengthy to include in this note. Griffiths briefly discusses the example of the rectangular wave packet. See D. J. Griffiths, *Introduction to Quantum Mechanics* (Prentice Hall, Upper Saddle River, NJ, 2005), pp. 62–63.

⁶The imaginary error function is defined by $\operatorname{erfi}(z)=\operatorname{erf}(iz)/i$, where $\operatorname{erf}(z)$ is the error function.

⁷See, for example, F. Reif, *Fundamentals of Statistical and Thermal Physics* (McGraw-Hill, Boston, MA, 1965), pp. 37–40.

Comment on “Quantum mechanics of the $1/x^2$ potential,” by Andrew M. Essin and David J. Griffiths [Am. J. Phys. 74 (2), 109–117 (2006)]

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A recent paper¹ on the quantum mechanical properties of the attractive $-1/x^2$ potential explains in simple terms the unusual quantum properties we would expect from a system described by a singular potential. These properties include the need for considering the restrictions imposed by the Hamiltonian H and the renormalization that is required to obtain physically proper (or “true” as they are called in Ref. 1) solutions. Reference 1 also discusses the need to guarantee not only the Hermiticity but also the self-adjointness of H —an operator is self-adjoint if the action of H is the same as that of H^\dagger and both operators have the same domain, $\mathcal{D}_H=\mathcal{D}_{H^\dagger}$. That is, both H and H^\dagger need to be defined over exactly the same set of functions in Hilbert space.

We will show that the $-1/x^2$ potential can also be used to exhibit at least one more unusual feature of some singular quantum systems, namely, the existence of a superselection rule. To this end, we need to regard the problem as defined on the whole x -axis and not only on the positive real axis, $0\leq x<\infty$, as done in Ref. 1.

The conditions established in Ref. 1 restrict the set of functions, $\psi(x)$, for which H is physically appropriate to those vanishing at the origin $\psi(0)=0$ with a finite derivative at $x=0$ [we have simplified the condition stated in Eq. (73) of Ref. 1]. Because the boundary condition on the wave function, $\psi(0)=0$, is the same as the condition when there is an infinite potential at the origin, the physical consequences should be the same. That is, there must exist an effective separation of any physical effects occurring on the left from those on the right of the discontinuity. This feature has been called the *space-splitting effect* by some authors.^{2–4} Note that space-splitting also occurs when such potentials are studied on curved spaces, as has been recently proven for the potential $-1/|x|$ in Ref. 5. This effect also appears when the prob-

lem is analyzed using the deformed Heisenberg relation $[x,p]=i\hbar(1+\beta p^2)$ (β a real number) as shown in Ref. 6.

By using the detailed solution obtained in Ref. 1 and the symmetry under reflection which the set of eigenstates should satisfy, we can write the eigenfunctions as

$$\psi_-^h(x) = \begin{cases} F^h(-x), & \text{if } x \leq 0, \\ 0, & \text{if } x > 0, \end{cases} \quad (1a)$$

and

$$\psi_+^h(x) = \begin{cases} 0, & \text{if } x \leq 0, \\ F^h(x), & \text{if } x > 0, \end{cases} \quad (1b)$$

where $F^h(x)$ is any of the valid solutions, that is, those that can describe either bounded or scattering states as determined in Ref. 1. The superscript h (not necessarily an integer) serves to distinguish the different eigenstates. The form of the solutions given in Eqs. (1a) and (1b) indicates that the singularity acts as an impenetrable barrier, effectively splitting the configuration space available to the system into two independent regions. This feature can be checked by calculating the flux, $j \propto (\psi\psi'^* - \psi^*\psi')$,⁷ at the origin and noting that it always vanishes for the states in Eq. (1). According to the general analysis in Ref. 1, we can infer that even the scattering states comply with this peculiar space-splitting effect. Such an effect can be explained using the notion of superselection rules, another curious but important feature of quantum systems that establishes limitations on the general validity of the superposition principle.^{9,10}

To establish the setting for discussing the limitations on the superposition principle, let us consider the even and odd states of the problem. The reflection invariance of the $-1/x^2$

potential might lead us to expect the existence of such even and odd eigenstates. This conclusion is incorrect for this potential as we show in what follows.

From the eigenfunctions ψ_-^h and ψ_+^h , we can define even and odd functions

$$\psi_{\text{even}}(x) = \frac{1}{\sqrt{2}}(\psi_-^h(x) + \psi_+^h(x)), \quad (2a)$$

$$\psi_{\text{odd}}(x) = \frac{1}{\sqrt{2}}(\psi_-^h(x) - \psi_+^h(x)). \quad (2b)$$

The problem is that the functions in Eq. (2) cannot represent different eigenstates of the problem. If we accept Eqs. (2a) and (2b) as two distinct realizable states of the $-1/x^2$ potential, then those states should be completely independent of each other. However, it is easy to see that they are not independent solutions of the problem, because their Wronskian determinant vanishes,^{2,8}

$$W(\psi_-^h, \psi_+^{h'}) = \det \begin{bmatrix} \psi_-^h & \psi_+^{h'} \\ d\psi_-^h/dx & d\psi_+^{h'}/dx \end{bmatrix} = 0, \quad (3)$$

meaning that the functions ψ_-^h and $\psi_+^{h'}$ are not linearly independent. Hence, contrary to our assumption, they cannot describe independent states of the system. But, if we cannot distinguish between ψ_{even} and ψ_{odd} , it is clear that the relative phase of the components along the left and right eigenstates, ψ_-^h and $\psi_+^{h'}$, is fundamentally irrelevant. Therefore, if we extend the argument, any superposition of the form

$$a_-^h \psi_-^h + a_+^{h'} \psi_+^{h'}, \quad (4)$$

where a_-^h and $a_+^{h'}$ are complex numbers, is necessarily devoid of meaning as a coherent superposition.^{2,8,10} For the superposition (4) to make sense, either one of the coefficients must vanish or it has to be interpreted as a statistical mixed state (that is, as an incoherent superposition).^{7,11,12} We can see more clearly the dependence of the even and the odd states by calculating their probability densities and noting that they are identical:

$$|\psi_{\text{even}}|^2 = |\psi_{\text{odd}}|^2. \quad (5)$$

For a superselection rule to appear in a quantum system, there should exist an operator G that commutes with every other observable operator of the system and is *not* just a multiple of the identity. This property also implies that every physically realizable state of the system should be an eigenstate of G and, as a consequence, the superposition of some states is restricted. Moreover, any quantity not commuting with G cannot be an observable of the system.^{11,15} For the $-1/x^2$ problem, G is given by

$$G = \sum_h (|\psi_+^h\rangle\langle\psi_+^h| - |\psi_-^h\rangle\langle\psi_-^h|), \quad (6)$$

where we have used ket notation for the states (1); the sum may also mean integration if h is continuous. It is clear that $G|\psi_{\pm}^h\rangle = \pm|\psi_{\pm}^h\rangle$, and so we can interpret G as the operator that returns the side of the singularity on which the particle is moving. This property also exists in the classical case be-

cause a classical particle moving under a $-1/x^2$ potential will remain trapped forever on the same side where it started its motion.¹³

G commutes with all dynamical variables of the system, but does not commute with the parity operator \mathcal{P} , $[\mathcal{P}, G] \neq 0$, meaning that parity is not an observable property of the system and that parity eigenstates cannot exist in the system.^{9,10} Another way of stating this property is $\mathcal{P}|\psi_{\pm}^h\rangle = |\psi_{\mp}^h\rangle$; that is, the eigenstates $\psi_-^h(x)$ and $\psi_+^h(x)$ are “mirror images” of one another. That is, $\mathcal{P}|\psi_{\pm}^h\rangle$ describes particles located on the opposite side of the ones described by $|\psi_{\pm}^h\rangle$.

We have shown the existence of a superselection rule in the $-1/x^2$ potential using an argument similar to that used to forbid coherent superpositions of states describing photons (generally, bosons) with states describing electrons (generally, fermions). Such an argument is straightforward. Under rotations by 2π , $\mathcal{R}_{2\pi}$, photonic states remain unchanged, but electronic states are multiplied by a phase $e^{i\pi} = -1$.⁷ Thus, as long as the photonic and the electronic states are not mixed with one another, there are no consequences for the physics described by the state. If we are considering instead a superposition of the form

$$|M\rangle = a_p|\text{photon}\rangle + a_e|\text{electron}\rangle, \quad (7)$$

then a 2π rotation completely changes the physical content of the state, transforming it to

$$\mathcal{R}_{2\pi}|M\rangle = a_p|\text{photon}\rangle - a_e|\text{electron}\rangle. \quad (8)$$

Therefore, to maintain the consistency of quantum theory, we require that either $a_p = 0$ or $a_e = 0$. Thus, the coherent superposition $|M\rangle$ has to be forbidden. Any such state can only be interpreted as a statistical mixed state. This superselection rule is called *univalence*.^{11,12,14}

Superselection rules in nonrelativistic quantum theory explain the existence of properties such as the mass, electric charge, or the handedness of a molecular system, which do not require a quantum operator to be described. They also help to understand the existence of chiral molecules such as sugar or serine with a doubly degenerate ground state in which the component states differ from one another only in their handedness. Thus, superselection rules also explain the apparent paradox of optical isomers in molecular physics.^{11,12}

We believe that superselection rules should be explained in an intermediate course on quantum mechanics. In spite of the existence of pedagogical descriptions of superselection rules^{11,12} and of their importance, we know of only two textbooks that discuss the concept.^{15,16} In any case, we think the properties discussed in this comment would be an interesting addition to the discussion of Ref. 1 of the curious quantum features of the $1/x^2$ potential.

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