

Pair density functional theory

Á. Nagy

*Department of Theoretical Physics,
University of Debrecen,
H-4010 Debrecen, Hungary*

The pair density is a fundamental quantity. The Hohenberg-Kohn theorems have been extented and a pair density functional theory has been obtained [1, 2]. Auxiliary equations have been derived through adiabatic connection [3]. Thus the problem of an arbitrary system with even electrons can be reduced to a two-particle problem. The electron-electron cusp condition and asymptotic behaviour of the effective potential of the two-particle equation have been derived [4]. Exact differential and integral constraints for the kinetic energy pair density functional are presented [5].

References

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