ϕ507 Problems

1) [15 pts]. The ODE: $zf''+(b-z)f'-af=0$, a & b = cnsts, for $f=f(z)$, is the confluent hypergeometric equation. (A) By direct substitution, show that a series solution is: $f(z)=F(a;b;z)=\sum_{k=0}^{\infty}[(a)_k/(b)_k]\frac{z^k}{k!}$, w/ $(a)_k=a(a+1)\cdots(a+k-1)$ & $(a)_0=1$, the Pochhammer symbol. (B) Let $|z|\to$ large, and note $(a)_k=\Gamma(k+a)/\Gamma(a)$. By examining the dominant terms in the series for F, and using suitable approximations for the Γ-fcns, show that for k "large", the k^{th} term in the series is $\sim[\Gamma(b)/\Gamma(a)]\,z^k/(k-(a-b))!$ Use this to show that for large (+)ve z (z real): $F(a;b;z)\sim[\Gamma(b)/\Gamma(a)]\,z^{a-b}e^z$. (C) Use the result of part (B) to show that for large (−)ve z (again real): $F(a;b;z)\sim[\Gamma(b)/\Gamma(b-a)](-z)^{-a}$.

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(2) Verify that: $\mathrm{erf}(x)=(2/\sqrt{\pi})\,x\,F(\frac{1}{2};\frac{3}{2};-x^2)$, F = confluent hypergeometric fcn. Find an expression for erf(x), correct to $\mathcal{O}(x^3)$, as $x\to 0$.

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(3) A QM system consists of two particles, of masses m_1 & m_2. Express the operators for total momentum $\hat{\mathbf{P}}=\hat{\mathbf{p}}_1+\hat{\mathbf{p}}_2$ and total ∡ momentum $\hat{\mathbf{L}}=\hat{\mathbf{l}}_1+\hat{\mathbf{l}}_2$ in terms of the relative coordinate $\mathbf{r}=\mathbf{r}_1-\mathbf{r}_2$ and center-of-mass coordinate $\mathbf{R}=(m_1\mathbf{r}_1+m_2\mathbf{r}_2)/(m_1+m_2)$. Show that the kinetic energy part of the Hamiltonian, viz $\hat{K}=\frac{1}{2m_1}\hat{\mathbf{p}}_1^2+\frac{1}{2m_2}\hat{\mathbf{p}}_2^2$ can be put in the form: $\hat{K}=-(\hbar^2/2M)\nabla_R^2-(\hbar^2/2\mu)\nabla_r^2$, w/ $M=m_1+m_2$ & $\mu=m_1m_2/(m_1+m_2)$.

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(4) [15 pts]. Consider a central potential of form: $V(r)=-\frac{B}{r}+\frac{A}{r^2}$; B & A are (+)ve cnsts.

(A) Sketch V(r) vs. r. What physical system might be represented by such a potential?

(B) Write the radial eqtn in dimensionless variables ("atomic units" here are: length $a_0=\frac{\hbar^2}{mB}$, energy $E_0=\frac{B}{a_0}$). Find the radial wavefcn $R(\rho)$, and show that the bound state energies are: $\boxed{E_{nl}=-\frac{1}{2}E_0/(n+\Delta_l)^2}$, $n=1,2,3,\ldots$ and $l=0,1,\ldots,(n-1)$, just as for H-atoms. The "quantum defect" Δ_l lifts the l-degeneracy. Find an <u>exact</u> expression for Δ_l.

(C) Now approximate E_{nl} through terms of $\mathcal{O}(A)$. In a given state n, how are the l-states arranged? Sketch an energy-level diagram for n=1,2,3. What is the energy spread in level n?

ϕ507 Problems

⑤ [15pts]. This problem concerns details of H-atom radial wavefcns in Davydov ¶ 38.

(A) When $a=-N$, w/ $N=0,1,2,\ldots$, show that the confluent hypergeometric fcn $F(a;b;x)$ reduces to the polynomial: $F(-N;b;x)=\sum_{k=0}^{N}\frac{\Gamma(b)}{\Gamma(k+b)}\binom{N}{k}(-x)^k$, w/ $\binom{N}{k}=\frac{N!}{k!(N-k)!}$ the binomial coefficient. Using this result, find an explicit form for the full H-atom radial wavefcn $f_{n\ell}(\rho)=\frac{1}{\rho}R_{n\ell}(\rho)$ for the 3s state. Compare with Davydov Table 8.

(B) H-atom states $|n\ell\rangle$ with maximum allowed ∡ momentum $\ell=n-1$ are called "raster" states. Find the general form of the full radial wavefcn $f_{n\ell}(\rho)$ when $\ell=n-1$.

(C) Calculate expectation values of powers of ρ, viz. $\langle\rho^\lambda\rangle$, in the states $|n,\ell=n-1\rangle$ you found in part (B). For $\lambda=-3$, specifically, compare with Davydov's Eq. 38.17e.

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⑥ A QM ∡ momentum $\hat{\mathbb{J}}$ has eigenfcns $|jm\rangle$. Consider the ladder operators $\hat{J}_\pm=\hat{J}_x\pm i\hat{J}_y$.

(A) Show that $\hat{J}_\pm|jm\rangle$ is an eigenfcn of $\hat{\mathbb{J}}^2$, with j-value unchanged.

(B) Show that $\hat{J}_\pm|jm\rangle$ is an eigenfcn of $\hat{J}_z$, corresponding to eigenvalues $m\pm1$.

(C) Using the $\hat{J}_\pm$, find the most general matrix elements of $\hat{J}_x$ & $\hat{J}_y$ -- i.e. evaluate $\langle\alpha' j' m'|\hat{J}_{x,y}|\alpha j m\rangle$, with pertinent selection rules for the quantum #s $\alpha\alpha'$; jj', mm'.

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⑦ Consider the Pauli matrices $\vec{\sigma}=(\sigma_x,\sigma_y,\sigma_z)$ for spin $\frac{1}{2}$; they obey the commutation rule: $[\sigma_\alpha,\sigma_\beta]=2i\sigma_\gamma$, w/ $\alpha\beta\gamma$ = cyclic permutation of xyz [Sakurai, Sec 3.2].

(A) Prove the anti-commutation rule: $\{\sigma_\alpha,\sigma_\beta\}=\sigma_\alpha\sigma_\beta+\sigma_\beta\sigma_\alpha=2\delta_{\alpha\beta}$.

(B) If $\vec{A}$ & $\vec{B}$ are any two vector operators that commute with $\vec{\sigma}$, use $[\sigma_\alpha,\sigma_\beta]$ and $\{\sigma_\alpha,\sigma_\beta\}$ to prove the Dirac identity: $\boxed{(\vec{\sigma}\cdot\vec{A})(\vec{\sigma}\cdot\vec{B})=\vec{A}\cdot\vec{B}+i\,\vec{\sigma}\cdot(\vec{A}\times\vec{B})}$.

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⑧ If vector operators $\vec{A}$ & $\vec{B}$ are both $\vec{T}$-vectors w.r.t. a QM ∡ momentum operator $\vec{J}$, show that: $[\vec{J},\vec{A}\cdot\vec{B}]=0$. Why does this establish $\vec{A}\cdot\vec{B}$ as a "true scalar"?

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⑨ [5pts]. Given: noncommuting operators $\hat{P}$ & $\hat{Q}$ and a set of basis fcns $\{u_k(x)\}$. If $P_{ij}=\int dx\, u_i^*(x)\hat{P}u_j(x)$, verify the matrix eqtn: $(PQ)_{k\ell}=\sum_m P_{km}Q_{m\ell}$, directly. What assumption(s) must be made about the set $\{u_k(x)\}$?

(10) Consider the 2P states of a one-electron atom. Here, the orbital ∡ momentum $\vec{L}$ (eigenwerte $l=1$) and electron spin ∡ momentum $\vec{S}$ (eigenwerte $s=1/2$) couple to form $\vec{J}=\vec{L}+\vec{S}$, with j-values $3/2$ & $1/2$. By using the step-down operator J_-, and imposing orthonormality, explicitly do a Clebsch-Gordan transform^n from the uncoupled states $|lsm_lm_s\rangle$ to the coupled states $|lsjm_j\rangle$. Make a table of your results, i.e. each $|lsjm_j\rangle$ state in turn, as a linear combination of the $|lsm_lm_s\rangle$, with appropriate C-G coefficients.

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(11) [15pts]. To generalize prob. (10), let l have any value >0; then $j=l\pm\frac{1}{2}$. With $m_s=\pm\frac{1}{2}$ only, there are just two m_l values for a given m: viz. $m_l=m\mp\frac{1}{2}$ (here $m=m_j$). Let $\alpha=|s=\frac{1}{2},m_s=+\frac{1}{2}\rangle$ & $\beta=|s=\frac{1}{2},m_s=-\frac{1}{2}\rangle$ be the spin-up & spin-down eigenfcns. Then the eigenfcns of the coupled states have just two terms (suppress l & s, ad libitum):

$$\boxed{|n;lsjm\rangle = C_1(jm)|n;l,m_l=m-\tfrac{1}{2}\rangle\alpha + C_2(jm)|n;l,m_l=m+\tfrac{1}{2}\rangle\beta.}$$

The C-G transform in this case amounts to finding two pairs of constants C_k, one pair for each of $j=l\pm\frac{1}{2}$. By using the J_- operator, calculate the $C_k(jm)$ explicitly.

---

(12) In an atom where the orbital & spin ∡ momenta $\vec{L}$ & $\vec{S}$ couple to form $\vec{J}=\vec{L}+\vec{S}$, the magnetic moments $\vec{\mu}_L=-g_L\mu_0\vec{L}$ & $\vec{\mu}_S=-g_S\mu_0\vec{S}$ likewise couple to form a total $\vec{\mu}_J=\vec{\mu}_L+\vec{\mu}_S$. Use the Vector Model to show that (in an expectation-value sense): $\vec{\mu}_J=-g_J\mu_0\vec{J}$. Show that g_J -- which is called the Landé g-factor -- is given by:

$$\boxed{g_J=\left[\frac{j(j+1)+l(l+1)-s(s+1)}{2j(j+1)}\right]g_L+\left[\frac{j(j+1)+s(s+1)-l(l+1)}{2j(j+1)}\right]g_S.}$$

Calculate g_J-values for the hydrogen states $2P_{3/2}$, $2P_{1/2}$ & $2S_{1/2}$. What is the maximum observable μ_J in each state? If a weak magnetic field H were applied to this system how would the state energies vary with H? Draw a picture. [This is the Zeeman Effect].

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(13) Consider the hydrogenic states $2S_{\frac{1}{2}}$ [the $m=\pm\frac{1}{2}$ levels are denoted α & β] and $2P_{3/2}$ [$m=+\frac{3}{2}$, $+\frac{1}{2}$, $-\frac{1}{2}$, $-\frac{3}{2}$ levels denoted a, b, c, d]. Some of the m-levels are coupled by a Stark interaction $V=\vec{\mathcal{E}}\cdot\vec{r}$, w/ $\vec{r}$ = position and $\vec{\mathcal{E}}$ = cnst. Find the absolute value of all matrix elements $\mathcal{M}=|\langle 2S_{\frac{1}{2}}|V|2P_{\frac{3}{2}}\rangle|$ allowed between the six m-levels, up to a reduced matrix element R. If $\Gamma\propto\mathcal{M}^2$ is the transition rate induced by V, establish the equalities:

$$\boxed{\Gamma(\alpha\to b)=\Gamma(\beta\to c),\quad \Gamma(\alpha\to a)=\Gamma(\beta\to d)=3\Gamma(\alpha\to c)=3\Gamma(\beta\to b).}$$

(17) [15 pts]. For a particle (q,m) in an EM field specified by a 4-potential $(A_\mu)=(\vec{A},i\phi)$, the Klein-Gordon wave equation and continuity equation are [$\psi(x_\mu)=(\mathbf{r},ict)$]...

$$\left[\!\left[\begin{array}{l} \left[\left(\frac{\partial}{\partial x_\mu}-\frac{iq}{\hbar c}A_\mu\right)^2-k_0^2\right]\psi=0, \text{ w/ } k_0=mc/\hbar; \\ \partial S_\mu/\partial x_\mu=0, \text{ w/ } S_\mu=\frac{\hbar}{2im}\left[\psi^*\left(\frac{\partial}{\partial x_\mu}-\frac{iq}{\hbar c}\right)\psi-\text{c.c.}\right].\end{array}\right]\!\right]$$

Consider the gauge transformation: $A_\mu \rightarrow A'_\mu = A_\mu + \partial\eta/\partial x_\mu$, η = arbitrary fcn. Given that $\psi\rightarrow\psi'=\psi\exp[i(q/\hbar c)\eta]$ under this transform, show that: (A) S_μ is gauge invariant, and: (B) the KG Eqtn itself is gauge covariant (form-invariant).

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(18) [15 pts]. Consider a particle of mass m in a 3D attractive spherical potential well of depth V and radius a. Using the Klein-Gordon Eqtn for S-states only (set the orbital ∡ momentum $l=0$), find the minimum well depth V_{KG} which just barely binds the particle. State your answer in terms of the well-known result from the Schrödinger Eqtn, viz: $V_S=\pi^2\hbar^2/8ma^2$. Interpret the difference between V_{KG} and V_S.

---

(19) [15 pts]. A Schrödinger-type form for the free-particle Klein-Gordon Eqtn can be manufactured as follows. Define a fcn ξ via: $(mc^2)\xi=i\hbar\,\partial\psi/\partial t$. Then the KG Eqtn is: $\frac{1}{m}[\vec{p}^{\,2}+(mc)^2]\psi=i\hbar\,\partial\xi/\partial t$. Next, define a two-component wavefunction by: $\Psi=\begin{pmatrix}\psi_+\\ \psi_-\end{pmatrix}=\frac{1}{2}\begin{pmatrix}\psi+\xi\\ \psi-\xi\end{pmatrix}$. In these terms, show the KG Eqtn can be written as:

$$\boxed{i\hbar\,\partial\Psi/\partial t=\mathcal{H}\Psi, \text{ w/ } \mathcal{H}=\begin{pmatrix}1&0\\0&-1\end{pmatrix}mc^2+\begin{pmatrix}1&1\\-1&-1\end{pmatrix}\frac{\vec{p}^{\,2}}{2m}}.$$

Notice that this "Hamiltonian" $\mathcal{H}$ is not Hermitian. For nonrelativistic particles ($\vec{p}^{\,2}/2m \ll mc^2$), evidently ψ_+ is the solution for positive energy states $E\simeq+mc^2$, while ψ_- is the solution for negative energy states $E\simeq(-)mc^2$. Now show that the KG "probability density": $\rho=-(\hbar/mc^2)\,\mathrm{Im}[\psi^*(\partial\psi/\partial t)]$, class notes p. fs 16, can be written as a charge density: $\tilde{\rho}=q\rho=q\{|\psi_+|^2-|\psi_-|^2\}$. Then (+)ve energy solutions (ψ_+ dominant) have $\tilde{\rho}\doteq+q$, while (−)ve energy solutions (ψ_- dominant) have $\tilde{\rho}\doteq(-)q$. We will see that the Dirac Eqtn has similar features.

(20) To approximate the ground state of the simple harmonic oscillator (SHO), use the trial wavefunction: $\underline{\phi(x) = A[1-(|x|/\alpha)]}$, $\underline{\text{for } |x| \leq \alpha}$, and $\phi(x) \equiv 0$, for $|x| > \alpha$. Here A = cnst and α = variable (length) parameter. Calculate $E(\alpha) = \frac{\langle \phi | \mathcal{H}(\text{SHO}) | \phi \rangle}{\langle \phi | \phi \rangle}$ and -- for optimum α -- show that this energy lies less than 10% above the exact value.

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(21) [Davydov Ch. VII #6, p. 205]. Use the trial wavefunction: $\underline{\phi(\alpha, r) = Ae^{-\frac{1}{2}\alpha r^2}}$, to estimate the ground state energy of the hydrogen atom. <u>NOTE</u>: here you are approximating the atom's radial motion by that of an "equivalent" 1D SHO.

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(22) In a QM system with Hamiltonian $\mathcal{H}$, let the eigenfunctions & 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 the trial function: $\underline{\psi = \psi_0 + \lambda\phi}$, w/ ψ_0 = actual ground state wavefcn, λ is a small (real) parameter, and ϕ is 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.: $E(\lambda) = E_0 + \lambda \mathcal{E}_1 + \lambda^2 \mathcal{E}_2 + \lambda^3 \mathcal{E}_3 + \ldots$, then $\mathcal{E}_1 \equiv 0$, while $\mathcal{E}_2$ is the positive quantity: $\mathcal{E}_2 = \sum_n |c_n|^2 (E_n - E_0)$. <u>CONCLUSION</u>: for any perturbation on $\mathcal{H}$ which shifts $\psi_0 \to \psi_0 + \lambda\phi$ by a term <u>first</u> order in some small parameter λ, the ground state energy $E_0 \to E_0 + \lambda^2 \mathcal{E}_2$ shift is only a <u>second</u> order correction.

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(23) (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, $\nu = \frac{1}{n+2}$, $\zeta = \left(\frac{2\sqrt{\alpha}}{n+2}\right) \xi^{\frac{1}{2}(n+2)}$. $J_\nu(\zeta)$ is the Bessel fcn of order ν. (B) Assume the asymptotic form: $y(\xi) \sim \xi^{-k} e^{-a\xi^\ell}$, as $\xi \to \infty$. By proper choice of the cnsts k, ℓ & a, show that as $\xi \to \infty$, this form satisfies the differential eqtn: $y''(\xi) + \alpha \xi^n y(\xi) = \frac{n}{4}\left(\frac{n}{4}+1\right) \xi^{-2} y(\xi) \to 0$.

(D) 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 <u>approximate</u> solution for the Bessel fcn $y \simeq J_\nu(x)$ by the WKB method. Find an asymptotic form for $J_\nu(x)$ as $x \to$ "large" (specifically: $x \gg |\nu|$). You may assume $|\nu| \gg \frac{1}{2}$.

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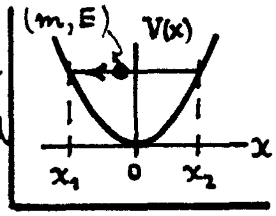
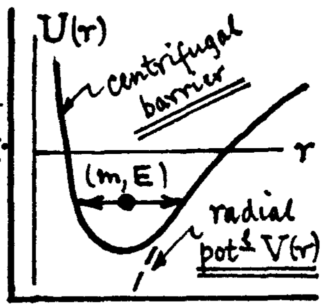
(25) In "Notes on the WKB Method", pp. 7-10, we solved the WKB problem $\ddot{v}+\Omega^2 v=0$ by transforming variables: $t\to s=\int\Omega(t)\,dt$, $v\to u=v\sqrt{\Omega}$, so the diff. eq. is $u''+[1+b(s)]u=0$, with $b(s)$ defined in Eq. (20) of Notes. For $b(s)=0$, we get the zeroth-order (WKB) solution: $u(s)\simeq u_0(s)=Ae^{+is}+Be^{-is}$. We then iterated to get: $u_1\simeq u_0+\int_0^s u_0 K\,d\sigma$, with K defined in Eq. (27). After $n+1$ iterations: $u_{n+1}=u_n+\int_0^s u_n K\,d\sigma$. Write out u_{n+1} explicitly as a series of $(n+2)$ terms, in successively higher "powers" of $b(s)$. Show that: $u_{n+1}(s)=u_0(s)+\sum_{k=1}^{n+1}\binom{n+1}{k}\int_0^s d\sigma_1\int_0^{\sigma_1}d\sigma_2\cdots\int_0^{\sigma_{k-1}}d\sigma_k\, u_0(\sigma_k)\,\mathcal{K}(\sigma_k,\ldots,\sigma_1,s)$. Identify $\mathcal{K}$.

(26) A QM particle of mass m and energy E moves in a 1D SHO, w/ potential $V(x)=\frac{1}{2}m\omega^2x^2$, where ω = SHO natural frequency. Use Bohr-Sommerfeld quantization [i.e. $\int_{x_1}^{x_2}k(x)\,dx=(n+\frac{1}{2})\pi$, w/ $n=0,1,2,\ldots$] to find the eigenenergies E_n for this motion. How does your result compare with the known E_n (SHO)?



(27) [30 pts]. For a QM particle (mass m, energy E) moving in >1D, and in an attractive radial pot$^{\underline{l}}$ $V(r)$, the effective potential $U(r)=V(r)+\frac{\mu^2\hbar^2}{2mr^2}$. The term in $\frac{1}{r^2}$ is the "centrifugal barrier", present because of m's rotational K.E. μ is a quantum # related to m's $\measuredangle$lar momentum [in 3D: $\mu^2=l(l+1)$, w/ $l=0,1,2,\ldots$; in 2D: $\mu^2=m^2-\frac{1}{4}$, w/ $m=\pm1,\pm2,\ldots$]. Here, just take $\mu^2\geqslant 0$.



(A) Let length r_0 be the "size" of $U(r)$, and define a dimensionless variable: $x=r/r_0$. Write $V(r)=V_0 f(x)$, V_0 = cnst & $f(x)$ arbitrary. Show the Bohr-Sommerfeld condition becomes:

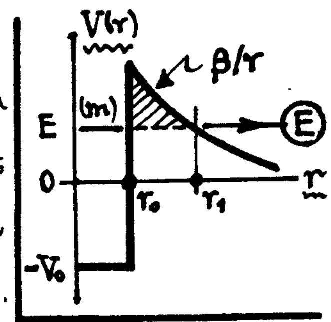
$$\boxed{\int_{x_1}^{x_2}\sqrt{\epsilon-[\sigma f(x)+\mu^2/x^2]}\,dx=(n+\tfrac{1}{2})\pi}$$

$\int$ w/ x_1 & x_2 = solutions to: $\sigma f(x)+\mu^2/x^2=\epsilon$. Specify ϵ & σ in terms of $m, r_0, \hbar, E$ & V_0.

(B) Specialize to $f(x)=\ln x$ [log potentials are use to model quark confinement -- see Quigg & Rossner, Phys. Lett. 71B, 153 (1977)]. Sketch $U(x)$ vs. x, and find the minimum, x_0. Expand $U(x)$ about x_0, find the effective "spring constant" near x_0, and calculate the quantized energies $E_{n\mu}$ of a quark trapped near x_0. You have a SHO here. Why?

(C) For large vibrations: $\sigma\gg\mu^2$. Evaluate the above integral to find how $E_{n\mu}$ varies w/ n.

(D) For large rotations: $\mu^2\gg\sigma$. Find $E_{n\mu}$, approximately, to see how it varies w/ μ & n.

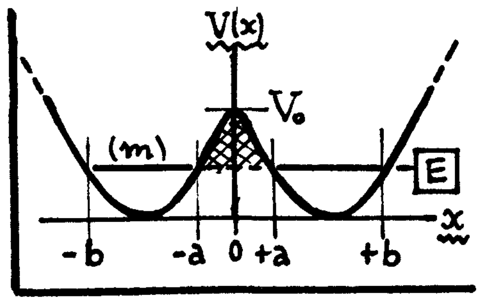


(28) [20pts]. A particle of mass m and total energy $E>0$ is initially bound in a nuclear potential well of depth V_0 and radial size r_0. m tunnels thru the Coulomb barrier β/r, emerging at r_1 with zero ∢ momentum.

(A) Per WKB, calculate the probability $T(E)$ that the tunneling occurs. Show that for high barriers ($E \ll \beta/r_0$): $T(E) \simeq \exp\left\{-\frac{\pi\beta}{\hbar}\sqrt{2m/E}\right\}$, independent of r_0.

(B) Consider deuterium fusion: ${}_1H^2 + {}_1H^2 \rightarrow {}_2He^3 + n$ (3.2 MeV), by collisions between ${}_1H^2$ nuclei. Calculate the tunneling factor for ${}_1H^2 \rightarrow {}_1H^2$ penetration at room temperature (300°K).

(C) Consider ${}_1H^2$ gas at STP, w/ density n & thermal speed $\bar{v}$. The probability/unit time of ordinary collisions is: $\Gamma_0 = n\sigma_A\bar{v}$, w/ σ_A = atomic collision cross-section. The fusion rate is: $\Gamma_f = n\sigma_D\bar{v}\,T(\bar{v})$, w/ σ_D = ${}_1H^2$ nuclear cross-section. Approximate σ_A & σ_D as geometrical, and estimate Γ_f/Γ_0. Is "cold fusion" plausible?



(29) [30pts]. A symmetric potential $V(x)$ consists of two wells separated by a barrier of height V_0 as shown. A particle of mass m and energy $E < V_0$ is initially placed in one well. m can tunnel thru the barrier ($-a \leq x \leq a$), coupling the wells.

(A) Use the WKB method to show that the condition determining the system eigenenergies is:

$$\boxed{\operatorname{ctn}\phi = \pm\frac{1}{2}e^{-\theta}} \quad \text{w/} \quad \begin{aligned} \phi &= \int_a^b k(x)\,dx, \quad k(x) = \sqrt{(2m/\hbar^2)[E-V(x)]}\,; \\ \theta &= \int_a^b \kappa(x)\,dx, \quad \kappa(x) = \sqrt{(2m/\hbar^2)[V(x)-E]}\,. \end{aligned}$$

Please use this notation.

HINT: establish this condition by starting out with $\psi_1 = (A/\sqrt{\kappa})\,e^{-\int_x^{-b}\kappa\,dx'}$ in the region $x < -b$, and connecting $\psi_1 \rightarrow \psi_2 \rightarrow \psi_3 \rightarrow \psi_4 \rightarrow \psi_5$ in $x > b$. Make sure ψ_5 doesn't diverge.

(B) For $V_0 \gg E$, $\theta \rightarrow$ "large", and the condition of part (A) is: $\phi \simeq (n+\frac{1}{2})\pi \pm \frac{1}{2}e^{-\theta}$. Let $E_n^{(0)}$ be the n^{th} energy level of either well alone (w/o barrier). Show that the presence of a penetrable barrier perturbs $E_n^{(0)}$ by an amount which is approximated to lowest order by: $\Delta E_n = \pm(\hbar\omega_n/2\pi)\exp\left\{-\int_{-a}^{+a}\sqrt{(2m/\hbar^2)[V(x)-E_n^{(0)}]}\,dx\right\}$. Here ω is the classical natural frequency of motion in the well, defined by: natural period $= \frac{2\pi}{\omega} = 2\int_a^b dx/[p(x)/m]$.

(C) Suppose the well is: $V(x) = \frac{1}{2}m\omega^2(|x|-x_0)^2$ [double SHO well]. Calculate the splitting ΔE_0 (in the $n=0$ ground state) explicitly in terms of ω & $V_0 = \frac{1}{2}m\omega^2 x_0^2$.

(30) In stationary-state (non-degenerate) perturbation theory for $\mathcal{H}_0 \psi_k^{(0)} = E_k^{(0)} \psi_k^{(0)}$, the first-order correction to the system wavefunctions when $\mathcal{H}_0 \to \mathcal{H} = \mathcal{H}_0 + V$ is: $\underline{\psi_k^{(0)} \to \psi_k = \psi_k^{(0)} + \psi_k^{(1)}}$, w/ $\psi_k^{(1)} = \sum_{n \neq k} a_{nk}^{(1)} \psi_n^{(0)}$, $a_{nk}^{(1)} = V_{nk}/(E_k^{(0)} - E_n^{(0)})$, $V_{nk} = \langle n|V|k\rangle$. Show that this ψ_k, correct to $\mathcal{O}(V)$, is sufficient to give an energy correct to $\mathcal{O}(V^2)$ by calculating: $\underline{E_k = \langle \psi_k|\mathcal{H}|\psi_k\rangle / \langle \psi_k|\psi_k\rangle}$.

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(31) [15pts, ~Davydov #5, p.205]. The proton has a finite size; its (rms) radius: $R_p \simeq 0.8 \times 10^{-13}$ cm. At distances $r \sim R_p$ the e-p interaction is thus not Coulombic, but is modified to: $\underline{-e^2/r + U(r)}$, w/ $U(r)$ the perturbation due to the proton charge distribution. $U(r)$ shifts the hydrogen atom energy levels E_n by small amounts.

(A) Assume the proton is a uniformly charged spherical <u>shell</u> of radius R_p. Show that the $n S_{1/2}$ state energies shift by: $\underline{\Delta E_n \simeq \frac{4}{3}(Z^2/n)[R_p/a_0]^2|E_n|}$, E_n = Bohr energy.

(B) What is ΔE_n of part (A) if the proton is a uniformly charged <u>sphere</u> of radius R_p?

(C) How big is ΔE_n (comparatively) for states with ∡ momentum $l > 0$?

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(32) The Stark Effect on the ground state of hydrogen perturbs the energy $E_0^{(0)}$ to $\mathcal{O}(\mathcal{E}^2)$ as: $E_0 = E_0^{(0)} - e^2 \mathcal{E}^2 S_z$, where: $S_z = \sum_{n>0} |\langle n|z|0\rangle|^2 / (E_n^{(0)} - E_0^{(0)})$, for a field $\vec{\mathcal{E}}$ along the z-axis. We showed in class that the sum was just: $S_z = -\langle 0|zF|0\rangle$, <u>if</u> a function F could be found such that: $\underline{z|0\rangle = [F, \mathcal{H}_0]|0\rangle}$, w/ $\mathcal{H}_0$ = unperturbed Hamiltonian. Assume: $F = (ma^2/\hbar^2)(\lambda\rho + \mu)z$, w/ $a = \hbar^2/me^2$, $\rho = r/a$, $z = r\cos\theta$, and λ & μ = numerical coefficients to be found. Find λ & μ by writing out the differential eqtn for F, and show: $\underline{F = -(ma/2\hbar^2)(r + 2a)z}$, as was used in class.

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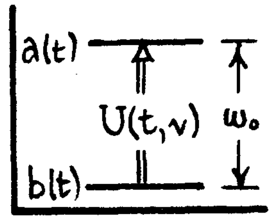
(33) [<u>Schmidt orthogonalization</u>]. Consider an N-fold set of eigenfcns $\{u_i\}$, $1 \leq i \leq N$, that are <u>degenerate</u> (each has same eigenenergy E: $\mathcal{H}u_i = Eu_i$), and <u>not</u> orthogonal: $\langle u_i|u_j\rangle \neq 0$. We want a set $\{v_k\}$, constructed from linear comb$^{\underline{n}}$s of the u_i, which <u>is</u> orthogonal.

(A) Start with $v_1 = u_1$. Set $v_2 = u_2 + a_{21} v_1$ and find a_{21} such that $\langle v_1|v_2\rangle = 0$. Next, set $v_3 = u_3 + a_{31} v_1 + a_{32} v_2$, and find a_{31} & a_{32} such that $\langle v_1|v_3\rangle = 0$ & $\langle v_2|v_3\rangle = 0$.

(B) Show by induction that the $n^{\underline{th}}$ member of the orthogonal set $\{v_k\}$ is, for $n > 1$: $\underline{v_n = u_n - \sum_{k=1}^{n-1} (\langle v_k|u_n\rangle / \langle v_k|v_k\rangle) v_k}$.

37 [20 pts]. Ref. class notes on tD Pert$^{\underline{b}}$n Theory, pp. tD 11-12. A two-level QM system (energy gap $\hbar\omega_0$) is subjected to a "chirped" coupling pulse $U(t,\nu) = \mathcal{E}(t)\, e^{-i[\nu - \theta(t)]t}$. The envelope $\mathcal{E}(t)$ has finite duration $\sim T$, and the main frequency $\nu \sim \omega_0$ drives transitions $b \to a$ as usual. What's new is that the "chirp" fcn $\theta(t)$ can modulate ν during the pulse.



(A) Find the spectral fcn δ corresponding to the rf carrier $e^{-i[\nu-\theta(t)]t}$ in the case where the chirp is : $\theta(t) = \Delta\nu \cdot \frac{t}{\tau}$, w/ $\Delta\nu$ (bandwidth) & τ (risetime) = cnsts. Show : $\underline{\delta(\omega) = (\alpha/\sqrt{\pi})\, e^{i\pi/4}\, e^{-i\alpha^2\omega^2}}$, and find α in terms of $\Delta\nu$ & τ. Show that δ becomes a Dirac delta fcn as $\alpha \to \infty$. What is the significance of this limit?

(B) If the envelope fcn is $\mathcal{E}(t) = \mathcal{E}_0\, e^{-(t/T)^2}$, find the transition amplitude $a(\Omega)$ for the chirp of part (A). $\Omega = \omega_0 - \nu$ is the detuning frequency.

(C) Analyse the transition lineshape, i.e. $|a(\Omega)|^2$ vs. Ω. Under what conditions on $\Delta\nu$, τ & T does the envelope dominate $|a(\Omega)|^2$? When does the chirp dominate?

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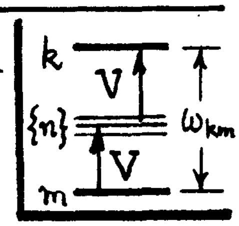
38 [20 pts.]. A pulsed harmonic perturbation $V(x,t) = 2\hbar\Omega(x)\cos\omega t$, over $0 \leq t \leq T$, drives QM transitions $m \to k$. In class [class notes p. tD6, Eq. (18)], we found the 1st order transition amplitude $a_k^{(1)}(t)$, which describes direct single-photon $m \to k$ processes. Here we analyse the 2nd order amplitude $a_k^{(2)}(t)$, describing two-photon processes : $m \to \{n\}$, $\{n\} \to k$, through a set of intermediate states $\{n\}$. To fix ideas, let the transition be absorptive, and let the driving frequency $\omega \sim \omega_0$, w/ $\omega_0 = \frac{1}{2}\omega_{km} > 0$ = half the resonant freq. Define the detuning as $\Delta\omega = \omega - \omega_0$.



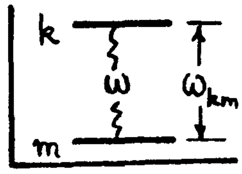
(A) Calculate the 2nd order amplitude $a_k^{(2)}(t)$ for the pulsed harmonic pert$^{\underline{b}}$n $V(x,t)$.

(B) Denote $\delta_{nm} = \omega - \omega_{nm}$. Show that the resonant parts of $a_k^{(2)}(t)$ contribute :

$$\boxed{a_k^{(2)}(t) \simeq \sum_n \frac{\Omega_{kn}\Omega_{nm}}{\delta_{nm}}\left[\frac{1-e^{-i(2\Delta\omega-\delta_{nm})t}}{2\Delta\omega-\delta_{nm}} - \frac{1-e^{-i(2\Delta\omega)t}}{2\Delta\omega}\right]}, \text{ for } m \to \{n\} \to k \ @\ \omega \simeq \frac{\omega_{km}}{2}.$$

(C) In $a_k^{(2)}(t)$ of part (B), we can have $\Delta\omega \to 0$ (by tuning) and $\delta_{nm} \to 0$ (by "accident"). Find the limiting forms of $a_k^{(2)}(t)$ for the following 3 cases : (I) $\delta_{nm} \to 0$, for some n, and $\Delta\omega \to 0$; (II) $\delta_{nm} \to 0$, for some n, but $\Delta\omega \neq 0$; (III) $\delta_{nm} \neq 0$, for any n, while $\Delta\omega \to 0$. Show that $a_k^{(2)}(t)$ is always finite, but its behavior depends critically on the δ_{nm}.

(39) [20 pts]. Consider a pulsed harmonic perturbation $V_{ij}(t) = 2\hbar\Omega_{ij}\cos\omega t$, applied at $t=0$ to a QM system, in the case where ω approaches an exact resonance for transitions $m \leftrightarrow k$, i.e. $\nu = (\omega_{km} - \omega) \to 0$. In class, we remarked [NOTES, p. tD6] that the first-order transition amplitude is $a_k^{(1)}(t) \simeq -i\Omega_{km} t$, and hence cannot be correct as $t \to$ large. Here we remedy that situation by solving a new version of the $m \to k$ transition problem very near resonance ($\nu \simeq 0$). We make an exactly solvable two-level problem out of $m \leftrightarrow k$.



(A) When $\nu = (\omega_{km} - \omega) \to 0$, basically only the states m & k participate in transitions, to good approximation. Show then that the "exact" eqtns for the amplitudes are: $\boxed{i\dot{a}_k = \Omega_{km}\, a_m\, e^{i\nu t}, \quad i\dot{a}_m = \Omega_{mk}\, a_k\, e^{-i\nu t}}$; the approximation is that all other states are so far off resonance they can be ignored. We have a two-level problem.

(B) The problem in part (A) can be solved exactly (assuming Ω_{km} is independent of t). Find $a_k(t)$, assuming the system was initially in state m: $a_m(0)=1$, $a_k(0)=0$. Define and use the quantity: $Q = [1 + (2|\Omega_{km}|/\nu)^2]^{1/2}$. Also find $a_m(t)$.

(C) Sketch the $m \to k$ transition probability $|a_k|^2$ vs. ν. Now what happens as $\nu \to 0$?

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(40) A QM state of nominal energy E_n which undergoes exponential decay at rate Γ_n is represented by a wavefcn: $\Psi_n(x,t) = [\phi_n(x)\, e^{-(i/\hbar)E_n t}]\, e^{-\frac{1}{2}\Gamma_n t}$; $|\Psi_n|^2 = |\phi_n|^2 e^{-\Gamma_n t}$ decays with a "lifetime" $\tau_n = 1/\Gamma_n$. Fourier transform $\Psi_n(x,t) \to \tilde{\Psi}_n(x,\omega)$ to a frequency variable $\omega = E/\hbar$. Then $|\tilde{\Psi}_n(x,E)|^2$ vs. E should give the spectrum of photon energies which can be emitted during the decay. Find and analyse this spectrum. Also, evaluate $\int_{-\infty}^{\infty} |\tilde{\Psi}(x,E)|^2 dE$. Why is this "interesting"?

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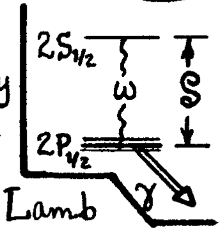
(41) A QM harmonic oscillator (1D, mass m & spring cnst k) is initially in its ground state, with (normalized) wavefcn: $\phi(x) = (\alpha/\pi)^{1/4} e^{-\frac{1}{2}\alpha x^2}$, w/ $\alpha = \sqrt{km}/\hbar$. The spring cnst is suddenly changed from k to Nk, w/ $N>0$ some numerical factor. Find the probability P_0 that the oscillator will remain in its (new) ground state. Calculate P_0 for $N=2$, and $N=\frac{1}{2}$. Over what range of N-values will P_0 be greater than 50%?



(42) [20 pts]. The $2S_{1/2}$ level in hydrogen is metastable (lifetime $\tau_{2S} \sim \frac{1}{7}$ sec for decay $2S \to 1S$ by two photons). The nearby $2P_{1/2}$ level decays rapidly: the lifetime for $2P \to 1S + Ly\alpha$ (1216 Å) is $\tau_{2P} = 1.6 \times 10^{-9}$ sec. The levels are separated by the Lamb Shift S (in circular freq. $S = 2\pi \times 1058$ MHz) and can be coupled by an rf electric field via $V = [e\mathbf{r}\cdot\mathbf{E}(t)]\cos\omega t$, at freq. $\omega \simeq S$. Since the next nearest level, $2P_{3/2}$, lies $\simeq 10^4$ MHz above $2S_{1/2}$, the $2S_{1/2}$–$2P_{1/2}$ coupling is well-represented by a two-level problem, viz.

$$\boxed{i\dot{S} = \Omega^*(t)\,P\,e^{i\nu t}, \quad i\dot{P} = \Omega(t)\,S\,e^{-i\nu t} - \tfrac{1}{2}i\gamma P}$$

w/ $\nu = (S - \omega)$, detuning frequency; $\gamma = 1/\tau_{2P}$, $2P \to 1S$ decay rate.

$S(t)$ & $P(t)$ are the $2S_{1/2}$ & $2P_{1/2}$ amplitudes, and $\Omega(t) = \frac{1}{2\hbar}\langle\phi_{2P}|\,e\mathbf{r}\cdot\mathbf{E}(t)\,|\phi_{2S}\rangle$ is the envelope of the E-field pulse. The term in γ is added phenomenologically, so that -- when the coupling $\Omega \to 0$ -- $2P_{1/2}$ decays naturally, according to: $|P(t)|^2 = |P(0)|^2 e^{-\gamma t}$.

(A) A sample of $2S_{1/2}$ atoms experiences a weak rf pulse $\Omega = $ cnst, over $0 \leq t \leq T$, w/ $\tau_{2P} \ll T \ll \tau_{2S}$. Solve the above two-level problem to find the fraction $|S(t>T)|^2$ of $2S_{1/2}$ atoms remaining after the pulse. Sketch $|S(\text{after})|^2$ vs. ω. What is the <u>width</u> of this resonance?

(B) What fractional resolution in the linewidth [part (A)] is needed to measure S to 100 ppm?

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(43) [20 pts]. The <u>time-dependent</u> Schrödinger Eq. can be solved by Green's fcns. At $t<0$, start with a known stationary system: $\mathcal{H} u_n(\mathbf{r}) = \omega_n u_n(\mathbf{r})$, w/ $\mathcal{H} = -\frac{1}{2m}\nabla^2 + V(\mathbf{r})$ [units: $\hbar = 1$]. At $t \geq 0$, add coupling $W = W(\mathbf{r},t)$, so $\mathcal{H} \to \mathcal{H} + W$, and consider the time-dept Schrodinger Eq: $\underline{(\mathcal{H} - i\frac{\partial}{\partial t})\psi = -W(\mathbf{r},t)\psi}$. Now <u>define</u> K via: $\underline{(\mathcal{H} - i\frac{\partial}{\partial t})K = -i\,\delta(\mathbf{r}-\mathbf{r}_0)\,\delta(t-t_0)}$, for $t > t_0$, and $K \equiv 0$ for $t < t_0$. $K = K(\mathbf{r},t;\mathbf{r}_0,t_0)$ is the Green's fcn for the problem.

(A) Show that: $\psi(\mathbf{r},t) = \phi(\mathbf{r},t) - i\int_0^{t+} dt_0 \int_\infty d^3x_0\, K(\mathbf{r},t;\mathbf{r}_0,t_0)\,W(\mathbf{r}_0,t_0)\,\psi(\mathbf{r}_0,t_0)$, where $\phi(\mathbf{r},t) = \int_\infty d^3x_0\, K(\mathbf{r},t;\mathbf{r}_0,0)\,\psi(\mathbf{r}_0,0)$, and $t+ = \lim_{\epsilon\to 0}(t+\epsilon)$.

(B) Verify that: $\underline{\underline{K(\mathbf{r},t;\mathbf{r}_0,t_0) = \theta(t-t_0)\sum_n u_n^*(\mathbf{r}_0)\,u_n(\mathbf{r})\,e^{-i\omega_n(t-t_0)}}}$, satisfies the equation which defines K. <u>NOTE</u>: the $\{u_n\}$ are assumed to be a complete set of eigenfcns.

(C) Specify the initial state of the system by: $\psi(\mathbf{r}_0,0) = \sum_k a_k u_k(\mathbf{r}_0)$, the $\{a_k\}$ = cnsts. With K of part (B), show that the first term in the solution for ψ in part (A) amounts to: $\underline{\underline{\phi(\mathbf{r},t) = \sum_n a_n u_n(\mathbf{r})\,e^{-i\omega_n t}}}$. Clearly, $\phi(\mathbf{r},t)$ is the evolution of the <u>unperturbed</u> state $\psi(\mathbf{r},0)$.

(D) Write down ψ of part (A) in the first Born Approxn. Discuss briefly how you would proceed to find ψ to terms higher order in W.

(44) Using the first Born approximation, find the differential and total scattering cross-sections for the central potentials: (A) $V(r) = V_0 e^{-\alpha r}$, (B) $V(r) = V_0 e^{-\alpha^2 r^2}$. With α held cnst, adjust V_0 so that each potential has the same "volume", i.e. so that $\int_0^\infty V(r) \cdot 4\pi r^2 dr = \Lambda$, cnst. Intercompare your results for $\frac{d\sigma}{d\Omega}$ & σ in parts (A) & (B).

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(45) [20 pts]. The Green's fcn K for the time-dependent Schrödinger Eq. in prob #(43), viz. $K(\mathbf{r},t;\mathbf{r}_0,t_0) = \theta(t-t_0)\sum_n u_n^*(\mathbf{r}_0)u_n(\mathbf{r})e^{-i\omega_n(t-t_0)}$ is hard to evaluate explicitly. Here we reformulate the "scattering problem" [i.e. how $\psi(\mathbf{r},t)$ evolves from some initial state $\psi(\mathbf{r}_0,0)$ by repeated interactions with a potential V] in terms of K_0, the Green's fcn for a free particle, which can be handled. As a compact notation, let $\xi = (x,t)$ stand for a space-time point ($x = x$ in 1D, $x = \mathbf{r}$ in 3D, etc.). Let $\hbar = 1$, and write $\mathcal{H}_0 = -(1/2m)\partial^2/\partial x^2$ for the free-particle Hamiltonian. The free-particle Green's fcn is then defined (1): $(i\frac{\partial}{\partial t} - \mathcal{H}_0)K_0(\xi,\xi') = i\,\delta(\xi-\xi')$, for $t > t'$, and zero otherwise. The Schrödinger Eq. (2): $(i\frac{\partial}{\partial t} - \mathcal{H}_0)\psi(\xi) = U(\xi)\psi(\xi)$, where now $U(\xi)$ now contains all interactions [$U(\xi) = V(\mathbf{r})$\{binding\} + $W(\xi)$\{coupling\}, W on @ $t=0$].

(A) Show that Eqs. (1) & (2) together give the usual integral equation for ψ, i.e. $\underline{\psi(\xi) = \phi(\xi) - i\int d\xi' K_0(\xi,\xi')U(\xi')\psi(\xi')}$. Here $\phi(\xi) = \int d^3x_0\, K_0(\mathbf{r},t;\mathbf{r}_0,0)\psi(\mathbf{r}_0,0)$ is the initial state, and $\int d\xi' = \int_0^{t+} dt' \int_\infty dx'$. We could reference ϕ to $t' = (-)\infty$ [when free].

(B) Now construct K_0. Use above bound-state K, with $u_n(x) \rightarrow (1/\sqrt{2\pi})e^{ikx}$ for a free particle with energy $\omega_n \rightarrow k^2/2m$ in 1D [delta-fcn norm for the plane waves]. Show, when $\sum_n \rightarrow \int_{-\infty}^{+\infty} dk$, that: $K_0(\xi,\xi') = \frac{1}{2\pi}\int_{-\infty}^{+\infty} dk \exp[ik(x-x') - i\frac{k^2}{2m}(t-t')]$. By judicious choice of a convergence factor, evaluate this integral, and show that in 1D: $K_0(\xi,\xi') = \left(\frac{m/2\pi i}{t-t'}\right)^{1/2}\exp\left[\frac{im}{2}(x-x')^2/(t-t')\right]$. What would K_0 be in 3D? Sketch a graph of how K_0(1D) evolves in space & time.

(C) Briefly discuss the sucessive (Born-type) iterations to the $\psi(\xi)$ integral equation in part (A). The resultant perturbation series is the Feynman-Hellman approach to QM.