

### Quantum Chemistry Exam I – Solutions

1.) (16 points) Explain or provide an example illustrating each of the following concepts.

a.) Born probability interpretation

The Born probability interpretation states that the probability of finding a particle in the volume  $d\tau = dx dy dz$  between  $(x, y, z)$  and  $(x + dx, y + dy, z + dz)$  is given by  $\psi^* (x, y, z) \psi(x, y, z) d\tau$ .

b.) Normalization

Normalization refers to the scaling of a wavefunction so that the total probability "sums" to 1. Since the wavefunction is expressed in terms of continuous variables, the sum becomes an integral, and the normalization requirement is

$$\int \psi^* \psi d\tau = 1.$$

and the integral is over all space.

c.) Orthogonal functions

Two functions  $f$  and  $g$  are said to be orthogonal if the integral of their product (with one function as the complex conjugate) equals 0.

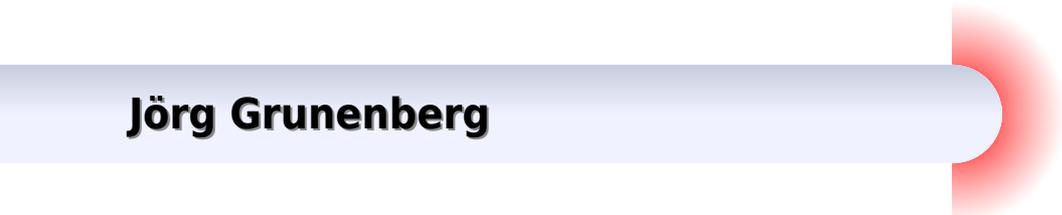
$$\int f^* g d\tau = 0.$$

d.) Tunneling

Tunneling is the penetration of the wavefunction into a classically forbidden region (i.e., a region in which  $E < V$ ).

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**Jörg Grunenberg**



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