Problema 1

Parte 1
Le funzioni d'onda $\psi_S(\vec{r}_1, \vec{r}_2)$ e $\psi_T(\vec{r}_1, \vec{r}_2)$ sono reali.

$$\psi_S(\vec{r}_1, \vec{r}_2) = C_S(\psi_a(\vec{r}_1)\psi_b(\vec{r}_2) + \psi_b(\vec{r}_1)\psi_a(\vec{r}_2))$$
$$\psi_T(\vec{r}_1, \vec{r}_2) = C_T(\psi_a(\vec{r}_1)\psi_b(\vec{r}_2) - \psi_b(\vec{r}_1)\psi_a(\vec{r}_2))$$

$$\langle \psi_S \mid \psi_S \rangle = 1 \qquad\qquad \langle \psi_T \mid \psi_T \rangle = 1$$

$$\int d^3r_1 d^3r_2 \psi_S^*(\vec{r}_1, \vec{r}_2)\psi_S(\vec{r}_1, \vec{r}_2) =$$
$$\int d^3r_1 d^3r_2 \psi_S(\vec{r}_1, \vec{r}_2)\psi_S(\vec{r}_1, \vec{r}_2) =$$
$$C_S^2 \int d^3r_1 d^3r_2 \left(\psi_a(\vec{r}_1)\psi_b(\vec{r}_2) + \psi_b(\vec{r}_1)\psi_a(\vec{r}_2)\right)\left(\psi_a(\vec{r}_1)\psi_b(\vec{r}_2) + \psi_b(\vec{r}_1)\psi_a(\vec{r}_2)\right) =$$
$$= C_S^2 \left(\int d^3r_1 d^3r_2 \psi_a^2(\vec{r}_1)\psi_b^2(\vec{r}_2) + \int d^3r_1 d^3r_2 \psi_b^2(\vec{r}_1)\psi_a^2(\vec{r}_2) + 2\int d^3r_1 d^3r_2 \psi_a(\vec{r}_1)\psi_b(\vec{r}_1)\psi_a(\vec{r}_2)\psi_b(\vec{r}_2)\right)$$

Le funzioni (...) sono già normalizzate, quindi i primi due integrali danno 1.

$$C_S^2 \left(2 + 2\int d^3r_1 \psi_a(\vec{r}_1)\psi_b(\vec{r}_1) \int d^3r_2 \psi_a(\vec{r}_2)\psi_b(\vec{r}_2)\right) = C_S^2 \left(2 + 2S^2\right)$$

Dove abbiamo definito
$$S \equiv \int d^3r \psi_a(\vec{r})\psi_b(\vec{r})$$

Per ψ_T i calcoli sono quasi identici, l'unica differenza è che il terzo integrale ha il meno, quindi si trova

$$\int d^3r_1 d^3r_2 \psi_T(\vec{r}_1, \vec{r}_2)\psi_T(\vec{r}_1, \vec{r}_2) = C_T^2(2 - 2S^2)$$

$$C_S = \frac{1}{\sqrt{2(1+S^2)}} \qquad\qquad C_T = \frac{1}{\sqrt{2(1-S^2)}}$$

Parte 2

$$S = \int d^3r \psi_a(\vec{r})\psi_b(\vec{r}) = \int d^3r \left(\frac{1}{\sqrt{\pi a^3}} \exp\left(-\frac{|\vec{r} - \vec{r}_a|}{a}\right)\right)\left(\frac{1}{\sqrt{\pi a^3}} \exp\left(-\frac{|\vec{r} - \vec{r}_b|}{a}\right)\right) =$$
$$= \frac{1}{\pi a^3} \int d^3r \exp\left(-\frac{|\vec{r} - \vec{r}_a| + |\vec{r} - \vec{r}_b|}{a}\right)$$

$$\begin{cases} \xi = \frac{|\vec{r}-\vec{r}_a|+|\vec{r}-\vec{r}_b|}{R} \\ \eta = \frac{|\vec{r}-\vec{r}_a|-|\vec{r}-\vec{r}_b|}{R} \\ \phi = \text{prova} \end{cases}$$

dove $R \equiv |\vec{r}_a - \vec{r}_b|$

Lo Jacobiano di questa trasformazione è $\frac{R^3}{8}(\xi^2-\eta^2)$

$$\begin{aligned}
\frac{1}{\pi a^3}\int d^3r\exp\left(-\frac{|\vec{r}-\vec{r}_a|+|\vec{r}-\vec{r}_b|}{a}\right) &= \frac{1}{\pi a^3}\int d^3r\exp\left(-\frac{R}{a}\frac{|\vec{r}-\vec{r}_a|+|\vec{r}-\vec{r}_b|}{R}\right) = \\
&= \frac{1}{\pi a^3}\int_0^{2\pi}d\phi\int_{-1}^{1}d\eta\int_1^\infty d\xi\exp\left(-\frac{R}{a}\xi\right)\frac{R^3}{8}(\xi^2-\eta^2) = \\
= \frac{R^3}{8\pi a^3}\left(\int_0^{2\pi}d\phi\int_{-1}^{1}d\eta\int_1^\infty d\xi\exp\left(-\frac{R}{a}\xi\right)\xi^2 - \int_0^{2\pi}d\phi\int_{-1}^{1}d\eta\,\eta^2\int_1^\infty d\xi\exp\left(-\frac{R}{a}\xi\right)\right) &= \\
= \frac{R^3}{8\pi a^3}\left(2\pi\cdot 2\cdot\int_1^\infty d\xi\exp\left(-\frac{R}{a}\xi\right)\xi^2 - 2\pi\cdot\left[\frac{\eta^3}{3}\right]_{-1}^{1}\left[\frac{\exp\left(-\frac{R}{a}\xi\right)}{-\frac{R}{a}}\right]_1^\infty\right) &= \\
&= \frac{R^3}{8\pi a^3}\left(4\pi\int_1^\infty d\xi\exp\left(-\frac{R}{a}\xi\right)\xi^2 - 2\pi\cdot\frac{2}{3}\cdot\frac{\exp\left(-\frac{R}{a}\right)}{\frac{R}{a}}\right) = \\
&= \frac{R^3}{8\pi a^3}\left(4\pi\cdot\frac{2!\exp\left(-\frac{R}{a}\right)}{\left(\frac{R}{a}\right)^3}\sum_{k=0}^{2}\frac{\left(\frac{R}{a}\right)^k}{k!} - \frac{4\pi}{3}\cdot\frac{\exp\left(-\frac{R}{a}\right)}{\frac{R}{a}}\right) = \\
&= \frac{R^3\exp\left(-\frac{R}{a}\right)}{2a^3}\left(\frac{2}{\left(\frac{R}{a}\right)^3}\sum_{k=0}^{2}\frac{\left(\frac{R}{a}\right)^k}{k!} - \frac{1}{3}\frac{1}{\frac{R}{a}}\right) = \\
&= \exp\left(-\frac{R}{a}\right)\left(\sum_{k=0}^{2}\frac{\left(\frac{R}{a}\right)^k}{k!} - \frac{1}{6}\left(\frac{R}{a}\right)^2\right) = \\
&= \exp\left(-\frac{R}{a}\right)\left(1+\frac{1}{2}\left(\frac{R}{a}\right)+\frac{1}{6}\left(\frac{R}{a}\right)^2-\frac{1}{6}\left(\frac{R}{a}\right)^2\right) = \\
&= \exp\left(-\frac{R}{a}\right)\left(1+\frac{1}{2}\left(\frac{R}{a}\right)\right)
\end{aligned}$$

Parte 3

$$\frac{\partial}{\partial r_i}|\vec{r}-\vec{r}_a| = \frac{r_i - r_{a_i}}{|\vec{r}-\vec{r}_a|} = \frac{(\vec{r}-\vec{r}_a)_i}{|\vec{r}-\vec{r}_a|}$$

$$\nabla|\vec{r}-\vec{r}_a| = \frac{\vec{r}-\vec{r}_a}{|\vec{r}-\vec{r}_a|}$$

$$\begin{aligned}
\nabla\exp\left(-\frac{|\vec{r}-\vec{r}_a|}{a}\right) &= \exp\left(-\frac{|\vec{r}-\vec{r}_a|}{a}\right)\nabla\left(-\frac{|\vec{r}-\vec{r}_a|}{a}\right) = \\
&= -\frac{1}{a}\exp\left(-\frac{|\vec{r}-\vec{r}_a|}{a}\right)\frac{\vec{r}-\vec{r}_a}{|\vec{r}-\vec{r}_a|}
\end{aligned}$$

$$
\begin{aligned}
&\frac{\partial}{\partial r_i}\left(-\frac{1}{a}\exp\left(-\frac{|\vec{r}-\vec{r}_a|}{a}\right)\frac{(\vec{r}-\vec{r}_a)_i}{|\vec{r}-\vec{r}_a|}\right)=\\
&=-\frac{1}{a}\left[\frac{(\vec{r}-\vec{r}_a)_i}{|\vec{r}-\vec{r}_a|}\frac{\partial}{\partial r_i}\exp\left(-\frac{|\vec{r}-\vec{r}_a|}{a}\right)+\exp\left(-\frac{|\vec{r}-\vec{r}_a|}{a}\right)\frac{\partial}{\partial r_i}\frac{(\vec{r}-\vec{r}_a)_i}{|\vec{r}-\vec{r}_a|}\right]\\
&=-\frac{1}{a}\exp\left(-\frac{|\vec{r}-\vec{r}_a|}{a}\right)\left[\frac{(\vec{r}-\vec{r}_a)_i}{|\vec{r}-\vec{r}_a|}\frac{\partial}{\partial r_i}\left(-\frac{|\vec{r}-\vec{r}_a|}{a}\right)+\frac{\partial}{\partial r_i}\frac{(\vec{r}-\vec{r}_a)_i}{|\vec{r}-\vec{r}_a|}\right]\\
&=-\frac{1}{a}\exp\left(-\frac{|\vec{r}-\vec{r}_a|}{a}\right)\left[-\frac{1}{a}\frac{(\vec{r}-\vec{r}_a)_i}{|\vec{r}-\vec{r}_a|}\frac{(\vec{r}-\vec{r}_a)_i}{|\vec{r}-\vec{r}_a|}+\frac{1\cdot|\vec{r}-\vec{r}_a|-(\vec{r}-\vec{r}_a)_i\cdot\frac{(\vec{r}-\vec{r}_a)_i}{|\vec{r}-\vec{r}_a|}}{|\vec{r}-\vec{r}_a|^2}\right]\\
&=-\frac{1}{a}\exp\left(-\frac{|\vec{r}-\vec{r}_a|}{a}\right)\left[-\frac{1}{a}\frac{(\vec{r}-\vec{r}_a)_i^2}{|\vec{r}-\vec{r}_a|^2}+\frac{1}{|\vec{r}-\vec{r}_a|}-\frac{(\vec{r}-\vec{r}_a)_i^2}{|\vec{r}-\vec{r}_a|^3}\right]
\end{aligned}
$$

$$
\begin{aligned}
&-\frac{1}{a}\exp\left(-\frac{|\vec{r}-\vec{r}_a|}{a}\right)\sum_i\left[-\frac{1}{a}\frac{(\vec{r}-\vec{r}_a)_i^2}{|\vec{r}-\vec{r}_a|^2}+\frac{1}{|\vec{r}-\vec{r}_a|}-\frac{(\vec{r}-\vec{r}_a)_i^2}{|\vec{r}-\vec{r}_a|^3}\right]=\\
&=-\frac{1}{a}\exp\left(-\frac{|\vec{r}-\vec{r}_a|}{a}\right)\left[-\frac{1}{a}\frac{|\vec{r}-\vec{r}_a|^2}{|\vec{r}-\vec{r}_a|^2}+\frac{3}{|\vec{r}-\vec{r}_a|}-\frac{|\vec{r}-\vec{r}_a|^2}{|\vec{r}-\vec{r}_a|^3}\right]=\\
&=-\frac{1}{a}\exp\left(-\frac{|\vec{r}-\vec{r}_a|}{a}\right)\left(-\frac{1}{a}+\frac{2}{|\vec{r}-\vec{r}_a|}\right)=\\
&=\exp\left(-\frac{|\vec{r}-\vec{r}_a|}{a}\right)\left(\frac{1}{a^2}-\frac{2}{a\,|\vec{r}-\vec{r}_a|}\right)
\end{aligned}
$$

$$
V(\vec{r}_1,\vec{r}_2)\equiv e^2\left(\frac{1}{|\vec{r}_1-\vec{r}_2|}-\frac{1}{|\vec{r}_1-\vec{r}_a|}-\frac{1}{|\vec{r}_1-\vec{r}_b|}-\frac{1}{|\vec{r}_2-\vec{r}_a|}-\frac{1}{|\vec{r}_2-\vec{r}_b|}+\frac{1}{|\vec{r}_a-\vec{r}_b|}\right)
$$

$$
\begin{aligned}
&\int d^3r_1d^3r_2\psi_S(\vec{r}_1,\vec{r}_2)\left(-\frac{\hbar^2}{2m}(\nabla_1^2+\nabla_2^2)+V(\vec{r}_1,\vec{r}_2)\right)\psi_S(\vec{r}_1,\vec{r}_2)=\\
&\int d^3r_1d^3r_2\psi_S(\vec{r}_1,\vec{r}_2)\left(-\frac{\hbar^2}{2m}(\nabla_1^2+\nabla_2^2)\right)\psi_S(\vec{r}_1,\vec{r}_2)+\int d^3r_1d^3r_2V(\vec{r}_1,\vec{r}_2)\psi_S(\vec{r}_1,\vec{r}_2)\psi_S(\vec{r}_1,\vec{r}_2)
\end{aligned}
$$

$$
\begin{aligned}
&C_S^2\int d^3r_1d^3r_2\left(\psi_a(\vec{r}_1)\psi_b(\vec{r}_2)+\psi_b(\vec{r}_1)\psi_a(\vec{r}_2)\right)\left(-\frac{\hbar^2}{2m}(\nabla_1^2+\nabla_2^2)\right)\left(\psi_a(\vec{r}_1)\psi_b(\vec{r}_2)+\psi_b(\vec{r}_1)\psi_a(\vec{r}_2)\right)=\\
&=\int d^3r_1d^3r_2\left(\psi_a(\vec{r}_1)\psi_b(\vec{r}_2)+\psi_b(\vec{r}_1)\psi_a(\vec{r}_2)\right)\times\\
&\times\left(-\frac{\hbar^2}{2m}(\psi_b(\vec{r}_2)\nabla_1^2\psi_a(\vec{r}_1)+\psi_a(\vec{r}_2)\nabla_1^2\psi_b(\vec{r}_1)+\psi_b(\vec{r}_1)\nabla_2^2\psi_a(\vec{r}_2)+\psi_a(\vec{r}_1)\nabla_2^2\psi_b(\vec{r}_2))\right)
\end{aligned}
$$

Consideriamo solo la parentesi con il laplaciani

$$
\begin{aligned}
&-\frac{\hbar^2}{2m}(\psi_b(\vec{r}_2)\nabla_1^2\psi_a(\vec{r}_1)+\psi_a(\vec{r}_2)\nabla_1^2\psi_b(\vec{r}_1)+\psi_b(\vec{r}_1)\nabla_2^2\psi_a(\vec{r}_2)+\psi_a(\vec{r}_1)\nabla_2^2\psi_b(\vec{r}_2))=\\
&=-\frac{\hbar^2}{2m}\left(\psi_b(\vec{r}_2)\psi_a(\vec{r}_1)\left(\frac{1}{a^2}-\frac{2}{a\,|\vec{r}_1-\vec{r}_a|}\right)+\psi_a(\vec{r}_2)\psi_b(\vec{r}_1)\left(\frac{1}{a^2}-\frac{2}{a\,|\vec{r}_1-\vec{r}_b|}\right)\right.\\
&\left.+\psi_b(\vec{r}_1)\psi_a(\vec{r}_2)\left(\frac{1}{a^2}-\frac{2}{a\,|\vec{r}_2-\vec{r}_a|}\right)+\psi_a(\vec{r}_1)\psi_b(\vec{r}_2)\left(\frac{1}{a^2}-\frac{2}{a\,|\vec{r}_2-\vec{r}_b|}\right)\right)=\\
&=-\frac{\hbar^2}{2m}\left(\psi_a(\vec{r}_1)\psi_b(\vec{r}_2)\left(\frac{2}{a^2}-\frac{2}{a\,|\vec{r}_1-\vec{r}_a|}-\frac{2}{a\,|\vec{r}_2-\vec{r}_b|}\right)+\psi_b(\vec{r}_1)\psi_a(\vec{r}_2)\left(\frac{2}{a^2}-\frac{2}{a\,|\vec{r}_1-\vec{r}_b|}-\frac{2}{a\,|\vec{r}_2-\vec{r}_a|}\right)\right)=
\end{aligned}
$$

Moltiplicando per $(\psi_a(\vec{r}_1)\psi_b(\vec{r}_2) + \psi_b(\vec{r}_1)\psi_a(\vec{r}_2))$ si trova

$$= -\frac{\hbar^2}{2m}\left(\psi_a(\vec{r}_1)^2\psi_b(\vec{r}_2)^2\left(\frac{2}{a^2} - \frac{2}{a\,|\vec{r}_1 - \vec{r}_a|} - \frac{2}{a\,|\vec{r}_2 - \vec{r}_b|}\right) + \psi_b(\vec{r}_1)^2\psi_a(\vec{r}_2)^2\left(\frac{2}{a^2} - \frac{2}{a\,|\vec{r}_1 - \vec{r}_b|} - \frac{2}{a\,|\vec{r}_2 - \vec{r}_a|}\right)\right.$$
$$\left. + \psi_a(\vec{r}_1)\psi_b(\vec{r}_1)\psi_a(\vec{r}_2)\psi_b(\vec{r}_2)\left(\frac{4}{a^2} - \frac{2}{a\,|\vec{r}_1 - \vec{r}_a|} - \frac{2}{a\,|\vec{r}_2 - \vec{r}_b|} - \frac{2}{a\,|\vec{r}_1 - \vec{r}_b|} - \frac{2}{a\,|\vec{r}_2 - \vec{r}_a|}\right)\right)$$

$$\int d^3r_1 d^3r_2 V(\vec{r}_1, \vec{r}_2)\psi_S(\vec{r}_1, \vec{r}_2)\psi_S(\vec{r}_1, \vec{r}_2) =$$
$$C_S^2 \int d^3r_1 d^3r_2 V(\vec{r}_1, \vec{r}_2)\left(\psi_a(\vec{r}_1)\psi_b(\vec{r}_2) + \psi_b(\vec{r}_1)\psi_a(\vec{r}_2)\right) \cdot \left(\psi_a(\vec{r}_1)\psi_b(\vec{r}_2) + \psi_b(\vec{r}_1)\psi_a(\vec{r}_2)\right) =$$
$$C_S^2 \int d^3r_1 d^3r_2 V(\vec{r}_1, \vec{r}_2)\left(\psi_a^2(\vec{r}_1)\psi_b^2(\vec{r}_2) + \psi_b^2(\vec{r}_1)\psi_a^2(\vec{r}_2) + 2\psi_a(\vec{r}_1)\psi_b(\vec{r}_2)\psi_b(\vec{r}_1)\psi_a(\vec{r}_2)\right) =$$

Dato che

$$\int d^3r_1 d^3r_2 \psi_a(\vec{r}_1)^2\psi_b(\vec{r}_2)^2\left(\frac{2}{a^2} - \frac{2}{a\,|\vec{r}_1 - \vec{r}_a|} - \frac{2}{a\,|\vec{r}_2 - \vec{r}_b|}\right) = \int d^3r_1 d^3r_2 \psi_a(\vec{r}_2)^2\psi_b(\vec{r}_1)^2\left(\frac{2}{a^2} - \frac{2}{a\,|\vec{r}_2 - \vec{r}_a|} - \frac{2}{a\,|\vec{r}_1 - \vec{r}_b|}\right)$$

$$\int d^3r_1 d^3r_2 \psi_a(\vec{r}_1)\psi_b(\vec{r}_2)\psi_b(\vec{r}_1)\psi_a(\vec{r}_2)\left(\frac{2}{a^2} - \frac{2}{a\,|\vec{r}_1 - \vec{r}_a|} - \frac{2}{a\,|\vec{r}_2 - \vec{r}_b|}\right) =$$
$$= \int d^3r_1 d^3r_2 \psi_a(\vec{r}_1)\psi_b(\vec{r}_2)\psi_b(\vec{r}_1)\psi_a(\vec{r}_2)\left(\frac{2}{a^2} - \frac{2}{a\,|\vec{r}_2 - \vec{r}_a|} - \frac{2}{a\,|\vec{r}_1 - \vec{r}_b|}\right)$$

$$\int d^3r_1 d^3r_2 V(\vec{r}_1, \vec{r}_2)\left(\psi_a^2(\vec{r}_1)\psi_b^2(\vec{r}_2)\right) = \int d^3r_1 d^3r_2 V(\vec{r}_1, \vec{r}_2)\left(\psi_b^2(\vec{r}_1)\psi_a^2(\vec{r}_2)\right)$$