

# Modern Theory of Macroscopic Polarization and Berry's Phase

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## Quantum-Mechanical Position Operator in Extended Systems

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The position operator (defined within the Schrödinger representation in the standard way) becomes meaningless when periodic boundary conditions are adopted for the wave function, as usual in condensed matter physics. I show how to define the position expectation value by means of a simple many-body operator acting on the wave function of the extended system. The relationships of the present findings to the Berry-phase theory of polarization are discussed. [S0031-9007(98)05419-2]

$$\langle X \rangle = \langle \Phi_0 | \hat{X} | \Phi_0 \rangle = \int dx \, x n(x),$$

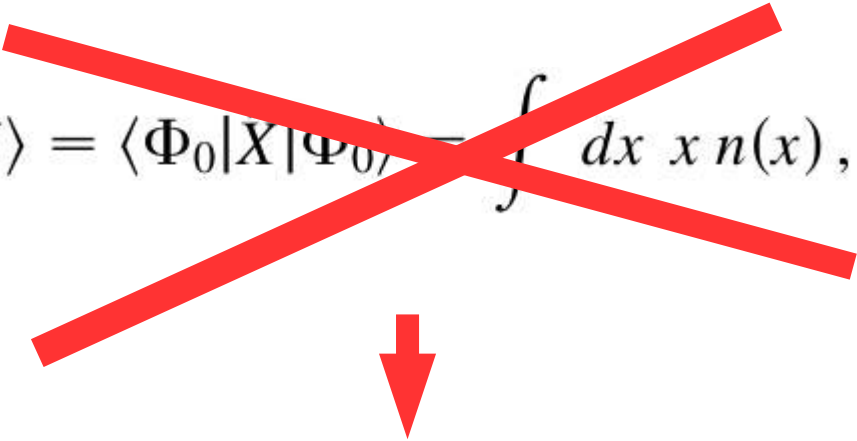
## Quantum-Mechanical Position Operator in Extended Systems

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$$\langle X \rangle = \langle \Phi_0 | X | \Phi_0 \rangle = \int dx \, x n(x),$$



$$\langle X \rangle = \frac{L}{2\pi} \operatorname{Im} \ln \langle \Psi_0 | e^{i \frac{2\pi}{L} \hat{X}} | \Psi_0 \rangle.$$

# Perturbation theory approach to electric fields

Dielectric constants, Born effective charges, piezoelectric constants are physical quantities that involves the treatment of macroscopic electric fields in the crystal.

Perturbation theory has been able to treat these quantities since ever.

- long wavelength approach

$$\exp(iqr)/iq \sim 1/iq + r + \dots, \quad q \rightarrow 0$$

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$$\exp(iqr)/iq \sim 1/iq + r + \dots, \quad q \rightarrow 0$$

- commutator trick

matrix elements of  $r$  are expressed in terms of its commutator with the Hamiltonian:  $[r, H] = i \hbar p + [r, V_{NL}]$



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Tricks only apply to off diagonal matrix elements !

Matrix elements of  $r$  are converted to operations comparing neighboring  $k$ -points  $\rightarrow$  Berry phase

## ***Ab initio* Molecular Dynamics in a Finite Homogeneous Electric Field**

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We treat homogeneous electric fields within density functional calculations with periodic boundary conditions. A nonlocal energy functional depending on the applied field is used within an *ab initio* molecular dynamics scheme. The reliability of the method is demonstrated in the case of bulk MgO for the Born effective charges, and the high- and low-frequency dielectric constants. We evaluate the static dielectric constant by performing a damped molecular dynamics in an electric field and avoiding the calculation of the dynamical matrix. Application of this method to vitreous silica shows good agreement with experiment and illustrates its potential for systems of large size.

$$E^{\mathcal{E}}[\{\psi_i\}] = E^{(0)}[\{\psi_i\}] - \mathcal{E} \cdot P[\{\psi_i\}],$$

$$P[\{\psi_i\}] = -\frac{L}{\pi} \text{Im}(\ln \det S[\{\psi_i\}]),$$

$$S_{ij} = \langle \psi_i | e^{2\pi i x/L} | \psi_j \rangle.$$