# von Laue's Theorem for the Density of States

M. von Laue, Annalen der Physik, **44**, p.1197 (1914)
also H. Weyl, Math. Ann., **71**, p. 441 (1911)
and Vol. 35, Solid State Physics (1980).

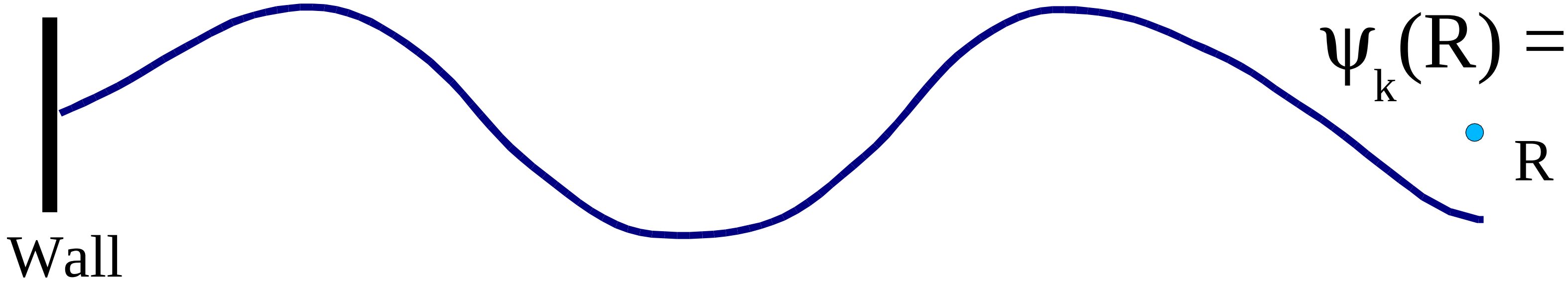
## Locality of Electronic Structure
## or any other wave phenomenon

- Range of the Density Matrix in Linear Scaling Methods.

- Calculations of properties independent of system size.

- Properties of correlated electrons.

# Example: A Free Electron near a Wall




$\psi_k(R) = \sin kR$

Local Density of States: $n(R, E) = (1/k)\sin^2 kR, \quad k = \sqrt{E}$

Change due to the wall: $\delta n(R, E) = -(1/2k)\cos 2kR$

Smoothing function: $f(E-E_0) = \Gamma / [(k - k_0)^2 + \Gamma^2]$

$k_0 = \sqrt{E_0}, \; k_0 R >> 1$, and $\Gamma << k_0$

Smoothed Change: $\int f(E-E_0)\, \delta n(R, E)\, dE = -e^{-2\Gamma R} \cos 2kR$

Effect of Wall decreases exponentially with distance!

# The Local Density of States

$$n(r, E) = \sum |\psi_\alpha(r)|^2 \, \delta(E - E_\alpha)$$

## The Smoothing Function

$f(E - E_0)$ must be analytic (smooth) for real E.

## The Theorem

$$\delta \int f(E-E_0)\, n(r, E)\, dE = \delta_0 \exp\{-\alpha R / \lambda_0\}$$

where R is the distance to a defect or boundary and $\lambda_0$ is the wavelength at $E_0$.

or

$$\delta \int f(E-E_0)\, n(r, E)\, dE = \delta_0 \exp\{-\alpha T / \tau_0\}$$

where T is the time it takes a disturbance to propagate to a defect or boundary and $\tau_0$ is the is the period of the wave at $E_0$.

# Compare to the Total Density of States

- The total density of states is the average of the local density of states over the whole system.
- For a system of side L, $\lambda$/L of the system is closer than one wavelength $\lambda$ to the boundary.
- So the total density of states converges only as 1/L, while while the local density of states converges exponentially in L.

# Conclusions

- The error in the smoothed local density of states decreases exponentially with number of wavelengths to the boundary.
- Or, the error decreases exponentially with the number of periods of the oscillation it takes a disturbance to propagate to the boundary
- Applies to any linear wave equation −Maxwell’s, Schrödinger’s, Heisenberg’s, ...