Electron Density and the One-Particle Density Matrix

The one particle density matrix is intimately related to the electron density in the system, in that the diagonal element, $\gamma(1,1)$, is equal to the spin density at point 1. Recall that the coordinate 1 means $\vec{r}_1\xi_1$ where $\vec{r}_1$ is the position vector to electron 1 and ξ_1 is the spin of electron 1, either α *or* β. The spin number density at point $\vec{r}\xi$ in this coordinate-spin space is given by the expectation value of the operator

$$\hat{\eta}(\vec{r}\xi) = \sum_{i=1}^{N} \delta(\vec{r}_i\xi_i - \vec{r}\xi)$$

or

$$\hat{\eta}(1,2,3,\cdots,N;1^{''}) = \sum_{i=1}^{N} \delta(i-1^{''})$$

The spin density at $1^{''}$ is given by the expectation value

$$\eta(1^{''}) = \left\langle \psi(1,2,3,\cdots,N) \middle| \hat{\eta} \middle| \psi(1,2,3,\cdots,N) \right\rangle = \left\langle \psi(1,2,3,\cdots,N) \middle| \sum_{i=1}^{N} \delta(i-1^{''}) \middle| \psi(1,2,3,\cdots,N) \right\rangle$$

and using the one particle density matrix, this becomes

$$\eta(1^{''}) = \int_{1^{'}\to 1} d\tau(1)\delta(1-1^{''})\gamma(1,1^{'}) = \int d\tau(1)\delta(1-1^{''})\gamma(1,1) = \gamma(1^{''},1^{''})$$

If we wanted the spatial electron density (number of electrons/volume) we would integrate over the spin coordinate in $\gamma(1,1)$

$$\rho(\vec{r}_1) = \int \gamma(1,1)\, d\xi_1$$