NATURAL SCIENCES TRIPOS Part II
EXPERIMENTAL AND THEORETICAL PHYSICS (1)

SECTION A

ADVANCED QUANTUM PHYSICS

A1 *Attempt **all** parts of this question. Answers should be concise, and relevant formulae may be assumed without proof.*

(a) The hydrogen atom's $n = 2$ levels are degenerate, so should use degenerate perturbation theory. Since two levels shift but two do not, the perturbing potential (electric field in z-direction, $[H^1 = qEr\cos\vartheta]$) must have zero matrix elements with two of the states so to first order there should be no shift in energy levels. However, since two shift linearly, they must have non-zero matrix elements [at second order], forming a two-dimensional degenerate subspace in which to diagonalise the perturbing Hamiltonian. [Bookwork] [1] [1] [1] [1]

(b) Electronic ground state of P ($Z = 15$), assuming LS coupling:
Z=15=2+8+2+3 so 3 electrons in 3p shell (given).

Hund's rules [Bookwork]: max S $\Rightarrow S = 3/2$. [1]

Max $L = 1 + 0 - 1 = 0$. [1]

Min J (since $\leq$ half-filled shell), $J = L + S = S = 3/2$. [1]

So ground state is ${}^{2S+1}L_S = {}^4\mathrm{S}_{3/2}$. [1]

(c) [Bookwork] 10^{th} excited state in a simple harmonic potential, indicating the features that can be explained within the WKB approximation [page 21] [or otherwise]:

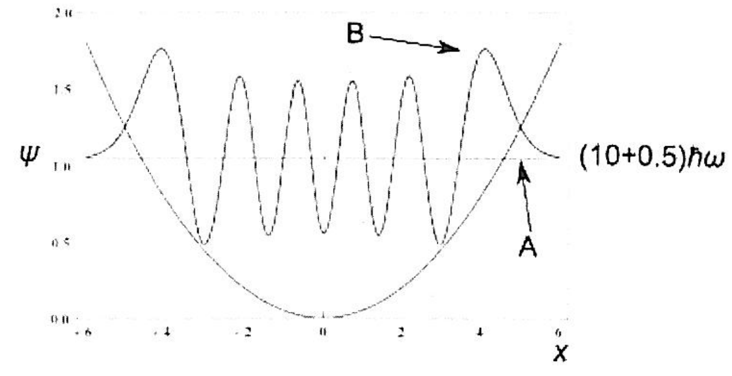

Figure 1: SHO for $n = 10$.

[2]

$\psi = \frac{C}{\sqrt{p(x)}} e^{(i/\hbar)\int^x p dx'}$.

A: extra [$\pi/4$ of] phase after turning point (in classically forbidden region) (in WKB this is due to matching across the turning point). [1]

B: amplitude grows as $1/\sqrt{p}$, as $p = \sqrt{[2m(E-V)]}$ decreases to zero at turning point. [1]

A2 *Attempt this question. Credit will be given for well-structured and clear explanations, including appropriate diagrams and formulae. Detailed mathematical derivations are not required.*

Write brief notes on **two** of the following: [One or two marks available for each bullet point depending on depth.]

(a) Uniform magnetic fields in quantum mechanics, including a discussion of the Aharonov-Bohm effect and Landau levels: [p53-57]

- Magnetic field B enters Schrödinger Equation by changing momentum $\boldsymbol{p}$ to $\boldsymbol{p} - q\boldsymbol{A}$ for charge q in magnetic vector potential $\boldsymbol{A}$ (free to choose gauge, which gives extra phase factor in the wavefunction).
- Aharonov-Bohm effect: split wavefunction (e.g. beam of electrons) up into two paths, with magnetic flux enclosed between the paths; phase change between beams due to flux [details marked as "info" (non-examinable) in notes].
- Landau levels: solve Schrödinger's Equation, classical cyclotron motion corresponds to simple-harmonic potential, energy levels $E_{n,p_z} = (n+1/2)\hbar\omega_c + \frac{p_z^2}{2m}$; the quantum number n labels states called Landau levels. $\omega_c = eB/m$.
- Degeneracy of Landau level is AB/Φ_0 where $\Phi_0 = h/e$ [says e/h in notes!]
- As increase B, fit more electrons into each LL since degeneracy increases.
- Zeeman effect splits energies of the two spins so LLs split into two at high B.
- Quantum Hall effect (marks available but not examinable).

(b) The Hartree method in the central-field approximation: [p91-94]

- Central-field approximation: electron interaction term in the Hamiltonian for an atom contains a large spherically symmetrical component arising from the core electrons—closed shells have isotropic density distributions.
- Treat core electrons as giving an average central potential $U_i(r_i)$ for i^{th} electron and write the Hamiltonian as $H = H_0 + H_1$ where H_0 includes $U_i(r_i)$ for each electron and the single-electron Schrödinger Equation for each electron—separable for each electron so wavefunction is a product of wavefunctions. Then H_1 is a small perturbation (full interactions minus $\Sigma U_i(r_i)$).
- Hartree: self-consistent field method—need to estimate $U_i(r_i)$; write wavefunction as product of wavefunctions for each electron –

unfortunately not a properly symmetrised Slater determinant; use this as a trial state in the variational method to find the variational energy $< \Psi|H|\Psi >$;

- Minimise set of individual wavefunctions subject to them being normalised; get Hartree equations; the set that minimises the energy are determined by the effective potential $U_i(r)$ [forced to be spherically symmetric].
- Recipe (page 93): 1. Guess common central potential, construct single-particle eigenstates, and then the self-consistent potentials $U_i(r)$. 2. Find eigenstates using $U_i(r)$. 3. Estimate ground-state energy by filling up the levels, taking account of the exclusion principle. 4. Make improved estimate of the potentials $U_i(r)$ and go back to step 2 until process converges.

(c) Coupling of matter to the electromagnetic field, including a discussion of emission and absorption of photons by atoms.

[p126-130]

- EM field gives time-dependent perturbation to atomic Hamiltonian; consider only coupling to electrons around the atom; paramagnetic and diamagnetic terms (ignore the latter since negligible).
- EM field quantised, can expand vector potential $\boldsymbol{A}$ in terms of ladder operators that create/annihiliate photons.
- Spontaneous emission of a photon can occur for an electron initially in an excited state; perturbing Hamiltonian $\approx e\boldsymbol{E}(\boldsymbol{r},t)\cdot\boldsymbol{r}$, the electric dipole approximation.
- Absorption and stimulated emission: FGR gives probability of absorbing a photon from the EM field. But it also gives an enhanced probability of emission if there are already identical photons in the EM field—stimulated emission.
- Einstein's A and B coefficients: spontaneous and stimulated emission rates from state k to state j $A_{k\to j}(\omega)$ and $B_{k\to j}(\omega)u(\omega)$, respectively, must be related ($u(\omega)$ is energy density of radiation per unit ω)—thermodynamic equilibrium, Boltzmann factor, Planck formula; if we calculate A can infer B (or *vice versa*).

A3 [Bookwork] The Pauli matrices form the components of a vector $\boldsymbol{\sigma}$. The component of the spin operator $\hat{S}$ in the direction of the unit vector $\hat{\boldsymbol{n}}$ is given by $\hat{S}\cdot\hat{\boldsymbol{n}} = \frac{\hbar}{2}\boldsymbol{\sigma}\cdot\hat{\boldsymbol{n}}$. So, if the basis states of $\hat{S}\cdot\hat{\boldsymbol{n}}$ are $|\alpha_\pm\rangle$, then $\boldsymbol{\sigma}\cdot\hat{\boldsymbol{n}}\,|\alpha_\pm\rangle = \pm\,|\alpha_\pm\rangle$, so $|\alpha_\pm\rangle$ can be found in the basis of the S_z operator. [3]

$$\sigma_x\,|X_\pm\rangle = \pm\,|X_\pm\rangle$$

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and

$$\sigma_z |\alpha\rangle = \pm |\alpha\rangle , \quad \sigma_z |\beta\rangle = \pm |\beta\rangle . \qquad [1]$$

Let $|X_\pm\rangle = a_\pm |\alpha\rangle + b_\pm |\beta\rangle$.

$$\therefore \sigma_x \begin{pmatrix} a_\pm \\ b_\pm \end{pmatrix} = \pm \begin{pmatrix} a_\pm \\ b_\pm \end{pmatrix} \qquad [1]$$

$$\therefore \begin{pmatrix} b_\pm \\ a_\pm \end{pmatrix} = \pm \begin{pmatrix} a_\pm \\ b_\pm \end{pmatrix}$$

$$\therefore b_+ = a_+ \quad \text{and} \quad b_- = -a_-. \qquad [1]$$

[Bookwork] Zeeman energy for $B = B_x$ is $E_Z = -\mu \cdot \boldsymbol{B}$. [1]
Let $\boldsymbol{\mu} = \gamma \boldsymbol{S}$, so $E_Z = -\gamma \boldsymbol{S} \cdot \boldsymbol{B} = -\gamma \boldsymbol{\sigma} \cdot \boldsymbol{B}\hbar/2 = \mp \gamma B\hbar/2$ for $|X_\pm\rangle$. [1]
The time-evolution operator

$$\hat{U}(t) = e^{-i\hat{H}t/\hbar} = e^{i\gamma \boldsymbol{\sigma} \cdot \boldsymbol{B}t/2} = e^{i\gamma\sigma_x Bt/2}. \qquad [1]$$

But [from hint],

$$\mathrm{e}^{\mathrm{i}\theta(\sigma_x)} = \boldsymbol{I} \cos\theta + \mathrm{i}(\sigma_x) \sin\theta$$

[Simple use of bookwork] So

$$\begin{aligned} e^{i\gamma\sigma_x Bt/2} &= \boldsymbol{I} \cos\omega t + i\sigma_x \sin\omega t \\ &= \begin{pmatrix} \cos\omega t & \cos\omega t \\ i\sin\omega t & \cos\omega t \end{pmatrix} \end{aligned}$$

where $\omega \equiv \gamma B/2$. [1]

So at time t, the wavefunction $|\psi(t)\rangle$ has evolved from $|\alpha\rangle$ to

$$\begin{pmatrix} c(t) \\ d(t) \end{pmatrix} = \hat{U}(t) \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} \cos\omega t \\ i\sin\omega t \end{pmatrix} \qquad [1]$$

i.e.

$$|\psi(t)\rangle = |\alpha\rangle \cos\omega t + \mathrm{i}\, |\beta\rangle \sin\omega t,$$

Expectation value:

$$
\begin{aligned}
<\boldsymbol{\mu}>(t) &= \langle\psi(t)|\,\gamma\boldsymbol{S}\,|\psi(t)\rangle = \langle\psi(t)|\,\gamma\hbar\boldsymbol{\sigma}/2\,|\psi(t)\rangle \\
&= \frac{\gamma\hbar}{2}\left\langle\begin{pmatrix}\cos\omega t & -i\sin\omega t\end{pmatrix}\begin{pmatrix}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\\ \begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}\\ \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\end{pmatrix}\begin{pmatrix}\cos\omega t\\ i\sin\omega t\end{pmatrix}\right\rangle \\
&= \frac{\gamma\hbar}{2}\begin{pmatrix}\cos\omega t, & -i\sin\omega t\end{pmatrix}\begin{pmatrix}\begin{pmatrix}i\sin\omega t\\ \cos\omega t\end{pmatrix}\\ \begin{pmatrix}\sin\omega t\\ i\cos\omega t\end{pmatrix}\\ \begin{pmatrix}\cos\omega t\\ -i\sin\omega t\end{pmatrix}\end{pmatrix} \\
&= \mu\begin{pmatrix}(i\sin\omega t\cos\omega t - i\sin\omega t\cos\omega t)\\ (\sin\omega t\cos\omega t + \sin\omega t\cos\omega t)\\ (\cos^2\omega t - \sin^2\omega t)\end{pmatrix} = \begin{pmatrix}0\\ \mu\sin 2\omega t\\ \mu\cos 2\omega t\end{pmatrix}
\end{aligned}
$$

since $\mu = \gamma\hbar/2$. [3]

[Straightforward calculation] $|\alpha\rangle$ is split into two beams $|\psi_1(t)\rangle$ and $|\psi_2(t)\rangle$:

$$|\psi_1(t)\rangle = \begin{pmatrix}\cos\omega t\\ i\sin\omega t\end{pmatrix}, |\psi_2(t)\rangle = \begin{pmatrix}1\\ 0\end{pmatrix}.$$ [1]

When recombined, total wavefunction is

$$|\psi\rangle = A(|\psi_1\rangle + |\psi_2\rangle) = A\begin{pmatrix}1+\cos\omega t\\ i\sin\omega t\end{pmatrix}.$$ [1]

Probability of finding a neutron is [3]

$$
\begin{aligned}
\langle\psi|\psi\rangle &= |A|^2\begin{pmatrix}1+\cos\omega t, & -i\sin\omega t\end{pmatrix}\begin{pmatrix}1+\cos\omega t\\ i\sin\omega t\end{pmatrix} \\
&= |A|^2((1+\cos\omega t)^2 + \sin^2\omega t) \\
&= |A|^2(1 + 2\cos\omega t + \cos^2\omega t + \sin^2\omega t) \\
&= 2|A|^2(1+\cos\omega t).
\end{aligned}
$$

[3]

Physical interpretation of the curves in terms of the components of the wavefunction $|\psi(t)\rangle$: When component of $|\alpha\rangle$ is much larger than that of $|\beta\rangle$, $\langle\mu_z\rangle$ is positive (in line with $|\alpha\rangle$), and when $|\alpha\rangle$ is much smaller than that of $|\beta\rangle$, $\langle\mu_z\rangle$ is negative (in line with $|\beta\rangle$). Zero probability of finding a neutron when one of the beams has changed its phase by π relative to the other. [3]

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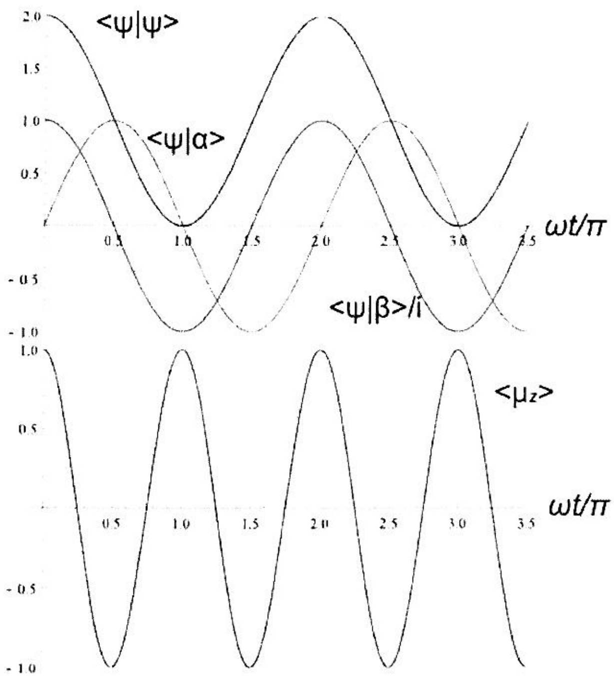

Figure 2: Graphs of the numbers of neutrons detected, and of $\langle \mu_z \rangle$ for the beam that was in the B field, against ωt. $< \mu_z >$ for beam not in B field is constant, at $+\mu$.

A4 [Bookwork; details not required] Expand time-dependent wavefunction (in the interaction representation) in the unperturbed basis $|n\rangle$:

$$|\psi(t)\rangle = \Sigma_n c_n(t)\,|n\rangle \qquad [1]$$

In time-dependent perturbation theory, $c_n(t)$ is expanded in powers of the interaction, and the first-order term is

$$c_n^{(1)}(t) = -\frac{i}{\hbar}\int_{t_0}^{t} \mathrm{d}t'\, e^{i\omega_{ni}t'}\, V_{ni}(t') \qquad [1]$$

So for an initial state $|\mathrm{i}\rangle$, perturbed by a potential $\widehat{V}(t)e^{-i\omega t}$ which is abruptly switched on at time $t = 0$, the coefficient for state $|\mathrm{f}\rangle$ at a later time t is

$$c_n^{(1)}(t) = -\frac{i}{\hbar}\int_{0}^{t} \mathrm{d}t'\, \langle \mathrm{f}|\,\widehat{V}\,|\mathrm{i}\rangle\, e^{i(\omega_{\mathrm{fi}}-\omega)t'} \qquad [1]$$

where $\hbar\omega_{\mathrm{fi}}$ is the energy difference between states $|\mathrm{f}\rangle$ and $|\mathrm{i}\rangle$.

The probability of a transition after a time t is therefore

$$P_{\mathrm{i}\to\mathrm{f}}(t) \simeq |c_n^{(1)}(t)|^2 = \frac{1}{\hbar^2}|\,\langle \mathrm{f}|\,\widehat{V}\,|\mathrm{i}\rangle\,|^2 \left(\frac{\sin((\omega_{\mathrm{fi}}-\omega)t/2)}{(\omega_{\mathrm{fi}}-\omega)t/2}\right)^2. \qquad [1]$$

This sinc function is strongly peaked and as $t \to \infty$ tends towards a delta function multiplied by t, i.e. the likelihood of transition is proportional to the time elapsed. So to find the transition rate $R_{\mathrm{i}\to\mathrm{f}}(t)$, divide $P_{\mathrm{i}\to\mathrm{f}}(t)$ by t and take the limit as $t \to \infty$. This is Fermi's Golden Rule, [1]

$$R_{\mathrm{i}\to\mathrm{f}}(t) = \frac{2\pi}{\hbar}|\langle \mathrm{f}|\widehat{V}|\mathrm{i}\rangle|^2 \delta(\omega_{\mathrm{fi}} - \omega)$$

[Page 120 of notes] Fermi's Golden Rule can be applied to the case of a continuous density of final states by summing the rate over all the final states, and turning the sum into an integral multiplied by the density of final states (in energy). [2]

[Bookwork] The differential scattering cross-section ${}^{\mathrm{d}\sigma}/{}_{\mathrm{d}\Omega}$ is defined as

$$^{\mathrm{d}\sigma}/_{\mathrm{d}\Omega} = \frac{\text{rate of scattering into solid angle } \mathrm{d}\Omega}{\text{incident flux } \times \mathrm{d}\Omega}.$$ [1]

To derive the Born approximation, start with FGR and consider a plane wave incident on a localised potential $V(\boldsymbol{r})$. The rate of scattering from $|\boldsymbol{k}\rangle$ to $|\boldsymbol{k}'\rangle$ in a small solid angle $\mathrm{d}\Omega$ is

$$\Gamma_{\boldsymbol{k}\to\boldsymbol{k}'\in\mathrm{d}\Omega} = \frac{2\pi}{\hbar}|\langle \boldsymbol{k}'|V|\boldsymbol{k}\rangle|^2 \delta(E_{k'} - E_k),$$

where $E_k = \hbar^2|\boldsymbol{k}|^2/2m$. [1]

The matrix element

$$\langle \boldsymbol{k}'|\widehat{V}|\boldsymbol{k}\rangle = \frac{1}{L^3}\int \mathrm{d}^3\boldsymbol{r} V(\boldsymbol{r}) e^{i(\boldsymbol{k}'-\boldsymbol{k})\cdot\boldsymbol{r}} \equiv \frac{1}{L^3}\widetilde{V}(\boldsymbol{q}),$$

where $\boldsymbol{q} = \boldsymbol{k}' - \boldsymbol{k}$ (given) and L^3 is the volume of the system. [1]

$$\begin{aligned}
\therefore \Gamma_{\boldsymbol{k}\to\boldsymbol{k}'\in\mathrm{d}\Omega} &= \frac{2\pi}{\hbar}\frac{1}{L^6}\sum_{\boldsymbol{k}'\in\mathrm{d}\Omega} |\widetilde{V}(\boldsymbol{q})|^2 \delta(E_{k'} - E_k) \\
&= \frac{2\pi}{\hbar}\frac{1}{L^6}\frac{L^3}{(2\pi)^3}\mathrm{d}\Omega \int_0^\infty k'^2 \mathrm{d}k' \, |\widetilde{V}(\boldsymbol{q})|^2 \delta\left(\frac{\hbar^2}{2m}(k'^2 - k^2)\right) && [1] \\
&= \frac{2\pi}{\hbar}\frac{1}{L^3}\frac{1}{(2\pi)^3}\mathrm{d}\Omega k^2 \frac{m}{\hbar^2 k}|\widetilde{V}(\boldsymbol{q})|^2 && [1]
\end{aligned}$$

using

$$\delta\left(\frac{\hbar^2}{2m}(k'^2 - k^2)\right) = \frac{2m}{\hbar^2(k + k')}\delta(k' - k).$$

and requiring from the δ-function that $|\boldsymbol{k}'| = |\boldsymbol{k}'|$. [1]

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Now, from the probability flux of a plane wave, the incident flux is $\hbar k/m$ (given) $\times 1/L^3$ (normalisation), so

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \frac{\Gamma_{\boldsymbol{k}\to\boldsymbol{k}'\in\mathrm{d}\Omega}}{(\hbar k/mL^3)\mathrm{d}\Omega} = \frac{1}{(2\pi)^2}\frac{mk}{\hbar^3}\frac{1}{L^3}\mathrm{d}\Omega|\widetilde{V}(\boldsymbol{q})|^2 \times \frac{mL^3}{\hbar k \mathrm{d}\Omega} \qquad [1]$$

$$= \left|\frac{m}{2\pi\hbar^2}\widetilde{V}(\boldsymbol{q})\right|^2 = \left|\frac{m}{2\pi\hbar^2}\int V(\boldsymbol{r})\mathrm{e}^{-\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}}\mathrm{d}^3\boldsymbol{r}\right|^2.$$

The Born approximation

[Not bookwork] To find $\mathrm{d}\sigma/\mathrm{d}\Omega$ for $V = V_0\exp(-r^2/a^2)$, use the above equation (setting $A = \frac{mV_0}{2\pi\hbar^2}$ and taking the z-axis along $\boldsymbol{q}$):

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \left|A\int e^{-r^2/a^2}\mathrm{e}^{-\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}}\mathrm{d}^3\boldsymbol{r}\right|^2$$

$$= \left|A\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\exp[-(x^2+y^2+z^2)/a^2 - \mathrm{i}qz]\,\mathrm{d}x\mathrm{d}y\mathrm{d}z\right|^2 \qquad [1]$$

$$= \left|A\int_{-\infty}^{\infty}\mathrm{e}^{-x^2/a^2}\mathrm{d}x\int_{-\infty}^{\infty}\mathrm{e}^{-y^2/a^2}\mathrm{d}y\int_{-\infty}^{\infty}\mathrm{e}^{-z^2/a^2}(\cos qz + \mathrm{i}\sin qz)\,\mathrm{d}z\right|^2 \qquad [2]$$

$$= \left|Aa^2\pi\int_{-\infty}^{\infty}\mathrm{e}^{-z^2/a^2}\cos qz\,\mathrm{d}z\right|^2 \quad \text{(since sin integral is an odd fn, gives 0)} \qquad [1]$$

$$= \left|Aa^3\pi\sqrt{\pi}\mathrm{e}^{-q^2a^2/4}\right|^2 = \left|\frac{mV_0a^3\sqrt{\pi}}{2\hbar^2}\mathrm{e}^{-q^2a^2/4}\right|^2 \qquad [1]$$

(using integrals given in the hint).

The momentum transfer $\boldsymbol{q}$ has $|\boldsymbol{q}| = 2|\boldsymbol{k}|\sin(\theta/2)$ since $|\boldsymbol{k}'| = |\boldsymbol{k}'|$ from the derivation above. Here θ is the scattering angle (between $\boldsymbol{k}'$ and $\boldsymbol{k}'$) (simple diagram of perpendicular bisector of isosceles triangle). [1]

Therefore $\mathrm{e}^{-q^2a^2/4} = \mathrm{e}^{-2k^2a^2\sin^2(\theta/2)}$. In the long-wavelength limit, $ka \ll 1$, so $\mathrm{e}^{-2k^2a^2\sin^2(\theta/2)} \approx 1 - 2k^2a^2\sin^2(\theta/2)$ since $|\sin^2(\theta/2)| \le 1$. [1]

To first order in ka, this is just one, and so $\mathrm{d}\sigma/\mathrm{d}\Omega \approx$ constant. [1]

The total scattering cross-section is $\sigma = \int(\mathrm{d}\sigma/\mathrm{d}\Omega)\,\mathrm{d}\Omega$. [1]

$$\therefore \sigma \approx \left(\frac{mV_0a^3}{2\hbar^2}\right)^2\pi\int\int(1 - 2k^2a^2\sin^2(\theta/2))\sin\theta\mathrm{d}\theta\mathrm{d}\phi$$

$$= B\,2\pi\int_0^{\pi}\mathrm{d}\theta(1 - 2k^2a^2\sin^2(\theta/2)) \qquad [1]$$

(setting $B = \left(\frac{mV_0a^3}{2\hbar^2}\right)^2\pi$, and doing ϕ integral)

$$\approx 2\pi B\left(\pi - 2k^2a^2\int_0^{\pi}\sin^2(\theta/2)\mathrm{d}\theta\right) = 2\pi B\left(\pi - 2k^2a^2\int_0^{\pi}(1-\cos\theta)/2\mathrm{d}\theta\right)$$

$$= 2\pi B(\pi - 2k^2a^2\pi/2) = 2\pi^3\left(\frac{mV_0a^3}{2\hbar^2}\right)^2(1 - k^2a^2). \qquad [1]$$

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