Assigned: 1/15. Due: 1/22/93.

(1) In a QM system with Hamiltonian $\mathcal{H}$, let the eigenfcns & eigenenergies be ψ_n & E_n, so: $\mathcal{H}\psi_n = E_n\psi_n$. To approximate the ground state energy E_0, suppose you use a trial fcn: $\underline{\psi = \psi_0 + \lambda\phi}$, w/ ψ_0 = actual ground state eigenfcn, λ = small (real) parameter, and ϕ = an arbitrary fcn with the expansion: $\phi = \sum_n c_n\psi_n$. Show that if the approximate (variational) energy $E(\lambda) = \langle\psi|\mathcal{H}|\psi\rangle / \langle\psi|\psi\rangle$ is expanded in a power series in λ, viz.: $\underline{E(\lambda) = E_0 + \lambda\mathcal{E}_1 + \lambda^2\mathcal{E}_2 + \lambda^3\mathcal{E}_3 + \cdots}$, then $\mathcal{E}_1 = 0$, while $\mathcal{E}_2$ is the positive quantity: $\boxed{\mathcal{E}_2 = \sum_n |c_n|^2 (E_n - E_0)}$. NOTE: this result $\Rightarrow$ that any perturbation on $\mathcal{H}$ which shifts $\psi_0 \to \psi_0 + \lambda\phi$ by a term $\underline{1^{st}}$ order in some small parameter λ, can only shift the ground state energy $E_0 \to E_0 + \lambda^2\mathcal{E}_2$ by a term $\underline{2^{nd}}$ order in λ.

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(2) On p. 2 of "Notes on the WKB Method", it is claimed that any 2^{nd} order homogeneous ODE of the form: $\underline{y'' + f(x)y' + g(x)y = 0}$, can be cast into the WKB form: $\underline{\psi'' + k^2(x)\psi = 0}$, if $\underline{\psi(x)} = y(x)\exp\left[+\frac{1}{2}\int_a^x f(\xi)\,d\xi\right]$, and $\underline{k(x)} = \pm\left\{g(x) - \frac{1}{2}\left[f'(x) + \frac{1}{2}f^2(x)\right]\right\}^{1/2}$. Verify this claim by substituting $y(x) = \psi(x)u(x)$ into the original ODE and then choosing $u(x)$ judiciously. Why is the lower limit a in the integral $\int_a^x f(\xi)\,d\xi$ essentially arbitrary?

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(3) Bessel's ODE is: $\underline{y'' + \frac{1}{x}y' + \left(1 - \frac{\nu^2}{x^2}\right)y = 0}$, w/ ν = real cnst. Find an $\underline{\text{approximate}}$ solution for the Bessel fcn $y = J_\nu(x)$ by the WKB method. Then find an asymptotic form for $J_\nu(x)$ as $x \to$ "large" (i.e. $x \gg |\nu|$). You may assume $|\nu| \gg 1/2$.

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(4) This exercise is connected with the WKB "turning point" problem. (A) Show -- by substitution -- that a solution to: $\underline{y''(\xi) + \alpha\xi^n y(\xi) = 0}$, w/ α & n = cnsts and $\xi \geq 0$, is given by: $\underline{y(\xi) = A\sqrt{\xi}\,J_\nu(\zeta)}$, w/ A = cnst, $\nu = 1/(n+2)$, $\zeta = \left(\frac{2\sqrt{\alpha}}{n+2}\right)\xi^{\frac{1}{2}(n+2)}$, and $J_\nu(\zeta)$ is the Bessel fcn of order ν. (B) Assume an asymptotic form: $y(\xi) \sim \xi^{-k}e^{-a\xi^l}$, as $\xi \to \infty$. By properly choosing the cnsts k, l & a, show that as $\xi \to \infty$ this form satisfies the ODE: $y''(\xi) + \alpha\xi^n y(\xi) = \frac{n}{4}\left(\frac{n}{4} + 1\right)\xi^{-2}y(\xi) \to 0$.

(1) For ground state (ψ_0, E_0), $O(\lambda)$ perturbation on wavefcn $\psi_0 \Rightarrow O(\lambda^2)$ correction to energy E_0.

1) Calculation is best done by putting in $\phi = \sum_n c_n \psi_n$ at the very end. Straightforwardly:

$$E(\lambda) = \langle\psi|\mathcal{H}|\psi\rangle / \langle\psi|\psi\rangle = \langle\psi_0+\lambda\phi|\mathcal{H}|\psi_0+\lambda\phi\rangle / \langle\psi_0+\lambda\phi|\psi_0+\lambda\phi\rangle$$

or

$$\rightarrow E(\lambda) = \frac{\overset{(1)}{\langle\psi_0|\mathcal{H}|\psi_0\rangle} + \lambda\left[\overset{(2)}{\langle\psi_0|\mathcal{H}|\phi\rangle} + \overset{(3)}{\langle\phi|\mathcal{H}|\psi_0\rangle}\right] + \lambda^2\langle\phi|\mathcal{H}|\phi\rangle}{\underset{(4)}{\langle\psi_0|\psi_0\rangle} + \lambda\underbrace{\left[\langle\psi_0|\phi\rangle + \langle\phi|\psi_0\rangle\right]}_{N} + \lambda^2\langle\phi|\phi\rangle}. \qquad (1)$$

We've used λ = real here. Term (1) $\equiv E_0$, and in terms (2) & (3), use $\langle\psi_0|\mathcal{H} = E_0\langle\psi_0|$ & $\mathcal{H}|\psi_0\rangle = E_0|\psi\rangle$, resp. ($\mathcal{H}$ is Hermitian). Term (4) $\equiv 1$, by normalization. With the shorthand notation $N = \langle\psi_0|\phi\rangle + \langle\phi|\psi_0\rangle$, Eq. (1) becomes...

$$\underline{\underline{E(\lambda) = \left[(1+\lambda N)E_0 + \lambda^2\langle\phi|\mathcal{H}|\phi\rangle\right] / \left[(1+\lambda N) + \lambda^2\langle\phi|\phi\rangle\right]}}. \qquad (2)$$

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2) In Eq. (2), $\lambda \rightarrow$ small. If we define the quantity: $\kappa = \lambda^2/(1+\lambda N)$, then

$$\left[\begin{array}{l} E(\lambda) = E_0\left[1 + \frac{\kappa}{E_0}\langle\phi|\mathcal{H}|\phi\rangle\right] / \left[1 + \kappa\langle\phi|\phi\rangle\right], \\ \text{w/ } \kappa = \lambda^2/(1+\lambda N) \simeq \lambda^2\left[1 - \lambda N + (\lambda N)^2 - \dots\right]. \end{array}\right. \qquad (3)$$

The leading term in κ is $O(\lambda^2)$ in smallness. To $O(\lambda^2)$, $E(\lambda)$ expands as...

$$E(\lambda) \simeq E_0\left[1 + \frac{\lambda^2}{E_0}\langle\phi|\mathcal{H}|\phi\rangle\right]\left[1 - \lambda^2\langle\phi|\phi\rangle\right] \simeq E_0 + \lambda^2\varepsilon_2,$$

$$\text{w/ } \underline{\underline{\varepsilon_2 = \langle\phi|\mathcal{H}|\phi\rangle - E_0\langle\phi|\phi\rangle}}. \qquad (4)$$

As advertised, the first correction to E_0 is $O(\lambda^2)$, <u>not</u> $O(\lambda)$.

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3) Calculate ε_2 in Eq. (4) by putting in $\phi = \sum_n c_n\psi_n$. Since $\{\psi_n\}$ is an orthonormal set: $\langle\psi_m|\psi_n\rangle = \delta_{mn}$, we get...

$$\underline{\underline{\varepsilon_2}} = \sum_{m,n} c_m^* c_n\left[\langle\psi_m|\mathcal{H}|\psi_n\rangle - E_0\langle\psi_m|\psi_n\rangle\right] = \underline{\underline{\sum_n |c_n|^2(E_n - E_0)}}, \qquad (5)$$

as required. $\varepsilon_2 \geqslant 0$, since $E_n - E_0 \geqslant 0$. So $E(\lambda)$ in Eq. (4) lies <u>above</u> E_0.

② Verify conversion of $y''+f(x)y'+g(x)y=0$ to WKB form.

1. Put $y(x)=\psi(x)u(x)$, so: $y'=\psi'u+\psi u'$, etc. into the ODE, gather terms as coefficients of ψ, ψ', ψ'' and divide by u to obtain...

$y=\psi u$, into: $y''+fy'+gy=0$ ⇒

$$\rightarrow \psi''+\left[f+\frac{2u'}{u}\right]\psi'+\left[g+\frac{1}{u}(fu'+u'')\right]\psi=0. \qquad (1)$$

2. By choice of u, we can eliminate either the term in ψ', or the term in ψ. In our case, we want to get rid of the ψ' term, so we impose...

$$f+\frac{2u'}{u}=0 \Rightarrow \underline{\underline{u(x)=\exp\left[-\frac{1}{2}\int_a^x f(\xi)\,d\xi\right]}}; \qquad (2)$$

so $y(x)=\psi(x)\,e^{-\frac{1}{2}\int_a^x f(\xi)\,d\xi}$, and the diff. eqtn (1) is... (3)

$$\rightarrow \psi''+k^2(x)\psi=0, \text{ w/ } k(x)=\pm\left\{g(x)+\frac{1}{u}(fu'+u'')\right\}^{1/2}. \qquad (4)$$

3. It remains to verify the specific form of $k(x)$. With u of Eq. (2)...

$$\left.\begin{aligned} u'&=-\tfrac{1}{2}fu\\ u''&=-\tfrac{1}{2}\left(f'u-\tfrac{1}{2}f^2u\right)\end{aligned}\right\} \text{ so } \frac{1}{u}(fu'+u'')=-\frac{1}{2}\left(f'+\frac{1}{2}f^2\right). \qquad (5)$$

When this result is used in (4), we find -- as advertised...

$$\underline{\underline{k(x)=\pm\left\{g(x)-\frac{1}{2}\left[f'(x)+\frac{1}{2}f^2(x)\right]\right\}^{1/2}}} \qquad (6)$$

4. So, indeed, $y''+fy'+gy=0$ converts to $\psi''+k^2\psi=0$, w/ $\psi=y\,e^{\frac{1}{2}\int_a^x f(\xi)\,d\xi}$, and k^2 given in Eq. (6). This verifies the claim made on p. 2 of "Notes... WKB". Changing the lower limit a in the $\int_a^x f(\xi)\,d\xi$ integral merely introduces a multiplicative cnst for ψ; since the ψ'' eqtn is linear, this does not invalidate the solution. So a is arbitrary, to be fixed by boundary conditions.

③ Find an asymptotic form for the Bessel fcn $J_\nu(x)$, $x \to$ "large", via WKB.

1) Bessel's Eqtn: $y'' + (1/x)y' + [1 - (\nu^2/x^2)]y = 0$, converts to WKB form, via:

$\rightarrow y(x) = \psi(x) \exp\left(-\frac{1}{2}\int \frac{dx}{x}\right) = \psi(x)/\sqrt{x}$,

$$\Rightarrow \boxed{\psi'' + k^2(x)\psi = 0, \text{ w/ } k(x) = \left[1 - \frac{1}{x^2}\left(\nu^2 - \frac{1}{4}\right)\right]^{1/2}.} \qquad (1)$$

This eqtn is exact. A WKB approxn to $\psi(x)$ [and thus to $y = \psi/\sqrt{x}$] will work at values of x where k is "slowly-varying", i.e.

$$\rightarrow \left|\frac{1}{k^2}(dk/dx)\right| = \left|\frac{1}{k^3x^3}\left(\nu^2 - \frac{1}{4}\right)\right| \ll 1, \text{ or } |(kx)^3| \gg \left|\nu^2 - \frac{1}{4}\right|$$

This works OK when $|x| \to$ "large", so long as i.e. $\underline{\underline{\left|x^2 - \left(\nu^2 - \frac{1}{4}\right)\right|^{\frac{3}{2}} \gg \left|\nu^2 - \frac{1}{4}\right|}}$ (2)

ν = some cnst. Then a WKB form for ψ should be good for $\frac{1}{2} \ll |\nu| \ll x \to \infty$.

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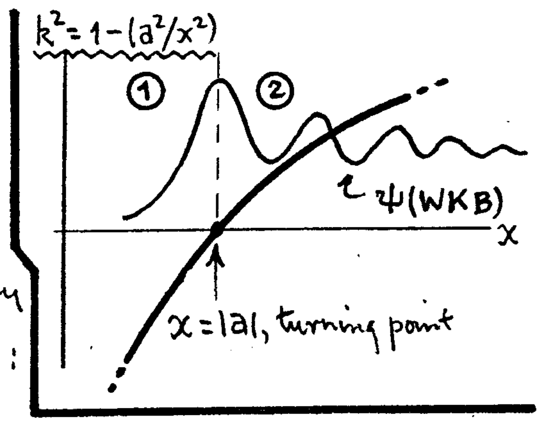
2) Let $\underline{\underline{a}} = \left(\nu^2 - \frac{1}{4}\right)^{1/2}$, so $k(x) = [1 - (a^2/x^2)]^{\frac{1}{2}}$.

$x = |a|$ is a "turning point" for the prob^m [$k(a) = 0$], and we want ψ(WKB) for $x > |a|$. To be an acceptable solution, ψ should decrease exponentially in region ①, and oscillate in region ②. So we write:



$\rightarrow \psi(x > |a|) \simeq (A/\sqrt{k}) \sin\left(\int_a^x k(\xi)d\xi + \beta\right)$; k as above, ampl. A & phase β = cnsts;

but $\int_a^x k(\xi)d\xi = \int_a^x \frac{d\xi}{\xi}(\xi^2 - a^2)^{1/2} = (x^2 - a^2)^{1/2} - a\cos^{-1}\left(\frac{a}{x}\right) \simeq x - \frac{\nu\pi}{2}$ for $x \gg |a|$ & $a \simeq \nu$.

so Since $k \simeq 1$ as $x \to$ "large", then: $\underline{\underline{\psi(x > |a|) \simeq A\sin\left(x - \frac{\nu\pi}{2} + \beta\right)}}$. (3)

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3) Since $y = \psi/\sqrt{x}$, the WKB solution to Bessel's Eqtn, for $\frac{1}{2} \ll |\nu| \ll x \to \infty$, is

$$\boxed{y(x) = J_\nu(x) \simeq \frac{\text{cnst}}{\sqrt{x}} \sin\left(x - \frac{\nu\pi}{2} + \beta\right)} \quad (4)$$

When the phase $\beta = \pi/4$, this is a standard result; see NBS Math. Handbook #(9.2.1). The phase β can be fixed by the WKB Connection Formulas.

④ Solution to: $y''+\alpha\xi^n y=0$ for $y=y(\xi)$. Asymptotic form for $\xi\to\infty$.

This problem appears in the WKB turning point problem, for $\alpha=-1$, $n=1$ (Airy's ODE).

(A) 1) Let: $x(\xi)=\sqrt{\xi}\,J_\nu(\zeta)$, w/ $\nu=1/(n+2)$ & $\zeta=\left(\frac{2\sqrt{\alpha}}{n+2}\right)\xi^{\frac{1}{2}(n+2)}$. By direct differentiation...

$$\rightarrow \frac{dx}{d\xi}=\sqrt{\xi}\left(\frac{d\zeta}{d\xi}\right)\frac{d}{d\zeta}J_\nu(\zeta)+\frac{1}{2}\xi^{-\frac{1}{2}}J_\nu(\zeta). \quad (1)$$

But: $\left(\frac{d\zeta}{d\xi}\right)=\sqrt{\alpha}\,\xi^{\frac{n}{2}}$, and: $\frac{d}{d\zeta}J_\nu(\zeta)=-\frac{\nu}{\zeta}J_\nu(\zeta)+J_{\nu-1}(\zeta)$ {Mathews & Walker Eq. (7-54). So...

$$\rightarrow \frac{dx}{d\xi}=\sqrt{\alpha}\,\xi^{\frac{1}{2}(n+1)}\left[-\frac{\nu}{\zeta}J_\nu(\zeta)+J_{\nu-1}(\zeta)\right]+\frac{1}{2}\xi^{-\frac{1}{2}}J_\nu(\zeta)$$

$$=\sqrt{\alpha}\,\xi^{\frac{1}{2}(n+1)}J_{\nu-1}(\zeta)-\underbrace{\left[\sqrt{\alpha}\,\xi^{\frac{1}{2}(n+1)}\frac{1/(n+2)}{\left(\frac{2\sqrt{\alpha}}{n+2}\right)\xi^{\frac{1}{2}(n+2)}}\right]}_{=\frac{1}{2}\xi^{-1/2}}J_\nu(\zeta)+\frac{1}{2}\xi^{-\frac{1}{2}}J_\nu(\zeta)$$

cancels

So//
$$\frac{dx}{d\xi}=\sqrt{\alpha}\,\xi^{\frac{1}{2}(n+1)}J_{\nu-1}(\zeta). \quad (2)$$

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2) The second derivative is calculated as...

$$\rightarrow \frac{1}{\sqrt{\alpha}}\frac{d^2x}{d\xi^2}=\xi^{\frac{1}{2}(n+1)}\left(\frac{d\zeta}{d\xi}\right)\frac{d}{d\zeta}J_{\nu-1}(\zeta)+\frac{n+1}{2}\xi^{\frac{1}{2}(n-1)}J_{\nu-1}(\zeta). \quad (3)$$

Use $\left(\frac{d\zeta}{d\xi}\right)=\sqrt{\alpha}\,\xi^{\frac{n}{2}}$ as above, and: $\frac{d}{d\zeta}J_{\nu-1}(\zeta)=\frac{\nu-1}{\zeta}J_{\nu-1}(\zeta)-J_\nu(\zeta)$ {M & W (7-55). So...

$$\frac{1}{\sqrt{\alpha}}\frac{d^2x}{d\xi^2}=\sqrt{\alpha}\,\xi^{n+\frac{1}{2}}\left[\left(\frac{\nu-1}{\zeta}\right)J_{\nu-1}(\zeta)-J_\nu(\zeta)\right]+\frac{n+1}{2}\xi^{\frac{1}{2}(n-1)}J_{\nu-1}(\zeta) \quad (4)$$

$$=-\sqrt{\alpha}\,\xi^n x(\xi)+\Big[\underbrace{\sqrt{\alpha}\,\xi^{n+\frac{1}{2}}\left(\frac{\nu-1}{\zeta}\right)}+\frac{n+1}{2}\xi^{\frac{1}{2}(n-1)}\Big]J_{\nu-1}(\zeta) \quad (5)$$

$$=\sqrt{\alpha}\,\xi^{n+\frac{1}{2}}\frac{\frac{1}{n+2}-1}{\left(\frac{2\sqrt{\alpha}}{n+2}\right)\xi^{\frac{n}{2}+1}}=-\left(\frac{n+1}{2}\right)\xi^{\frac{1}{2}(n-1)}$$

cancels

So// $\frac{1}{\sqrt{\alpha}}\frac{d^2x}{d\xi^2}=-\sqrt{\alpha}\,\xi^n x(\xi)+\text{zero}$, or// $\boxed{\frac{d^2x}{d\xi^2}+\alpha\xi^n x=0}$, for// $x(\xi)=\sqrt{\xi}\,J_\nu(\zeta)$. (6)

) We have shown that $x(\xi)=\sqrt{\xi}\,J_\nu(\zeta)$, w/ $\nu=1/(n+2)$ & $\zeta=\left(\frac{2\sqrt{\alpha}}{n+2}\right)\xi^{\frac{1}{2}(n+2)}$, satisfies the ODE of interest, viz $x''+\alpha\xi^n x=0$. Then $y(\xi)=Ax(\xi)$ is also a soln, for $A=$ cnst. For the Airy problem: $y''-\xi y=0$, the soln is: $y(\xi)=A\sqrt{\xi}\,J_{1/3}\left(\frac{2i}{3}\xi^{3/2}\right)$.

④ (cont'd)

4) Now assume an asymptotic form: $x(\xi) \sim \xi^{-k} e^{-a\xi^{\ell}}$, as $\xi \to \infty$. Differentiate...

(B)

$$\rightarrow \frac{dx}{d\xi} = -k\xi^{-(k+1)} e^{-a\xi^{\ell}} + \xi^{-k}\left[-a\ell\xi^{\ell-1} e^{-a\xi^{\ell}}\right] = -(k\xi^{-1} + a\ell\xi^{\ell-1})\,x; \tag{7}$$

$$\rightarrow \frac{d^2x}{d\xi^2} = -\left[-k\xi^{-2} + a\ell(\ell-1)\xi^{\ell-2}\right]x + \left[k\xi^{-1} + a\ell\xi^{\ell-1}\right]^2 x$$

... gather terms to get...

$$\rightarrow \frac{d^2x}{d\xi^2} = \underbrace{(a\ell)^2 \xi^{2(\ell-1)}}_{①}\left[1 - \underbrace{\left(\frac{\ell-2k-1}{a\ell}\right)}_{②}\xi^{-\ell} + \underbrace{\frac{k(k+1)}{(a\ell)^2}}_{③}\xi^{-2\ell}\right]x. \tag{8}$$

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5) The parameters k, ℓ, a are free. We fix them by the following choices...

Set factor ① $= -\alpha\xi^n \Rightarrow \begin{cases} 2(\ell-1) = n, \text{ or: } \underline{\underline{\ell = \frac{1}{2}(n+2)}}; \\ (a\ell)^2 = -\alpha, \text{ or: } \underline{\underline{a = 2\sqrt{-\alpha}/(n+2)}}. \end{cases}$ (9a)

Set factor ② $\equiv 0 \Rightarrow \underline{\underline{k = \frac{1}{2}(\ell-1) = \frac{1}{4}n}}$. (9b)

Then factor ③: $k(k+1)/(a\ell)^2 = -\frac{1}{\alpha}\frac{n}{4}\left(\frac{n}{4}+1\right)$. (9c)

With the choices in Eq. (9), Eq. (8) becomes...

$$\frac{d^2x}{d\xi^2} = -\alpha\xi^n\left[1 - 0 - \frac{1}{\alpha}\frac{n}{4}\left(\frac{n}{4}+1\right)\xi^{-(n+2)}\right]. \tag{10}$$

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6) We can now state that: $x(\xi) = \xi^{-\frac{n}{4}} \exp\left[-\left(\frac{2\sqrt{-\alpha}}{n+2}\right)\xi^{\frac{1}{2}(n+2)}\right]$, satisfies the ODE:

$$\boxed{\frac{d^2x}{d\xi^2} + \alpha\xi^n x = \frac{n}{4}\left(\frac{n}{4}+1\right)\xi^{-2}x(\xi)} \rightarrow 0, \text{ as } \xi \to \infty, \tag{11}$$

as required. $x(\xi)$ is therefore an asymptotic form for $\sqrt{\xi}\, J_\nu(\xi)$ of part (A). For the Airy problem: $x'' - \xi x = 0$, the asymptotic form is as was used in Eq. (39), p. 14 of "Notes on the WKB Method", viz: $\underline{x(\xi) \sim \xi^{-\frac{1}{4}} \exp(-\frac{2}{3}\xi^{3/2})}$.