1.   A beam of neutrons of mass M_n ($M_n \simeq 167 \ 10^{-27}$ kg), of constant velocity and energy E, is incident on a linear chain of atomic nuclei, arranged in a regular fashion as shown in the figure (these nuclei could be, for example, those of a long linear molecule). We call l the distance between two consecutive nuclei, and d, their size ($d \ll l$). A neutron detector D is placed far away, in a direction which makes an angle of θ with the direction of the incident neutrons.
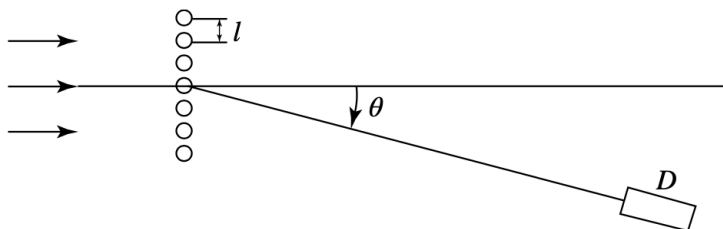
a) Describe qualitatively the phenomena observed at D when the energy E of the incident neutrons is varied.

b) The counting rate, as a function of E, presents a resonance about $E = E_1$. Knowing that there are no other resonances for $E < E_1$, show that one can determine l. Calculate l for $\theta = 30°$ and $E_1 = 13 \ 10^{-20}$ joule.

c) At about what value of E must we begin to take the finite size of the nuclei into account?

(a) To qualitatively understand the observation at D, we can assume that each nucleus in the atomic chain acts as a secondary source of waves, hence the linear atomic molecule acts as a diffraction grating, and the incident neutrons in terms of their wave-particle duality nature. Allow me to assume the atomic molecule (or the scattering center) has a diameter d, which will characterize its size as stated. In the approximation $d \ll \ell$, the Taylor expansion of the distance between nuclei then becomes

$$\ell - d = \ell \left(1 - \frac{d}{\ell} \right) \approx \ell. \tag{1.1}$$

Henceforth the neutrons will form a distribution of constructive and destructive fringes a distance L away from the linear molecule. The distance between constructive fringes shall remain constant because ℓ is not changing, and we can characterize this distance by a value Δy. It follows that

$$\tan \theta = \frac{\Delta y}{L} = \frac{\lambda}{\ell}. \tag{1.2}$$

By the de Broglie relation $E = h\nu = \dfrac{hc}{\lambda}$, where c is the speed of the neutrons (which is constant),

then $\lambda = \dfrac{hc}{E}$ which implies that, by substituting, $\dfrac{\Delta y}{L} = \dfrac{hc}{E\ell}$. This implies that

$$\Delta y \propto \frac{1}{E}. \tag{1.3}$$

Physically, this means that as the energy of the neutrons is increased, the spacing between the constructive fringes decreases, getting closer together. Similarly, as the energy of the neutrons decrease, the spacing of constructive fringes increases. Thus as the energy is varied, the detector D will measure a smooth pulse pattern of resonances and 'dead spots', similar to the amplitude of a sine wave.

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(b) Allow us to return to equation (1.2). With this relation we have that

$$\tan \theta = \frac{hc}{E\ell} \implies \ell = \frac{hc}{E \tan \theta}. \tag{1.4}$$

Since the neutrons are non-relativistic, we can make the classical assumption that $E = \dfrac{1}{2} M_n c^2$, or that

$$c = \sqrt{\frac{2E}{M_n}} \tag{1.5}$$

Taking (1.5) into (1.4) yields that

$$\ell = \frac{h}{E \tan \theta} \cdot \sqrt{\frac{2E}{M_n}} = \sqrt{\frac{2}{EM_n}} \frac{h}{\tan \theta}. \tag{1.6}$$

Taking our values $\theta = \dfrac{\pi}{6}, E = E_1 = 1.3 \times 10^{-20} \, J$, $M_n = 1.67 \times 10^{-27} \, kg$, and lastly $h = 6.63 \times 10^{-34} \, J \cdot s$, then we can calculate the slit width:

$$\ell = \sqrt{\frac{2}{(1.3 \times 10^{-20} \, J \cdot 1.67 \times 10^{-27} \, kg)}} \cdot \frac{6.63 \times 10^{-34} \, J \cdot s}{\tan(\pi/6)} = 3.48 \times 10^{-10} \, m.$$

Equivalently, $\boxed{\ell = 3.48 \text{Å}.}$

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(c) Allow me to return to the single-slit light diffraction experiment as an analogue to coherent neutron scattering. In short, the relationship between constructive or desctrive fringes and the angle relative to the symmetric axis is given by

$$\sin \theta = \frac{m\lambda}{d}, \qquad m \in \mathbb{Z}^+$$

where d is the width of the slit and θ is the angle relative to the normal axis. Note that when $\lambda \to d$, or even if $\lambda > d$, there does not exist an angle $\theta \in (-\pi/2, \pi/2)$ for which an interference fringe occurs on the screen. Equivalently for two slits, the relationship is similar. If the slits are too

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wide, not enough overlap between waves occurs to produce sufficient interference. In said analogue, thus the value of E for when we must take into account the finite size of the scattering centers is when $\lambda \simeq d$. That is,

$$\boxed{E = \frac{hc}{d}.}$$

5.   Well consisting of two delta functions

Consider a particle of mass m whose potential energy is

$$V(x) = -\alpha\,\delta(x) - \alpha\,\delta(x - l) \qquad \alpha > 0$$

where l is a constant length.

a) Calculate the bound states of the particle, setting $E = -\dfrac{\hbar^2\rho^2}{2m}$. Show that the possible energies are given by the relation

$$e^{-\rho l} = \pm\left(1 - \frac{2\rho}{\mu}\right)$$

where μ is defined by $\mu = \dfrac{2m\alpha}{\hbar^2}$. Give a graphic solution of this equation.

(i) *Ground state.* Show that this state is even (invariant with respect to reflection about the point $x = l/2$), and that its energy E_S is less than the energy $-E_L$ introduced in problem 3. Interpret this result physically. Represent graphically the corresponding wave function.

(ii) *Excited state.* Show that, when l is greater than a value to be specified, there exists an odd excited state, of energy E_A greater than $-E_L$. Find the corresponding wave function.

(iii) Explain how the preceding calculations enable us to construct a model which represents an ionized diatomic molecule (H_2^+, for example) whose nuclei are separated by a distance l. How do the energies of the two levels vary with respect to l? What happens at the limit where $l \longrightarrow 0$ and at the limit where $l \longrightarrow \infty$? If the repulsion of the two nuclei is taken into account, what is the total energy of the system? Show that the curve that gives the variation with respect to l of the energies thus obtained enables us to predict in certain cases the existence of bound states of H_2^+, and to determine the value of l at equilibrium. The calculation provides a very elementary model of the chemical bond.

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The time-independent schrodinger equation initially gives that

$$E\varphi(x) = -\frac{\hbar^2\rho^2}{2m}\varphi(x) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\varphi(x) - \alpha[\delta(x) - \delta(x - l)]\varphi(x). \tag{2.1}$$

The potential characterizes three regions:

$$x < 0, \qquad 0 < x < l, \text{ and } x > l.$$

We shall solve (2.1) in each the three cases. Allow for each to guess the solution $\varphi(x) = Ae^{kx}$. Then, by substituting into (2.1),

$$-\frac{\hbar^2 \rho^2}{2m} \cdot Ae^{kx} = -\frac{\hbar^2}{2m} Ak^2 e^{kx} \implies k = \pm\rho,$$

and we do not need to specify a complex exponential since $E < 0$. Thus $\varphi(x) = Ae^{\rho x} + A'e^{-\rho x}$ in each general region. Due to the struture of the delta function potential, however, our function $\varphi(x)$ will be discontinuous of the first order derivative at $x = 0$ and $x = l$, so our wavefunction will have a point of symmetry or antisymmetry around $x = l/2$. Therefore

$$\varphi(x) = \begin{cases} A_1 e^{\rho x} + A_1' e^{-\rho x} & (x < 0) \\ A_2 e^{\rho x} + A_2' e^{-\rho x} + A_2'' e^{\rho(x-l)} + A_2''' e^{-\rho(x-l)} & (0 < x < l) \\ A_3 e^{\rho(x-l)} + A_3' e^{-\rho(x-l)} & (x > l) \end{cases} . \quad (2.2)$$

Since $\varphi(x)$ must not diverge to $\pm\infty$ and remain bounded in these regions to account for energy conservation, we require that $A_1' = A_2 = A_2''' = A_3 = 0$. (2.2) then becomes

$$\varphi(x) = \begin{cases} A_1 e^{\rho x} & (x < 0) \\ A_2' e^{-\rho x} + A_2'' e^{\rho(x-l)} & (0 < x < l) \\ A_3' e^{-\rho(x-l)} & (x > l) \end{cases} . \quad (2.3)$$

The discontinuity of φ at the locations of the delta function potential regions are given by integrating the eigenvalue equation (2.1) over a region centered around the location of the delta function. Consider $-\alpha\delta(x)$, taken across the open interval $(-\varepsilon, \varepsilon)$ as $\varepsilon \to 0$. Then:

$$E \int_{-\varepsilon}^{\varepsilon} dx\, \varphi(x) = -\frac{\hbar^2}{2m} \int_{-\varepsilon}^{\varepsilon} dx\, \frac{\partial^2 \varphi(x)}{\partial x^2} - \alpha \int_{-\varepsilon}^{\varepsilon} dx\, \delta(x)\varphi(x)$$

$$\varepsilon \to 0:$$

$$0 = -\frac{\hbar^2}{2m} \left[\left.\frac{\partial \varphi}{\partial x}\right|_{\varepsilon} - \left.\frac{\partial \varphi}{\partial x}\right|_{-\varepsilon} \right] - \alpha\varphi(0)$$

$$\implies \left.\frac{\partial \varphi}{\partial x}\right|_{\varepsilon} - \left.\frac{\partial \varphi}{\partial x}\right|_{-\varepsilon} = -\frac{2m\alpha}{\hbar^2}\varphi(0). \quad (2.4)$$

By symmetry, a similar calculation can be made at $x = l$:

$$\left.\frac{\partial \varphi}{\partial x}\right|_{l+\varepsilon} - \left.\frac{\partial \varphi}{\partial x}\right|_{l-\varepsilon} = -\frac{2m\alpha}{\hbar^2}\varphi(l). \quad (2.5)$$

And thus the wavefunction's first derivative is discontinuous at $x = 0$ and $x = l$ of magnitude $-\frac{2m\alpha}{\hbar^2}\varphi(0)$ and $-\frac{2m\alpha}{\hbar^2}\varphi(l)$, respectively. The values of the coefficients are determined by the boundary conditions imposed on the wavefunction at $x = 0$ and $x = l$. We require the wavefunction to be continuous both at $x = 0, l$, and thus

$$A_1 = A_2' + A_2'' e^{-\rho l}, \qquad \text{and} \quad (2.6)$$

$$A_3' = A_2' e^{-\rho l} + A_2''. \quad (2.7)$$

Similarly, continuity relations (2.4) and (2.5) yield boundary conditions:

$$-A_2' + A_2'' e^{-\rho l} - A_1 = -\frac{2m\alpha}{\rho\hbar^2} A_1 \qquad \text{and} \quad (2.8)$$

$$-A_3' - A_2'e^{-\rho l} - A_2'' = -\frac{2m\alpha}{\rho\hbar^2}A_3'. \tag{2.9}$$

Determining the ratios of these coefficients yield an implicit relationship between energies. Allow us to manipulate:

$$(2.8) \longrightarrow \qquad -A_2' + A_2''e^{-\rho l} = A_1\left[1 - \frac{2m\alpha}{\rho\hbar^2}\right] \xrightarrow{(2.6)} = A_2' + A_2''e^{-\rho l}\left[1 - \frac{2m\alpha}{\rho\hbar^2}\right] \tag{2.10}$$

$$(2.9) \longrightarrow \qquad A_2'e^{-\rho l} - A_2'' = A_3'\left[1 - \frac{2m\alpha}{\rho\hbar^2}\right] \xrightarrow{(2.7)} = A_2'e^{-\rho l} + A_2''\left[1 - \frac{2m\alpha}{\rho\hbar^2}\right]. \tag{2.11}$$

Let us solve for $\dfrac{A_2''}{A_2'}$:

$$(2.10) \longrightarrow \qquad A_2'\left[-1 + \frac{A_2''}{A_2'}e^{-\rho l}\right] = A_2'\left[1 + \frac{A_2''}{A_2'}e^{-\rho l}\right]\left[1 - \frac{2m\alpha}{\rho\hbar^2}\right]$$

$$\implies \qquad -1 + \frac{A_2''}{A_2'}e^{-\rho l} = \left(1 - \frac{2m\alpha}{\rho\hbar^2}\right) + \frac{A_2''}{A_2'}e^{-\rho l}\left(1 - \frac{2m\alpha}{\rho\hbar^2}\right)$$

$$\implies \qquad \frac{A_2''}{A_2'}e^{-\rho l} - \frac{A_2''}{A_2'}e^{-\rho l}\left(1 - \frac{2m\alpha}{\rho\hbar^2}\right) = 2 - \frac{2m\alpha}{\rho\hbar^2}$$

$$\implies \qquad \frac{A_2''}{A_2'}e^{-\rho l}\left(\frac{2m\alpha}{\rho\hbar^2}\right) = 2\left(1 - \frac{m\alpha}{\rho\hbar^2}\right)$$

$$\implies \qquad \frac{A_2''}{A_2'} = \frac{1 - \frac{m\alpha}{\rho\hbar^2}}{e^{-\rho l}\cdot\frac{m\alpha}{\rho\hbar^2}} = \frac{\rho\hbar^2 e^{\rho l}}{m\alpha} - e^{\rho l}$$

$$= e^{\rho l}\left(\frac{\rho\hbar^2}{m\alpha} - 1\right) \tag{2.12}$$

By a similar calculation:

$$(2.11) \longrightarrow \qquad A_2'\left[e^{-\rho l} - \frac{A_2''}{A_2'}\right] = A_2'\left[e^{-\rho l} + \frac{A_2''}{A_2'}\right]\left[1 - \frac{2m\alpha}{\rho\hbar^2}\right]$$

$$\implies \qquad e^{-\rho l} - \frac{A_2''}{A_2'} = e^{-\rho l}\left(1 - \frac{m\alpha}{\rho\hbar^2}\right) + \frac{A_2''}{A_2'}\left(1 - \frac{m\alpha}{\rho\hbar^2}\right)$$

$$\implies \qquad e^{-\rho l} - e^{-\rho l}\left(1 - \frac{2m\alpha}{\rho\hbar^2}\right) = \frac{A_2''}{A_2'} + \frac{A_2''}{A_2'}\left(1 - \frac{m\alpha}{\rho\hbar^2}\right)$$

$$\implies \qquad e^{-\rho l}\left(1 - 1 + \frac{2m\alpha}{\rho\hbar^2}\right) = 2\frac{A_2''}{A_2'}\left(1 - \frac{m\alpha}{\rho\hbar^2}\right)$$

$$\implies \qquad \frac{A_2''}{A_2'} = e^{-\rho l}\cdot\frac{m\alpha}{\rho\hbar^2}\cdot\frac{1}{1 - \frac{m\alpha}{\rho\hbar^2}}. \tag{2.13}$$

Equation (2.12) with (2.13) yields

$$e^{\rho l}\left(\frac{\rho\hbar^2}{m\alpha} - 1\right) = e^{-\rho l}\cdot\frac{\frac{m\alpha}{\rho\hbar^2}}{1 - \frac{m\alpha}{\rho\hbar^2}}.$$

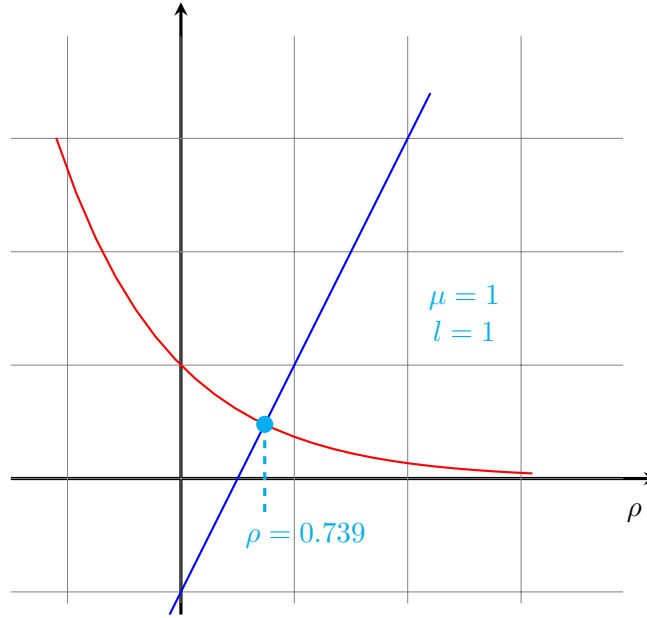Then:

$$e^{-2\rho l} = \frac{\left(\frac{\rho\hbar^2}{m\alpha} - 1\right)\left(1 - \frac{m\alpha}{\rho\hbar^2}\right)}{\frac{m\alpha}{\rho\hbar^2}}$$

$$= \frac{\frac{\rho\hbar^2}{m\alpha} - 1 - 1 + \frac{m\alpha}{\rho\hbar^2}}{\frac{m\alpha}{\rho\hbar^2}}$$

$$= \frac{\rho^2\hbar^2}{m^2\alpha^2} - 2\frac{\rho\hbar^2}{m\alpha} + 1$$

$$= \left(1 - \frac{\rho\hbar^2}{m\alpha}\right)^2. \tag{2.14}$$

The result of (2.14) directly yields the relation $\boxed{e^{-\rho l} = \pm\left(1 - \frac{2\rho}{\mu}\right),}$ with $\mu = \frac{2m\alpha}{\hbar^2}$, as desired.

It is important to note that this relation is known as a transcendental equation and cannot be algebraically manipulated to solve for ρ; it must be solved graphically for specified values of μ and l. [i] Allow us first to consider the ground state (energy) of the wavefunction, given by the solution of $e^{-\rho l} = \frac{2\rho}{\mu} - 1$.

$$\mu = 1$$
$$l = 1$$

$$\rho = 0.739$$

Now, since every physically possible value of ρ lies somewhere on the line $e^{-\rho l} > 0$, then it must be that the value $\frac{2\rho}{\mu} - 1 > 0$. Rearranging gives the inequality that $\rho > \frac{\mu}{2}$, and thus we have

$$\rho > \frac{\mu}{2} \implies -\rho^2 < -\frac{1}{4}\cdot\left(\frac{2m\alpha}{\hbar^2}\right)^2$$

$$\implies -\rho^2 < \frac{m^2\alpha^2}{\hbar^4}$$

$$\implies -\frac{\hbar^2}{2m}\rho^2 < -\frac{m\alpha^2}{\hbar^2} < -\frac{m\alpha^2}{2\hbar^2}$$

$$\implies -E_S < -E_L, \tag{2.15}$$

as specified in the previous question $\left(-E_L = -\frac{m\alpha^2}{2\hbar^2}\right)$. Therefore the ground state energy of the wavefunction located in a double delta function potential well is less than that of the single delta

potential well. Now to show that this state is given as an even wavefunction about the point $x = l/2$. As given by equation (2.12), we have that:

$$\frac{A_2''}{A_2'} = e^{\rho l}\left(\frac{\rho \hbar^2}{m\alpha} - 1\right) = \frac{1}{\frac{2\rho}{\mu} - 1} \cdot \left(\frac{\rho \hbar^2}{m\alpha} - 1\right)$$

$$= \frac{1}{\frac{2\rho}{\mu} - 1} \cdot \left(\frac{2\rho}{\mu} - 1\right)$$

$$= 1 \implies A_2' = A_2'' \tag{2.16}$$

and similarly for the relation $\dfrac{A_3'}{A_1}$, equations (2.6) and (2.7) give

$$\frac{A_3'}{A_1} = \frac{A_2' + A_2'' e^{-\rho l}}{A_2' e^{-\rho l} + A_2''} = \frac{A_2'(1 + e^{-\rho l})}{A_2'(1 + e^{-\rho l})} = 1,$$

and therefore the ratios of coefficients of the wavefunction are positive and unitary, hence the wavefunction is even about $x = l/2$. The wavefunction looks like:
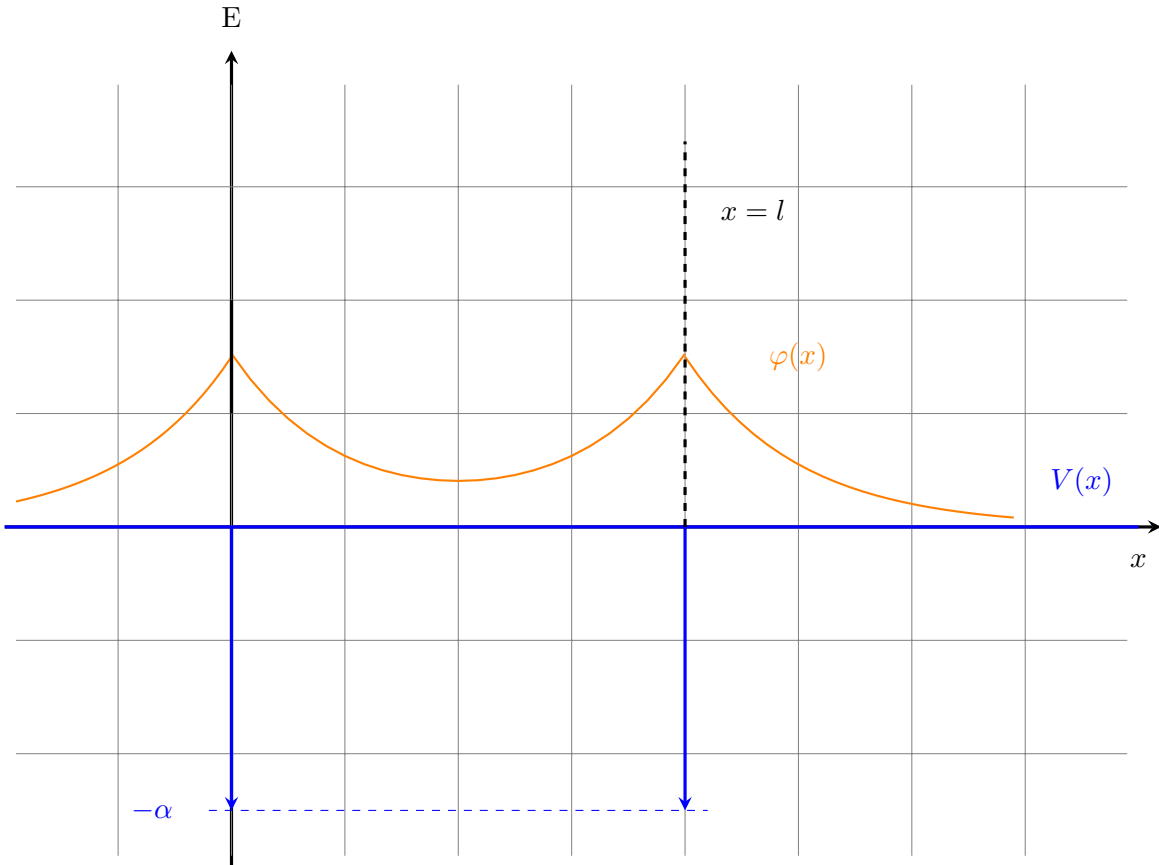
$[ii]$ On the other hand, the excited state of the wavefunction is characterized by the solution of the relation $e^{-\rho l} = 1 - \dfrac{2\rho}{\mu}$:
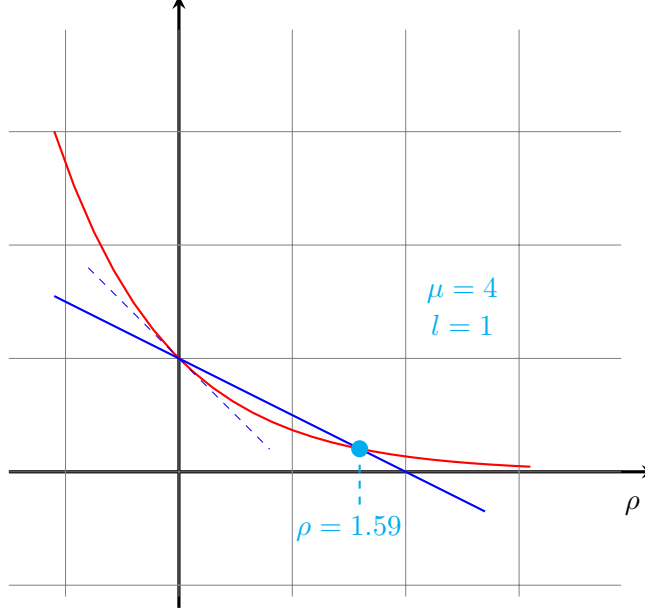
From this plot, we can see that there exists an excited state only when the slope of $e^{-\rho l}$ at $x = 0$ is equal to that of $\dfrac{2}{\mu}$. That is, there exists an excited state only when $l > \dfrac{2}{\mu}$ (see the blue dashed line in the figure above). Employing the same argument as the previous case, we know that the whole function $e^{-\rho l} > 0$ on its domain, and thus the value $1 - \dfrac{2\rho}{\mu} > 0$. Rearranging yields the inequality $\rho < \dfrac{\mu}{2}$. The similar calculation to yield equation (2.15) now gives

$$\rho < \frac{\mu}{2} \implies -\rho^2 > -\frac{m^2\alpha^2}{\hbar^4} \implies -\frac{\hbar^2\rho^2}{2m} > -\frac{m\alpha^2}{2\hbar^2} \implies \left| -\frac{\hbar^2\rho^2}{2m} \right| > -\frac{m\alpha^2}{2\hbar^2} \implies E_A > -E_L.$$

(2.17)

Thus the energy of the excited state is greater than that of the ground state energy of the single delta function potential well. It then follows to show that the wave function is odd about $x = l/2$, that the ratio of the coefficients are negative and unitary. We find:

$$\frac{A_2''}{A_2'} = e^{\rho l}\left(\frac{\rho\hbar^2}{m\alpha} - 1 \right) = \frac{1}{1 - \frac{2\rho}{\mu}} \cdot \left(\frac{\rho\hbar^2}{m\alpha} - 1 \right)$$

$$= -\frac{1}{\frac{2\rho}{\mu} - 1} \cdot \left(\frac{2\rho}{\mu} - 1 \right)$$

$$= -1 \implies A_2' = -A_2'' \qquad (2.18)$$

and simiarly for the relation $\dfrac{A_3'}{A_1}$, equations (2.6) and (2.7) yield

$$\frac{A_3'}{A_1} = \frac{A_2' + A_2''e^{-\rho l}}{A_2'e^{-\rho l} + A_2''} = -\frac{A_2'(1 - e^{-\rho l})}{A_2'(1 - e^{-\rho l})} = -1,$$

and therefore the wavefunction is odd about $x = l/2$. The corresponding wavefunction appears as:

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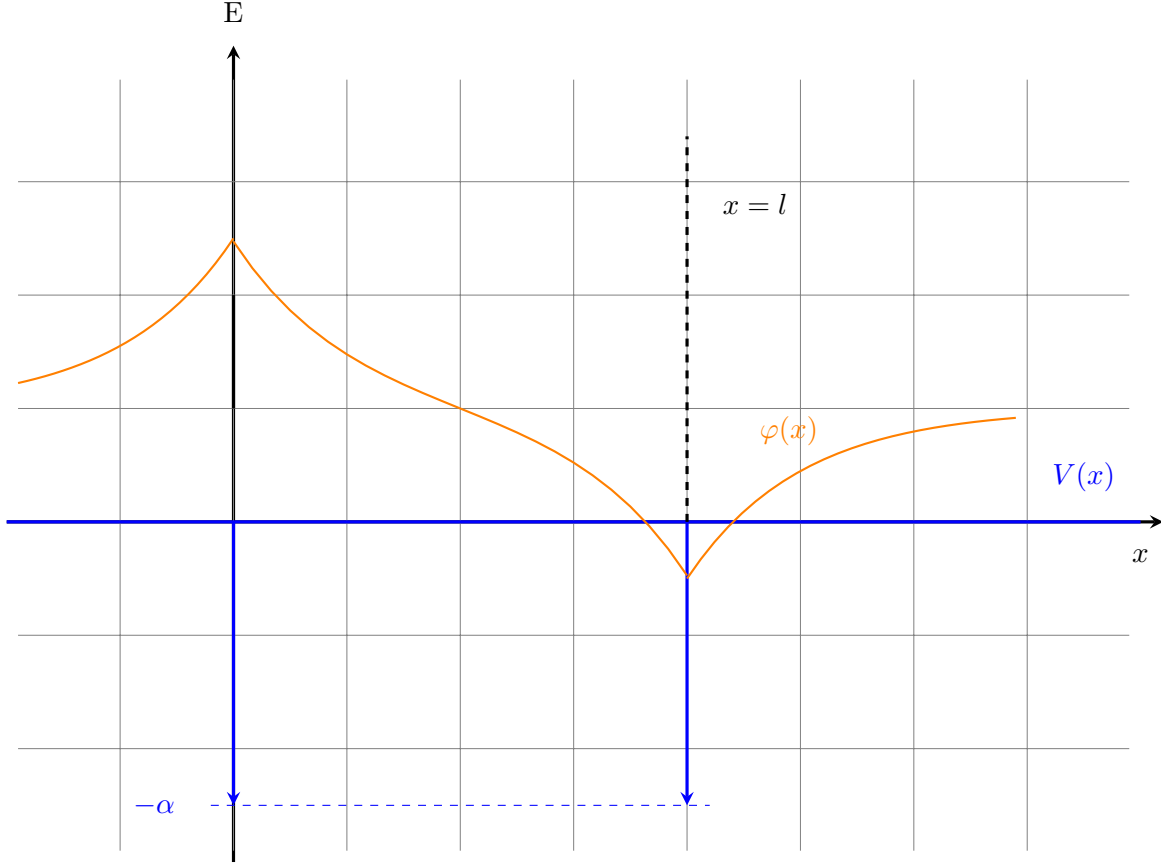
Here I shifted the wavefunction up the energy scale to indicate the energy $E_A > E_S$ of the first excited state being greater than that of the ground state.

[iii] The calculations above allow us to depict a model of an ionized atomic molecule, such as H_2^+. If said nuclei are separated by a distance l, we can represent their atomic potentials as delta functions, and the electron(s) as corresponding wave functions. Physically, a diatomic molecule invokes a stronger bond on electrons than a regular atom of the same type would, hence it would require a greater energy to ionize a diatomic molecule (once and twice) than that of a single atom of same type. The correlating model is shown in the previous calculations, since a first ionization energy (exicted state, only for a specific value of l) requires less energy than that of E_L, and second ionization (ionization of an electron in the ground state) requires more energy than E_L.

The model tells us that there will always exist a ground state for any value of l, however only when $l > \dfrac{2}{\mu}$ there exists an excited state. As l decreases, the intersecting value of ρ will increase for the ground state, and decrease for the excited state until that value dips beneath $\dfrac{2}{\mu}$. Likewise, as l increases, the intersecting value of ρ for the ground state decreases, and increases for the excited state. A smaller ρ corresponds to a smaller value of E, while a large value of ρ to a large value of E. Therefore as l decreases, E_S increases and E_A decreases, and vice versa when l increases.

Let us examine the limiting cases. In the limit when $\ell \to 0$, then $e^{-\rho l} \to 1$ so the energy relation becomes

$$l \to 0 \implies 1 = \pm\left(1 - \frac{2\rho}{\mu}\right). \tag{2.19}$$

In the '+' case, we find $\rho = 0$ which is trival. On the other hand, the '−' case yields that $\rho = \mu$.

This implies that only a ground state energy exists, and no excited state exists. We find that

$$\rho = \mu = \frac{2m\alpha}{\hbar^2} \implies -E_{l\to 0} = -\frac{\hbar^2}{2m} \cdot \frac{4m^2\alpha^2}{\hbar^4} = -\frac{2m\alpha^2}{\hbar^2} = -4E_L,$$

that is, four times the ground state energy of a single delta function potential at $x = 0$. Now as $l \to \infty$, then $e^{-\rho l} \to 0$ so the energy relation becomes

$$l \to \infty \implies 0 = \pm \left(1 - \frac{2\rho}{\mu}\right). \tag{2.20}$$

We can see here regardless the $\pm$, we find that $\rho = \frac{\mu}{2}$, hence there is only one bound state of the wavefunction. The value of the energy of this state is

$$\rho = \frac{\mu}{2} = \frac{m\alpha}{\hbar^2} \implies -E_{l\to\infty} = -\frac{\hbar^2}{2m} \cdot \frac{m^2\alpha^2}{\hbar^4} = -\frac{m\alpha^2}{2\hbar^2} = -E_L,$$

which is equivalently that of the only bound state of the single delta function potential well. Physically, this means that the infinite separation of two nuclei can be regarded as a single nucleus.

Allow us to now consider the total energy of such a molecule. The energy would be expressed as the sum of the energy of the repulsion of the nuclei, as well as the ground and excited state energies of the electrons around the nuclei. Given by a Coulomb potential energy, the total repulsion of the nuclei is then

$$V(l) = \frac{1}{4\pi\varepsilon_0} \frac{q^2}{l} \tag{2.21}$$

where l is their separation and q are the charges of the nuclei ($q = e$ for H_2^+), as taken in the model of their delta function potentials. The two energies of the ground state and excited state, respectively, are given by (2.15) and (2.17):

$$-E_S = -\frac{\hbar^2\rho_1^2}{2m} < E_L, \qquad E_A = -\frac{\hbar^2\rho_2^2}{2m} > -E_L,$$

where ρ_1 and ρ_2 are the solutions to the energy relation for the ground and exicted states, respectively. Then

$$E_{TOT} = V + E_{S/A} = \frac{1}{4\pi\varepsilon_0} \frac{q^2}{l} - \frac{\hbar^2\rho^2}{2m}. \tag{2.22}$$

Once again, in the case of the ionized diatomic molecule H_2^+, where one electron is present, then

$$E_{H_2^+} = \frac{1}{4\pi\varepsilon_0} \frac{e^2}{l} - \frac{\hbar^2\rho^2}{2m_e}, \tag{2.23}$$

where l and ρ should be specified and e^- can alter between the ground state and excited state. As stated before, the energy relation allows us to determine the existence of bound states (mainly, the existence of exicted states, because a ground state will always exist) for various values of l. I noted that an excited state exists only when $l > \frac{2}{\mu}$, which is the slope of the line $1 - \frac{2\rho}{\mu}$ at $\rho = 0$. The value of l at equilibrium may also be determined, since this corresponds to the value of l which minimizes the energy in (2.23). Physically, since the molecule requires more energy to house the electron in the excited state, then the only minimum value of E can occur when the electron is located in the ground state, so $\frac{\mu}{2} < \rho\mu$ according to (2.15). The energy relation yields that

$$l = -\frac{\log\left(\frac{2\rho}{\mu} - 1\right)}{\rho} \tag{2.24}$$

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in the ground state. Then (2.23) becomes

$$E(\rho) = \frac{e^2}{4\pi\varepsilon_0}\left[-\frac{\log\left(\frac{2\rho}{u}-1\right)}{\rho}\right]^{-1} - \frac{\hbar^2\rho^2}{2m_e}$$

with the corresponding value of l to ρ given by (2.24). This function can be plotted, and appears similar to
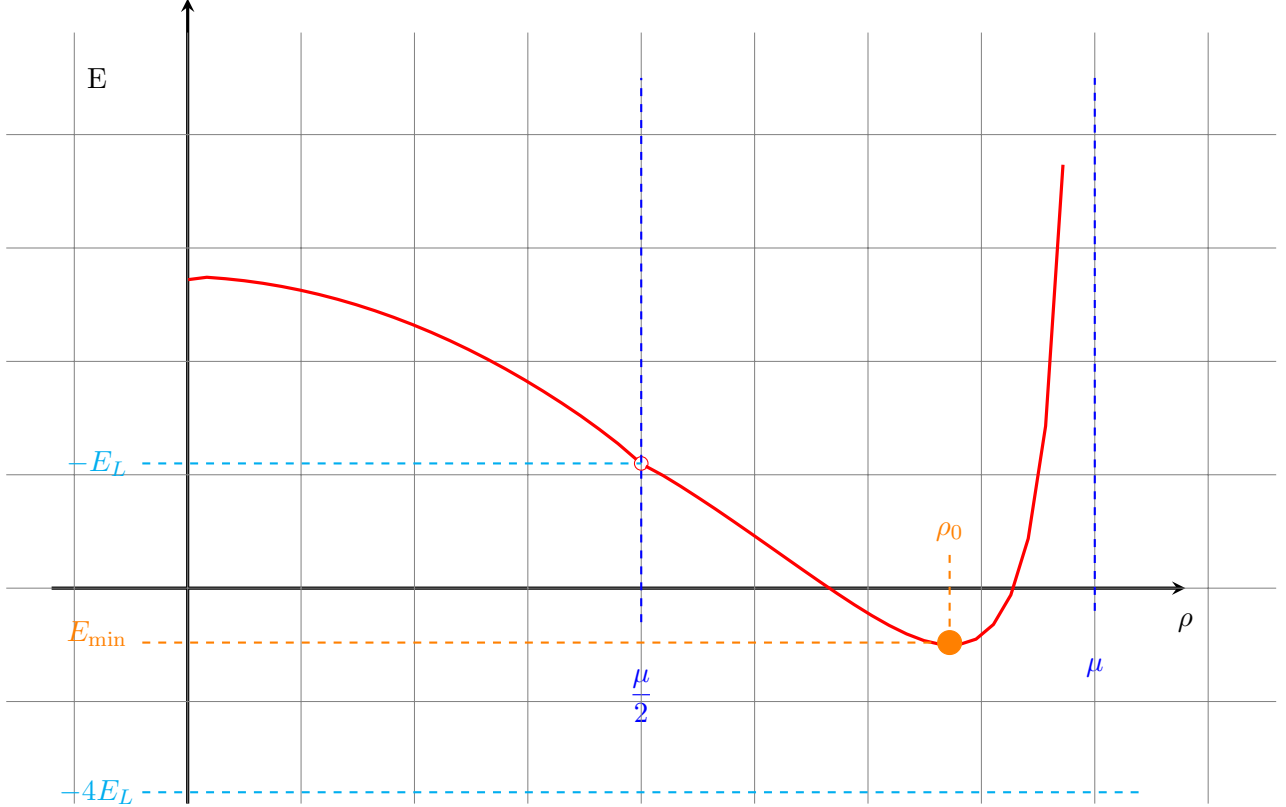
where the energy function is discontinuous at $\rho = \frac{mu}{2}$ and $\rho = \mu$. It should be regarded that $-4E_L < E_{\min} < -E_L$, as shown by the limiting cases. Now as $\ell \to 0$, there is an asymptote to $E \to \infty$ as $\rho \to \mu$, because physically we require an infinite amount of energy to 'push' the two nuclei together because they repel. However, the bound state energy still converges to $-4E_L$ as shown earlier.

Now suppose that $E(\rho = \rho_0)$ is the minimum energy for some specified value of μ. The corresponding value of l is

$$l = -\frac{\log\left(\frac{2\rho_0}{\mu}-1\right)}{\rho_0},$$

which would correspond to the value of l at equilibrium, or the value of l which requires the least amount of energy to bind the molecule. As μ varies (since $\mu \propto \alpha$), there will always exist an equilibrium value of l unless $\alpha \ll \hbar^2$, which can be shown graphically.