- ① In a QM system with Hamiltonian Hb, let the ligenfons & ligenenergies be  $\Psi_n \in E_n$ , so: Hb $\Psi_n = E_n \Psi_n$ . To approximate the ground state energy  $E_0$ , suppose you use a trial fon:  $\Psi = \Psi_0 + \lambda \Phi$ ,  $\Psi_0 = a$  actual ground state ligenfon,  $\lambda = small$  (real) parameter, and  $\Phi = an$  arbitrary fon 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  $\lambda$ ,  $Viz_0$ ::  $E(\lambda) = E_0 + \lambda E_1 + \lambda^2 E_2 + \lambda^3 E_3 + \cdots$ , then  $E_1 = 0$ , while  $E_2$  is the positive quantity:  $E_2 = \sum_n |C_n|^2 (E_n E_0)$ . NOTE: this result  $\Rightarrow$  that any perturbation on  $\mathcal{H}_0$  which shifts  $\Psi_0 \to \Psi_0 + \lambda \Phi$  by a term  $\frac{15t}{n}$  order in some small parameter  $\lambda$ , can only shift the ground state energy  $E_0 \to E_0 + \lambda^2 E_2$  by a term  $\frac{2nd}{n}$  order in  $\lambda$ .
- ② On p.2 of "Notes on the WKB Method", it is claimed that any  $2^{nd}$  order homogeneous ODE of the form: y'' + f(x)y' + g(x)y = 0, can be cast into the WKB form:  $y'' + k^2(x)\psi = 0$ , if  $y(x) = y(x) \exp\left[+\frac{1}{2}\int_{1}^{\infty}f(\xi)d\xi\right]$ , and  $y(x) = \frac{1}{2}\left[f'(x) + \frac{1}{2}f^2(x)\right]^{1/2}$ . Verify this claim by substituting  $y(x) = \psi(x)u(x)$  into the original ODE and then choosing u(x) indictionsly. Why is the lower limit a in the integral  $\int_{1}^{\infty}f(\xi)d\xi$  essentially arbitrary?
- 3 Bessel's ODE is:  $y'' + \frac{1}{x}y' + (1 \frac{v^2}{x^2})y = 0$ , v = real const. Find an approximate solution for the Bessel for  $y = J_v(x)$  by the WKB method. Then find an asymptotic form for  $J_v(x)$  as  $x \to "large"$  (i.e. x >> |v|). You may assume  $|v| >> \frac{v}{2}$ .
- This exercise is connected with the WKB "turning point" problem. (A) Show--by substitution-- that a solution to:  $y''(\xi) + \alpha \xi^n y(\xi) = 0$ ,  $y''(\xi) + \alpha \xi^n y(\xi) = 0$ ,  $y''(\xi) + \alpha \xi^n y(\xi) = 0$ ,  $y''(\xi) + \alpha \xi^n y(\xi) = 0$ , is given by:  $y(\xi) = AJ\xi J_v(\xi)$ ,  $y''(\xi) + \alpha \xi^n y(\xi) = 1/(n+2)$ ,  $\xi = (\frac{2J\alpha}{n+2})\xi^{\frac{1}{2}(n+2)}$ , and  $J_v(\xi)$  is the Bessel for of order v.(B) Assume an asymptotic form:  $y(\xi) \sim \xi^{-k}e^{-a\xi^{k}}$ , as  $\xi \to \infty$ . By properly choosing the costs  $k, l \notin a$ , show that as  $\xi \to \infty$  this form satisfies the ODE:  $y''(\xi) + \alpha \xi^n y(\xi) = \frac{n}{4}(\frac{n}{4}+1)\xi^{-2}y(\xi) \to 0$ .

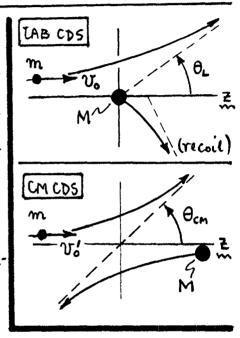
- DLet the Hamiltonian H=46+V, where Ho is a free-particle Hamiltonian, and V accounts for all interactions. Let ξ be the space-time point (x,t). The Schrödinger Eq. is: (it \frac{\particle}{\particle} \frac{\particle}{\particle})\psi(\xeta') = \frac{\particle}{\particle} \particle \text{V(ξ')\psi(\xeta')}. pacts as a source for for the otherwise free propagation of \psi. Now let Go(\xeta',\xeta) be the free-particle Green's for which satisfies the point-source extraction: (it \frac{\particle}{\particle} \frac{\particle}{\particle})\frac{\particle}{\particle} \text{Show that the general solution to the S. Extraction is: \frac{\particle}{\particle} = \particle \left(\xeta') \right(\xeta') \right) \frac{\particle}{\particle} \right) \text{V(\xeta')} + \int \frac{\particle}{\particle} \right) \right(\xeta') \right(\xeta') \right) \frac{\particle}{\particle} \right) \right) \right) \frac{\particle}{\particle} \right) \right) \right) \frac{\particle}{\particle} \right) \right) \right) \frac{\particle}{\particle} \right) \right)
- Det h=1. Consider a Schrödinger system with known eigenfons  $u_n(r)$  and eigenvalues  $w_n$  [generated as usual by  $y_0u_n=w_nu_n$ ]. In class, we claimed the Green's fon for this system was:  $G(r,t;r_0,t_0)=-i\,\theta(t-t_0)\sum u_n^*(r_0)u_n(r)e^{-i\,\omega_n(t-t_0)}$ ,  $u_n^*(r_0)u_n(r_0)e^{-i\,\omega_n(t-t_0)}$ ,  $u_n^*(r_0)u_n(r_0)e^{-i\,\omega_n(t-t_0)$

Interpret the motion of 4 physically le.g. draw pictures 1. What happens if 8 > 0?

BThis tidbit of complex variable arcana will be used in problem B. By evaluating an appropriate contonr integral in the complex  $\omega$ -plane, show that the unit step for can be represented by:  $\frac{|\theta(\tau)|^2}{|\theta(\tau)|^2} = \lim_{\epsilon \to 0+} \left(\frac{i}{2\pi}\right) \int_{-\infty}^{\infty} \frac{e^{-i\omega \tau} d\omega}{\omega + i\epsilon} = \begin{cases} 1, \text{ for } \tau > 0 \\ 0, \text{ for } \tau < 0 \end{cases}$  Yather than O+, show that the integral generates  $\theta(\tau) - 1$ , the often popular out-of-step fon. From the form for  $\theta(\tau)$ , what is the integral for the Dirac delta,  $\theta(\tau)$ ?

(F) A QM system consists of two particles, W masses  $m_1 \leqslant m_2$ . Express the operators for total momentum  $\hat{P} = \hat{p}_1 + \hat{p}_2$ , and total  $\chi$  momentum  $\hat{L} = \hat{L}_1 + \hat{L}_2$ , in terms of the relative cd.  $r = r_1 - r_2$  and center-of-mass cd.  $R = (m_1 r_1 + m_2 r_2)/(m_1 + m_2)$ . Show that the K. E, part of the Hamiltonian, vi3.  $\hat{K} = \frac{1}{2m_1} \hat{p}_1^2 + \frac{1}{2m_2} \hat{p}_2^2$ , can be put in the form:  $\hat{K} = -(h^2/2M) \nabla_R^2 - (h^2/2\mu) \nabla_r^2$ ,  $\frac{1}{2} M = (m_1 + m_2) \leqslant \mu = m_1 m_2/(m_1 + m_2)$ .

(18) [15 pts]. Most 2-body scattering events [M m (projectile) incident on M (twget)] are described in terms of the scattering & Ocm in the center-of-mass (CM) system. When m/M is finite, Ocm is generally & OL, the actual scattering & of m in the lab (L) system, because of M's recoil. Here we wish to relate OL to Ocm for a classical elastic scattering event. Assume that M is initially at rest on the Z-axis in lab, and m is incident at velocity voll Z-axis. Assume axial symmetry.



(A) After finding the CM velocity w. n.t. lab, and m's final velocity in CM (for an elastic event), Show that:  $tan \theta_L = sin \theta_{cm}/[cos \theta_{cm} + (m/M)]$ , is the required velotion. Evidently  $\theta_L \simeq \theta_{cm}$  when  $m \ll M$ . What is the relation when m = M? (B) If  $\frac{d\sigma}{d\Omega}$  is the differential scattering cross-section (#particles m scattered into solid  $\Delta \Omega = 2\pi \sin \theta d\theta$ , per  $d\Omega$ ), Show:  $\frac{(d\sigma/d\Omega)_L = (d\sigma/d\Omega)_{cm} \frac{d\cos \theta_{cm}}{d\cos \theta_L}}{d\cos \theta_L}$ . What does this relation reduce to when m = M? What is the maxm.  $\theta_L$  in this case?

<sup>19 [15</sup>pts]. Use the Born approx- to find the total cross section for an elastic Scattering by a spherical well: \(\formall \tau \) (r) = (-) \(\nabla\_0, r < a; \nabla\_1 \tau \) (r) = 0, \(\gamma > a, \text{NOTE}: \) it is handy to verify and use Eq. (31), \(\rho\_0, \text{ScT13}, \text{ of class notes -- following from Eq. (14), \(\rho\_0, \text{ScT7}, \text{ for elastic & spherically symmetric events. Find limiting forms for \(\sigma \text{lk}\)) for low energies [ka << 1] and high energies [ka >> 1].

- ② In  $prob^{m}$  ③, the Born Approxn (BA) provided cross-sections for scattering from a spherical well:  $V(r)=(-)V_0$ , r<a; V(r)=0, r>a. Evaluate the <u>validity</u> of the BA in this case, per class notes p. ScT 10, Eq.(22). Show that the BA can hold down to ~ zero incident energy, if the well is shallow enough. Discuss the shallowness condition on  $V_0$  w. p. t. formation of possible bound states in the well.
- 2 [15pts.]. Using the Born Approxn, find both the differential and total scattering cross-sections for the central potentials: (A)  $V(r) = V_0 e^{-\alpha r}$ , (B)  $V(r) = V_0 e^{-\alpha r}$ , Wa & Vo = enst. Now, with the range parameter a held the same for each V(r), adjust the amplitudes Vo so that each potential has the same "volume", i.e. so that:  $\int_0^\infty V(r) \cdot 4\pi r^2 dr = \Lambda = cnst$ . Finally, with this adjustment, intercompare and comment on the results for the V(r)'s in (A) & (B).
- (2) [15 pts]. Consider the scattering of an electron from a stationary charge distribution  $\rho(\theta)$  which generates a potential  $\phi$  per Poisson's egtn:  $\nabla^2 \phi = -4\pi \rho$ .
- (A) The scattering potential is  $V = -e\phi$ . Show that in Born Approx<sup>2</sup>, the differential cross-section is:  $\frac{d\sigma}{d\Omega} = |\frac{2me}{\hbar^2q^2}|\int \rho(\mathbf{r})e^{i\mathbf{q}\cdot\mathbf{r}}d^3x|^2 w/q = k_{before} k_{after}$ .
- (B) Let p(r) be due to an atomic ion W nucleus of charge Ze and N electrons distributed per their wavefens  $\Psi_{k}$ , i.e.  $\underline{p(r)} = \underline{Ze8(r)} \underline{e} \underbrace{\sum |\Psi_{k}(r)|^{2}}$ . The atom is randomly oriented, so only the radial dependence of  $\Psi_{k}$  is kept; the norm is  $\underbrace{\int |\Psi_{k}(r)|^{2}} + 4\pi r^{2} dr = 1$ . Show that  $d\sigma/d\Omega$  of part (A) can be written:  $\underline{d\sigma/d\Omega} = (4/a_{\sigma}^{2}q^{4})|Z-F(q)|^{2}$ ,  $\frac{2\pi}{2}$  and  $\frac{2\pi}{2}$ . F(q) is the "form factor" for the atomic electrons. Find F(q) and reduce it to a radial integral.
- (C) Evaluate Flq) for the single electron in the ground state of the FI-atom [i.e. for  $V(r) = (1/\sqrt{\pi a_0^2}) e^{-r/a_0}$ ]. Then, write down the cross-section (do/do2), and compare it with Sakurai's result ["Modern QM" (Mesley, 1985), p.448].

- ② In problem②, you showed that for an electron scattering from a charge distribution  $\rho(\mathbf{r})$ , the <u>transform</u> of the scattering potential important for the Born Approx<sup>2</sup> was:  $\tilde{V}(q) = -(4\pi e/q^2) \int \rho(\mathbf{r}) e^{iq\cdot \mathbf{r}} d^3x$ ,  $^{1/2}q = k(before) k(after)$ , the momentum transfer.
- (A) Put:  $\rho(r) = e8(r) e14(r)1^2$ , for e-scattering from a newhal H-atom, with the [10pts]. bound electron in a spherically symmetric eigenstate  $\Psi(r)$ . By inverting the transform  $\tilde{V}(q_1)$ , first show that the actual scattering potential can be written as:  $V(r) = -e^2\left[\frac{1}{r} \int \frac{d^3x'}{|r-r'|}|\Psi(r')|^2\right]$ . Interpret. Then, for the H-atom ground state:  $\Psi(r') = (1/\sqrt{\pi a_0^3})e^{-r'/a_0}$ ,  $\Psi(r') = (1/\sqrt{\pi a_0^3})e^{-r'/a_0}$ ,  $\Psi(r') = \frac{e^2}{a_0}(1+\frac{1}{\rho})e^{-2\rho}$ ,  $\Psi(r') =$
- (B) For the V(r) in part (A), evaluate the Born Approx<sup>2</sup> "validity criterion" (see class:  $\frac{10 \, \mathrm{pts.1}}{\mathrm{Eg.(22)}}$ ,  $\frac{1}{\mathrm{Eg.(22)}}$ ,  $\frac{1}{\mathrm{Eg.(22)}}$ ,  $\frac{1}{\mathrm{Eg.(22)}}$ . It is convenient to use the dimensionless energy parameter  $\frac{\lambda}{2} = \frac{k^2 a^2}{\mathrm{Eg.(22)}} = \frac{E}{\mathrm{Eh.(E=e^2/2a_0=H-atomionization)}}$ . Show that the Born Approxing fails at low energies,  $\lambda \to 0$ . Estimate a lower bound for  $\lambda$ , above which the Born Approxing  $\lambda \to 0$ .
- (C) Assume Sakurai's version of the <u>differential</u> cross-section for e→ H-atom scattering [10 pts]. (as quoted in prob. 22) is correct:  $\frac{d\sigma}{d\Omega} = (4a_o^2/Q^4)[1-16/(Q^2+4)^2]^2$ ,  $^{10}Q = qa_o$ ,  $^{10}Q =$ 
  - Consider scattering of an electron from a screened Coulomb potential:  $\frac{V(r) = -(2e^2/r)e^{-\alpha r}}{(2e^2/r)e^{-\alpha r}}, \text{ by means of partial wave analysis. Using Eq. (32),}$  b. PW9 of class notes, show that the  $l^{th}$  partial wave phase shift Se(k) is given by:  $\frac{2}{\tan 3e(k)} = \frac{2}{ka_0} Qe(1 + \frac{\alpha^2}{2k^2}), ^{35} a_0 = t^2/me^2, k = \sqrt{2mE/t^2}, and Qe(2) = \text{Legendre fen of } 2^{nd} \text{ kind. White } \tan 3e(k) = \text{explicitly, and find its limit for } k \to \infty \neq \alpha > 0.$  What happens to the analysis when  $\alpha \to 0$ ?

- ②[15 pts.] Phase shift analysis for hard-core scattering (notes, pp. PW 10-12) requires knowing the radial wavefor logarithmic derivative Rikela)/Rkela) at the cutoff r=a of the scattering potential. Consider the <u>dimensionless</u> logarithmic derivative: βe(k) = a Rkela)/Rkela). We wish to find how βe(k) depends on energy.
- (A) For a given x momentum l, consider two closely spaced energies:  $E_1 & E_2 = E_1 + \Delta E$ . If  $R_1 = R_{k,l}(r) & R_2 = R_{k,l}(r)$  are the corresponding interior radial wavefens, show that:  $\frac{d}{dr} \left[ r^2 (R_1 R_2' R_2 R_1') \right] + \frac{2m}{k^2} (E_2 E_1) r^2 R_1 R_2 = 0$ . [HINT: write the radial egths for  $R_1 & R_2$  from  $E_2(26)$ , p. PW 8. Recall:  $k^2 = 2mE/t^2$ . Then, think Green].

  (B) Intervals the identity in part (A) over  $0 \le r \le a$  to find an expression for  $\Delta B_1 / \Delta E = a$ .
- (B) Integrate the identity in part (A) over 0≤r≤a to find an expression for Δβ2/ΔE=
  [β2(k2)-β2(k1)]/(E2-E1). Pass to the limit k2→k1=k to derive the expression:

  Δβ2(k)/dE = -(2m/t²a) [[rRk2(r)/Rk2(a)]²dr. So, how does β2(k) vary \*/ Ε?
- (26) Find the exchange splitting of an energy level in a system of two electrons, by regarding the e-e interaction  $V(r_1-r_2)$  as a perturbation on the main electron binding terms. Use appropriate symmetrized wavefins for the electrons.
- (B) Show that the exchange-dependent terms in part (A) can be represented w.n.t. non-Symmetrized electron spin states (i.e. product states) as eigenvalues of the exchange operator:  $\frac{V_{ex} = -\frac{K}{2}(1+4\sigma_1.\sigma_2)}{1+4\sigma_2.\sigma_2}$ . Here, K is the exchange integral from part (A), and  $\sigma_1$  and  $\sigma_2$  are the (dimensionless) spin operators for electrons #1 \frac{4}{2}.
- \$\emptyseta [15 \text{pts.}]\$. Employ  $a_0 = \frac{\hbar^2}{me^2} (Bohr)$  as a length unit, and  $E_0 = \frac{e^2}{a_0} (2x Hatom)$  as an energy unit. Using the Thomas-Fermi model, estimate the average size of the following quantities [what's interesting is the scaling with Z]: (A) distance of an electron from the nucleus, (B) Co whomb interaction energy between two electrons, (C) kinetic energy of an electron, (D) energy needed to ionize the atom completely, (E) velocity of an electron in the atom, (F) angular momentum of an electron, (G) radial quantum number of an electron.

- [39] [15 pts]. In the Thomas-Fermi atom, the total e-e repulsion energy can be written:  $\frac{\text{Eee} = \frac{1}{2} \int U_e(r) \, n(r) \, dV}{\text{Ve}(r) = \text{potential energy of one e in the presence of the the other e's, and <math>n(r) = \text{number density of electron states} [n \text{ replaces the } p \text{ in Eq. } (39), p. ip 17, notes]. In turn: <math>U_e(r) = U(r) + \frac{Ze^2}{r}$ , W U(r) the full T-F potential [U(r) is (-) ve]; the nuclear attraction  $(-Ze^2/r)$  has been subtracted out.
- (A) Show that : Eee = \frac{1}{2} \text{Een} \frac{5}{6} \text{Ke}, \text{ \text{\text{Ke}} is the total electron-nuclear binding energy, and Ke is the total electronic kinetic energy.
- (B) Use the Virial Theorem for the Contomb field to show:  $\boxed{\text{Eee} = -\frac{1}{7}\text{Een}}$ . Thus, in the T-F atom, the e-e repulsion is relatively small compared to the binding.
- ② [25 pts]. In the ground state of a two-electron atom, both e's are in 1s orbitals ( $^{14}$  one spin up and the other down  $\Rightarrow$  spin singlet). If we neglect magnetic interactions, the system Hamiltonian is:  $\frac{16}{2} = -\frac{\hbar^2}{2m}(\nabla_i^2 + \nabla_z^2) 2e^2(\frac{1}{71} + \frac{1}{72}) + e^2/r_{12}$ ,  $^{14}$   $^{15}$   $^{15}$  the nuclear charge and  $^{17}$  the relative cd. If we neglect the e-e repulsion term, the problem reduces to each e moving separately in a Coulomb field  $-2e^2/r$ ; then for each e the energy is  $-\frac{1}{2}$   $\frac{1}{2}$   $\frac{1}{2}$
- (A) Use a trial waveform of form:  $\frac{\psi_{1,2}}{=N\exp\left[-\frac{\xi}{a_0}\left[r_1+r_2\right]\right]}$ ,  $\frac{W}{}$  5 a variational parameter. Adjust the norm const N so that:  $\int d^3x_1 \int d^3x_2 \left|\psi_{1,2}\right|^2 = 1$ .
- (B) Calculate the energy: E(3) = (4/16/4). The K.E. & P.E. integrals here are easy. Deal with the e-e repulsion term by expanding 1/2 via the Spherical Harmonic Addition Theorem [e.g. Jackson, Sec. 3.6]. Show: \( \int \delta^3 x\_1 \int \delta^3 x\_2 \right) \frac{1}{72} = \frac{5}{8} \int 1/20.
- (C) Minimize E(5) w.r.t.  $\zeta$  and find Emin. Ap- I(Z) H- He I(Z) Be<sup>2+</sup> B<sup>3+</sup> proximate the first ionization potential of the I(Z) 0.055 1.807 5.559 11.311 19.063 atom by:  $I(Z) = -E_{min} \frac{1}{2} \frac{Z^2 e^2}{a_0}$ . Calculate I(Z) in Rydbergs (i.e. energy units

of e<sup>2</sup>/2ao = 13.6 eV), and compare with the experimental values given in the box.

(D) Do your I(Z)'s agree 4 R.T. Robiscoe, Am. J. Phys. 43, 538 (1975)? Why not?

- 3) [15 pts]. The Dirac gamma matrices obey:  $\{Y_{\mu}, Y_{\nu}\} = Y_{\mu}Y_{\nu} + Y_{\nu}Y_{\mu} = 2S_{\mu\nu}, {}^{M}_{\mu}\mu\xi$  V=1,2,3,4. Assume that the  $\chi^{ls}$  are Hermitian, and show that their eigenvalues are at most  $\pm 1$ . Next, show that each  $Y_{\mu}$  has zero trace  $\{T_{\nu}Y_{\mu}=0\}$ ... what does this imply about (a) the number of  $\pm 1$  vs.  $\pm 1$  eigenvalues? (b) the allowed rank of the  $\chi^{ls}$ ? What is the <u>lowest</u> rank of a set of four  $\chi^{ls}$  which satisfy  $\{Y_{\mu}, Y_{\nu}\} = 2S_{\mu\nu}$ ?
- 38 In an external EM field with 4-potential  $A_{\mu} = (A, i\phi)$ , the Dirac Eqtr for a particle of charge  $q \notin mass m$  is:  $[\partial/\partial x_{\mu} i(q/kc)A_{\mu}] \gamma_{\mu} \psi + (mc/k) \psi = 0$ . Show trust for the adjoint wavefor  $\overline{\Psi} = \psi^{\dagger} \gamma_{4}$ , the eqtr is:  $[\partial/\partial x_{\mu} + i(q/kc)A_{\mu}] \overline{\psi} \gamma_{\mu} (mc/k) \overline{\psi} = 0$ . Now, in the usual fashim, derive a continuity equation  $\partial J_{\mu}/\partial x_{\mu} = 0$ , for a Dirac probability 4-current in the presence of  $A_{\mu}$  (HINT: multiply the adjoint eqtr on the right by  $\Psi$ , the original extr on the left by  $\Psi^{\dagger}$ , and combine). How does the present form for  $J_{\mu}$  compare with the current for a free particle?
- 39 Start from the Dirac Eqtn in an external EM potential Aµ as stated in problem #38. Confirm that the eqtn can be written in Hamiltonian form as 1  $\frac{i + \partial \Psi}{\partial t} = \frac{4}{5} \frac{4}{5$ 
  - By treating pp as a real eigenvalue, show that if 4 satisfies the egth for operator 36 (+q,+p), then the charge conjugate wavefor  $V_c = \gamma_2 V^*$  satisfies the egth for operator  $H_c = \gamma_1 V^*$ . Thus, charge conjugation reverses the sign of q and p.
- 40 [15 pts]. For a free Dirac particle, we have suggested that  $V_k = c\alpha_k$  is the velocity operator. If so, we could define a momentum operator by:  $b_k = mV_k = imc\beta\gamma_k$  (we've used  $\alpha_k = i\beta\gamma_k$ ). The value of  $\beta_k$  in state  $\psi$  is then the expectation value of  $imc\Psi\gamma_k\psi$ , W  $\Psi = \Psi^{\dagger}\beta$ . Calculate this quantity for the charge conjugate wavefor  $\Psi_c = \gamma_2 \Psi^*$ . Can you show:  $imc\Psi_c \gamma_k \Psi_c = (-) imc\Psi\gamma_k \Psi$ , as one would expect for this quantity? Comment on: (a) What works for a definition of  $\langle \beta_k \rangle$ ? (b) can  $V_k = c\alpha_k$  be a constant of the motion for a free particle?