ϕ507 MidTerm Preview

Tues. 3/14/95

The ϕ507 MidTerm will be given 7-9 PM on Mon. 3/20/95 in AJM 230. There will be no class lecture on that day.

The exam will be open-book, open-notes, and will consist of 5 problems worth 200 pts. total. Material covered is that in Secs. (1)-(5) of the Xerox notes for QM 507 (viz. Time-Dept. Perturbation Theory → QM Scattering Theory: Standard Approach). The problem areas are:

1. Transitions in an atom undergoing nuclear decay.
2. Radial distance scales in a one-electron atom.
3. The QM nature of $\mathbb{P}\cdot\mathbb{Q}$ as a rotational invariant.
4. The Schrödinger limit of a Klein-Gordon planewave.
5. Scattering, via 1st Born Approximation, for a very simple potential.

You may bring to the exam:

1. One QM text of your choice;
2. Your copy of ϕ507 CLASS NOTES & copies of Problems & Solutions;
3. A math reference table (or chair), calculator, and dictionary.

Good luck in your studies. The hints are pretty good, this time.

Dick Robiscoe

This exam is open-book, open-notes, and is worth 200 points total. For each of the 5 problems, $\boxed{\text{box}}$ the answer on your solution sheet. $\boxed{\text{Number}}$ your solution pages in sequence, put your $\boxed{\text{name}}$ on p.1, and $\boxed{\text{staple}}$ the pages before handing in.

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① [40 pts]. Atomic tritium, ${}^3H_1$, is an isotope of hydrogen where the nucleus undergoes spontaneous β-decay: ${}^3H_1 \to {}^3He_2 + e + \bar{\nu}$, i.e. the atomic nucleus changes from $Z=1$ to $Z=2$ upon ejecting an electron. The energy of the ejected electron is typically ~ 10 keV, so it leaves the atom "quickly." A question of interest is: in what state will we find the He^+ ion that is left behind?

(A) If the initial tritium atom is in its ground state ($n=1$), find the probability that the final He^+ ion is also in its ground state. HINT: the ground state wavefcn for a one-electron atom is: $\psi(r) \propto e^{-\kappa r}$, w/ $\kappa = Z/a_0$ & $a_0 = \hbar^2/me^2$.

(B) Why does the calculation in part (A) qualify for use of the sudden approximation?

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② [40 pts]. For a one-electron atom in its ground state (use $\psi(r)$ per HINT in ①):

(A) Evaluate the average value of the N^{th} power of the radius r, i.e. find $\langle r^N \rangle$ for N = integer ($N = 0, \pm 1, \pm 2$, etc.). Are there any restrictions on N?

(B) The "most probable" value of r is said to be $r_{mp} = a_0/Z$. Comment on how r_{mp} relates to any of the $\langle r^N \rangle$. How does r_{mp} qualify as a "most probable" r?

(C) Calculate the QM variance of r, i.e. $\Delta r = [\langle r^2 \rangle - \langle r \rangle^2]^{1/2}$. Compare this uncertainty in r with $\langle r \rangle$, or r_{mp}. Why is Δr so big?

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③ [40 pts]. Vector operators $\mathbb{A}$ & $\mathbb{B}$ are $\mathbb{T}$-vectors w.r.t. a QM ∡ momentum operator $\mathbb{J}$, i.e. they satisfy the commutators: $[J_\alpha, A_\beta] = i\hbar\, \epsilon_{\alpha\beta\gamma} A_\gamma$, and likewise for $\mathbb{B}$. $\mathbb{A}$ & $\mathbb{B}$ need not be commuting operators.

(A) For the scalar product, show that: $[\mathbb{J}, \mathbb{A}\cdot\mathbb{B}] \equiv 0$.

(B) On the strength of $[\mathbb{J}, \mathbb{A}\cdot\mathbb{B}] \equiv 0$, one refers to $\mathbb{A}\cdot\mathbb{B}$ as a "scalar invariant" under coordinate transformations. What does this reference mean?

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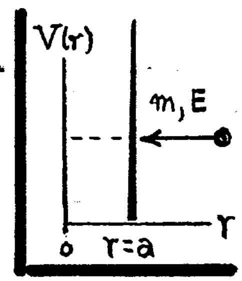
④ [40 pts.]. Let $\psi(\mathbf{r},t)$ be a solution to the free-particle Klein-Gordon equation for a particle of mass m, i.e. suppose that ψ satisfies

$$\left[\nabla^2 - \frac{1}{c^2}\frac{\partial^2}{\partial t^2} - (mc/\hbar)^2\right]\psi(\mathbf{r},t) = 0.$$

Transform this eqtn to a new wavefcn ϕ via: $\psi(\mathbf{r},t) = \phi(\mathbf{r},t)\, e^{-\frac{i}{\hbar}mc^2 t}$. What condition must you impose so that -- to good approximation -- ϕ will satisfy the nonrelativistic Schrödinger equation? If the original ψ is a simple plane wave solution, find a condition on the particle's energy such that ϕ (KG eqtn) is also a fairly reliable ϕ (Schröd^{r} eqtn).



⑤ [40 pts.]. A particle of mass m and energy E is incident on a hard spherical shell of radius a, whose center is fixed at the origin. The shell's scattering potential is taken to be: $V(r) = V_0\, a\, \delta(r-a)$, w/ V_0 & a = (+)ve constants, $r \geq 0$ the radial coordinate, and δ is the Dirac delta fcn. Analyse the scattering by the first Born Approximation.

(A) What condition on V_0 (and a) ensures that the Born Approximation is valid at all incident energies E? Assume this condition prevails in what follows.

(B) Find the differential scattering cross-section $(d\sigma/d\Omega)$ as a fcn of momentum transfer: $q = 2k\sin(\theta/2)$, w/ $k = \sqrt{2mE/\hbar^2}$ the wavenumber, and θ the (colatitude) scattering angle. Sketch $(d\sigma/d\Omega)$ vs. q over the allowed range of q. NOTE: $(d\sigma/d\Omega)$ vanishes at certain q-values. What physics is at work?

(C) Express the total scattering cross-section $\sigma = \int_{4\pi}(d\sigma/d\Omega)\,d\Omega$ as an integral over q (not Ω). The integral is not elementary. But find the leading terms in σ, including the E-dependence, in the low energy limit. HINT: prove and use the identity: $d\Omega = 2\pi\sin\theta\, d\theta = (2\pi/k^2)\, q\, dq$.

ϕ507 MidTerm Solutions (1995)

① [40pts.]. Atomic tritium decay: ${}^3H_1 \rightarrow {}^3He_2 + e + \bar{\nu}$; prob$^{\underline{y}}$ of He^+ ground state.

To set up the calculation, answer part (B) first.

(B) The electron bound in ${}^3H$; has an energy ~ 10 eV (13.6 eV to be precise) while the ejected electron travels away with $\sim 1000\times$ that energy... so the ejected electron is moving $\sim 30\times$ as fast as the orbiting electron, and it will leave the atom in a small fraction ($\sim 3\%$) of an orbital period. So the $Z=1\rightarrow 2$ perturbation takes place on a time scale much faster than that of $\mathcal{H}({}^3H_1)$; this qualifies us to use the "sudden approx$^{\underline{n}}$" ($\genfrac{}{}{0pt}{}{\text{CLASS}}{\text{NOTES}}$ p. tD 19) for transitions.

(A) Normalize the wavefcn: $\psi(r) = \mathcal{N}e^{-\kappa r}$, $\kappa = Z/a_0$:

$$\rightarrow \int_0^\infty |\psi(r)|^2 \cdot 4\pi r^2 dr = 4\pi \mathcal{N}^2 \int_0^\infty r^2 e^{-2\kappa r} dr = 4\pi \mathcal{N}^2 \cdot \frac{2!}{(2\kappa)^3} = 1,$$

so// $\mathcal{N} = (\kappa^3/\pi)^{1/2}$, and $\psi(r) = \mathcal{N}e^{-\kappa r}$ is normalized. (1)

To estimate that both initial & final states are ground states when $Z=1\rightarrow 2$, we need the overlap integral $\langle \psi_2 | \psi_1 \rangle$ i.e.

$$\rightarrow \langle \psi_Z | \psi_1 \rangle = \int_0^\infty \psi_Z^* \psi_1 \cdot 4\pi r^2 dr = 4\pi \left(\frac{Z^3}{\pi a_0^3}\right)^{\frac{1}{2}} \cdot \left(\frac{1}{\pi a_0^3}\right)^{\frac{1}{2}} \int_0^\infty r^2 e^{-\frac{Zr}{a_0}} e^{-\frac{r}{a_0}} dr$$

$$= \frac{4Z^{3/2}}{a_0^3} \int_0^\infty r^2 e^{-\left(\frac{Z+1}{a_0}\right)r} dr = \frac{4Z^{3/2}}{a_0^3} \cdot 2! \Big/ \left(\frac{Z+1}{a_0}\right)^3$$

i.e.// $\underline{\underline{\langle \psi_Z | \psi_1 \rangle = 8Z^{3/2}/(Z+1)^3}}$. (2)

By the "sudden approxn" [$\genfrac{}{}{0pt}{}{\text{CLASS}}{\text{NOTES}}$, p. tD 20, Eq (58)], the prob$^{\underline{y}}$ of $Z=1$ (ground) $\rightarrow Z=2$ (ground) is then...

$$\boxed{|\langle \psi_Z | \psi_1 \rangle|^2_{(Z=2)} = 64 \cdot 2^3/3^6 = 512/729 = 0.702}.$$ (3)

So this happens 70% of the time. The other 30% $\Rightarrow$ get excited states of He^+.

ϕ507 MidTerm Solutions (1995)

② [40 pts.]. Moments $\langle r^N \rangle$ for 1e atom ground state; r_{mp} & variance Δr.

We will use the normalized ground state wavefcn from problem ①...

$$\rightarrow \psi(r) = \mathcal{N} e^{-\kappa r}, \quad \underline{\underline{\kappa}} = \frac{Z}{a_0}, \text{ and: } \langle \psi | \psi \rangle = 1 \text{ if } \mathcal{N} = (\kappa^3/\pi)^{1/2}. \quad (1)$$

And we will use the well-known integral (defn of Gamma fcn):

$$\rightarrow \int_0^\infty x^n e^{-ax}\, dx = \Gamma(n+1)/a^{n+1} = n!/a^{n+1}, \quad n = \text{integer} > -1. \quad (2)$$

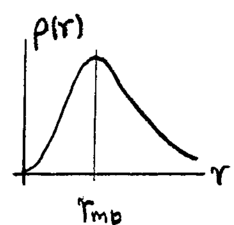
(A) The required N^{th} moment is...

$$\langle r^N \rangle = \int_0^\infty r^N |\psi(r)|^2 \cdot 4\pi r^2 dr = 4\pi \cdot \left(\frac{\kappa^3}{\pi}\right) \int_0^\infty r^{N+2} e^{-2\kappa r} dr$$

$$\text{by } (2) \quad \boxed{\langle r^N \rangle = 4\kappa^3 (N+2)!/(2\kappa)^{N+3} = \frac{(N+2)!}{2^{N+1}} \left(\frac{a_0}{Z}\right)^N.} \quad (3)$$

We've put in $\kappa = \frac{Z}{a_0}$. The moments do not exist for integers $N \leqslant -3$.

(B) $\langle r \rangle = \frac{3}{2}(a_0/Z)$ does not match $r_{mp} = (a_0/Z)$; neither does $\sqrt{\langle r^2 \rangle} = \sqrt{3}\,(a_0/Z)$, or any of the $\langle r^N \rangle^{\frac{1}{N}}$ for (+)ve N. In fact r_{mp} does not take its name as "most probable r" from any of the $\langle r^N \rangle$. Instead, r_{mp} locates the maximum in the electron radial charge density:



$$\rightarrow \rho(r) = e \cdot 4\pi r^2 |\psi(r)|^2 = \text{cnst} \times r^2 e^{-2\kappa r}; \ \rho \text{ is MAX @ } r = r_{mp}. \quad (4)$$

(C) The variance Δr is readily calculated from (3), using N = 1 & 2...

$$\rightarrow \Delta r = [\langle r^2 \rangle - \langle r \rangle^2]^{1/2} = [3 - (3/2)^2]^{1/2} (a_0/Z), \quad \boxed{\Delta r = \frac{\sqrt{3}}{2}(a_0/Z)}. \quad (5)$$

Δr is "large" insofar as: $\Delta r/\langle r \rangle = 1/\sqrt{3} = 0.5774$, or $\Delta r/r_{mp} = \frac{\sqrt{3}}{2} = 0.8660$. It must be so that $\Delta r = \nu(a_0/Z)$, with $\nu \sim 1$ a "large" fraction. Otherwise the e localization to Δr, which generates K.E. components $\Delta E \sim \frac{1}{2m}\left(\frac{\hbar}{2}/\Delta r\right)^2$, i.e. $\Delta E \sim \frac{1}{8\nu^2}(Z^2 e^2/a_0)$, would be enough to exceed the binding energy.

(3) [40 pts]. Show that $[\mathbb{J}, \mathbb{A}\cdot\mathbb{B}]=0$, if $\mathbb{A}$ & $\mathbb{B}$ are $\mathbb{T}$-vectors. Nature of $\mathbb{A}\cdot\mathbb{B}$.

Consider the α component of the commutator. It can be written as...

$$\rightarrow [\vec{J}, \vec{A}\cdot\vec{B}]_\alpha = \sum_\beta [J_\alpha, A_\beta B_\beta] = \sum_\beta \{A_\beta [J_\alpha, B_\beta] + [J_\alpha, A_\beta] B_\beta\}. \quad (1)$$

We have used the commutator identity: $[P, QR] = Q[P,R] + [P,Q]R$. Since $\vec{A}$ & $\vec{B}$ are both $\vec{T}$-vectors w.r.t. $\vec{J}$, then in Eq. (1) we can set...

$$\left[\begin{array}{l} [J_\alpha, B_\beta] = i \sum_\gamma \epsilon_{\alpha\beta\gamma} B_\gamma, \\ [J_\alpha, A_\beta] = i \sum_\gamma \epsilon_{\alpha\beta\gamma} A_\gamma. \end{array}\right\| \quad (2)$$

Here $\hbar=1$, and $\epsilon_{\alpha\beta\gamma}$ = Levi-Civita density.* The sum over γ is redundant (but useful).

$$\xrightarrow{\text{So}} [\vec{J}, \vec{A}\cdot\vec{B}]_\alpha = i \sum_{\beta,\gamma} \epsilon_{\alpha\beta\gamma} \{A_\beta B_\gamma + A_\gamma B_\beta\}$$

β & γ interchanged here

$$= i \left\{ \sum_{\beta,\gamma} \epsilon_{\alpha\beta\gamma} A_\beta B_\gamma - \sum_{\gamma,\beta} \epsilon_{\alpha\gamma\beta} A_\gamma B_\beta \right\}. \quad (3)$$

Each term on RHS of Eq. (3) is equivalent to $(\vec{A}\times\vec{B})_\alpha$. So, as required...

$$\boxed{[\vec{J}, \vec{A}\cdot\vec{B}] = i\{(\vec{A}\times\vec{B}) - (\vec{A}\times\vec{B})\} = 0.} \quad (4)$$

This result is independent of whether $\vec{A}$ & $\vec{B}$ commute with each other.

Under the ∞smal rotation operator (rotation by $\measuredangle\, \delta\varphi$ about axis $\hat{n}$), viz. $R(\delta\varphi) = 1 - i\,\delta\varphi(\hat{n}\cdot\vec{J})$, [Sakurai Eq. (3.1.15)], a scalar $\mathcal{S}$ transforms as

$$\left[\begin{array}{l} \mathcal{S} \rightarrow \mathcal{S}' = R^{-1}\mathcal{S}R = \mathcal{S} + i\,\delta\varphi[\hat{n}\cdot\vec{J}, \mathcal{S}], \text{ to } 1^{st} \text{ order in } \delta\varphi; \\ \text{so } \delta\mathcal{S} = \mathcal{S}' - \mathcal{S} = i\,\delta\varphi[\hat{n}\cdot\vec{J}, \mathcal{S}]. \end{array}\right. \quad (5)$$

If $\mathcal{S}$ is a "true scalar", it will be unaffected by such a rotation, i.e. $\delta\mathcal{S}=0$. This requires $[\hat{n}\cdot\vec{J}, \mathcal{S}]=0$... or that $\mathcal{S}$ commute with each component of $\vec{J}$, i.e. $[\vec{J}, \mathcal{S}]=0$. Then $\mathcal{S} = \vec{A}\cdot\vec{B}$ is a "true scalar" by virtue of Eq. (4).

* $\epsilon_{\alpha\beta\gamma} = \pm 1$ if $\alpha\beta\gamma = \left\{\begin{smallmatrix}\text{even}\\ \text{odd}\end{smallmatrix}\right\}$ permutation of 123. Otherwise $\epsilon_{\alpha\beta\gamma} \equiv 0$.

④ [40 pts]. Find Schrödinger limit on Klein-Gordon plane waves.

1. The free-particle KG eqtn is : $\left[\nabla^2 - \frac{1}{c^2}(\partial^2/\partial t^2) - (mc/\hbar)^2\right]\psi(\vec{r},t) = 0$ class notes p. fs 15.

If we substitute $\psi = \phi \exp(-\frac{i}{\hbar}mc^2 t)$, a straightforward calculation shows that

$$\rightarrow \frac{1}{c^2}(\partial^2\psi/\partial t^2) = \left[\frac{1}{c^2}(\partial^2\phi/\partial t^2) - \frac{2im}{\hbar}(\partial\phi/\partial t) - (mc/\hbar)^2\phi\right] e^{-\frac{i}{\hbar}mc^2 t}. \quad (1)$$

Plugging this into the free-particle KG eqtn for ψ, we find ϕ must satisfy

$$\rightarrow \left(\nabla^2 + \frac{2im}{\hbar}\frac{\partial}{\partial t}\right)\phi = \frac{1}{c^2}(\partial^2\phi/\partial t^2), \text{ for KG } \phi. \quad (2)$$

2. The Schrödinger equation for a free particle of mass m and wavefcn φ is :

$$\left[-\frac{\hbar^2}{2m}\nabla^2\varphi = i\hbar\frac{\partial\varphi}{\partial t}, \text{ or } \left(\nabla^2 + \frac{2im}{\hbar}\frac{\partial}{\partial t}\right)\varphi = 0. \quad (3)\right.$$

Comparison with Eq. (2) shows that the KG ϕ will satisfy the Schrödinger equation only if $\underline{\frac{1}{c^2}(\partial^2\phi/\partial t^2) \rightarrow \text{negligible}}$. More precisely, we need this term to be negligibly small compared the others... in particular :

$$\rightarrow \left|\frac{1}{c^2}\left(\frac{\partial^2\phi}{\partial t^2}\right)\right| \ll \left|\frac{2im}{\hbar}\left(\frac{\partial\phi}{\partial t}\right)\right|, \text{ or } \underline{\underline{\left|\frac{1}{\dot\phi}(\partial\dot\phi/\partial t)\right| \ll mc^2/\hbar.}} \quad (4)$$

3. A plane-wave solution to the free-particle KG eqtn is $\psi(\vec{r},t) = e^{\frac{i}{\hbar}(\vec{p}\cdot\vec{x} - Et)}$, where $\vec{p}$ is the relativistic particle momentum and E is the total (relativistic) energy. Then the plane-wave version of $\phi = \psi \exp(\frac{i}{\hbar}mc^2 t)$ is :

$$\rightarrow \phi(\vec{r},t) = \exp\left[\frac{i}{\hbar}(\vec{p}\cdot\vec{x} - \mathcal{E}t)\right], \quad \mathcal{E} = E - mc^2. \quad (5)$$

$\mathcal{E}$ is the "conventional" (actually relativistic) kinetic energy for the particle. For ϕ of Eq. (5), the condition in Eq. (4) prescribes

$$\boxed{\mathcal{E} \ll mc^2}, \text{ for KG } \phi \text{ to } \simeq \text{ satisfy Schrödinger Equation.} \quad (6)$$

Only very slowly moving m's, @ $v \ll c$, will qualify as Schrödinger-like.

Φ507 MidTerm Solutions (1995)

⑤ [40 pts]. Analyse scattering from potential $V(r) = V_0 a\,\delta(r-a)$, via Born Approxn.

(A) 1. Let $k = \sqrt{2mE/\hbar^2}$ be m's incident wave #. Born Approxn validity requires:

$$\rightarrow \left|\int_0^\infty [e^{2ikr} - 1]\,V(r)\,dr\right| \ll \hbar v = \hbar^2 k/m \leftarrow \text{Davydov Eq. (106.16), or Class notes p. ScT 10, Eq (22).} \quad (1)$$

... for $V(r) = V_0 a\,\delta(r-a)$, Eq (1) $\Rightarrow$ $\underline{\left(\frac{\sin ka}{ka}\right) V_0 \ll \frac{1}{2m}(\hbar/a)^2}$. (2)

Born Approxn is good at all energies (even $E \to 0$) if $\boxed{V_0 \ll \frac{1}{2m}(\hbar/a)^2}$. (3)

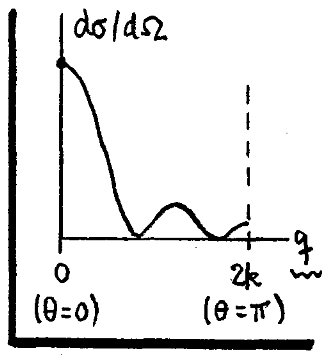
(B) 2. By class notes p. ScT (13), Eq. (31), the differential scattering cross-section is:

$$\rightarrow \frac{d\sigma}{d\Omega} = \left(\frac{m}{2\pi\hbar^2}\right)^2 |\tilde{V}(q)|^2, \quad w/\ q = 2k\sin(\theta/2) \int \begin{matrix} q = \text{momentum transfer}, \\ \theta = \text{scattering angle}. \end{matrix} \quad (4)$$

$$\text{and}/\!/ \quad \tilde{V}(q) = \frac{4\pi}{q}\int_0^\infty r\,V(r)\sin qr\,dr = [4\pi V_0 a^3]\left(\frac{\sin qa}{qa}\right) \int \begin{matrix} \text{for the given:} \\ V(r) = V_0 a\,\delta(r-a). \end{matrix} \quad (5)$$

In (5), $[4\pi V_0 a^3] = \int_0^\infty V(r)\cdot 4\pi r^2 dr = \underline{\Lambda}$, the "volume" of $V(r)$. So we get...

$$\boxed{\frac{d\sigma}{d\Omega} = \left(\frac{m\Lambda}{2\pi\hbar^2}\right)^2 \left(\frac{\sin qa}{qa}\right)^2} \int \begin{matrix} w/\ \Lambda = 4\pi V_0 a^3, \\ q = 2k\sin(\theta/2). \end{matrix} \quad (6)$$



By the inequality in (3), the coefficient $(m\Lambda/2\pi\hbar^2)^2 \ll a^2$. $(d\sigma/d\Omega)$ vs. q is sketched at right -- the scattering vanishes when $qa = n\pi$, $n = 1, 2, \ldots$ (and $q \leq 2k$). At these points, there is a sort of resonance condition, where an integral # of half-wavelengths of q fit inside the scattering potential, i.e. $\underline{n \cdot \frac{1}{2}(2\pi/q) = a}$, and $V(r)$ appears to be transparent.

(C) 3. The solid ∡ $d\Omega = 2\pi\sin\theta\,d\theta = (2\pi/k^2)\,q\,dq$ [prob. [redacted]], so the total cross-section is:

$$\rightarrow \sigma = \int_{4\pi} (d\sigma/d\Omega)\,d\Omega = \left(\frac{m\Lambda}{2\pi\hbar^2}\right)^2 \frac{2\pi}{k^2}\int_0^{2k}\left(\frac{\sin qa}{qa}\right)^2 q\,dq = \frac{2\pi}{k^2 a^2}\left(\frac{m\Lambda}{2\pi\hbar^2}\right)^2 \int_0^{2ka} \frac{dx}{x}\sin^2 x. \quad (7)$$

The integral is not an elementary fcn. When $a \to 0$ ($ka \ll 1$), put $\sin^2 x \simeq [x(1 - \frac{x^2}{6})]^2$ so that $\int_0^{2ka} (\sin^2 x)\frac{dx}{x} \simeq \int_0^{2ka} x(1 - \frac{x^2}{3})\,dx = 2(ka)^2[1 - \frac{2}{3}(ka)^2]$. Then leading terms in σ:

$$\boxed{\sigma \simeq 4\pi(m\Lambda/2\pi\hbar^2)^2\left[1 - \tfrac{2}{3}k^2a^2\right]} \quad (8)$$

σ falls off slowly with energy (at low energy).