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VARIATIONAL DERIVATION OF EQUATION FOR GENERALIZED PAIR CORRELATION FUNCTION

by

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Abstract

The wavefunction of a system is explicitly written down in a fully anti-symmetric way between a fermion pair and a medium, and the equations for each one of them are derived from the variation of total energy for bound systems and by forming appropriate scalar products for continuum states.

High-energy particles, such as protons, electrons, and nuclei impinging upon spacecraft, produce secondary radiations. In order to protect the internal environment of spacecraft from these radiations, their intensities are determined in many instances theoretically, and an appropriate program has been developed in the High Energy Science Branch [1]. The purpose of this research is to investigate the problem of indistinguishability of an incident projectile with one of the same in a target. For example, when a high-energy incident proton interacts directly with a target proton embedded in a medium, an appropriate scheme must be developed to incorporate the Pauli principle between the two colliding protons, as well as among all the protons in the medium. The natural scheme for this purpose is to partition the total wavefunction Ψ (1 . . . . n), into an anti-symmetrized, two-proton wavefunction, ϕ_α (ij) and an anti-symmetric target wavefunction ψ_β. A completely anti-symmetric wavefunction under this partitioning scheme may be obtained by generalizing the work of references [2, 3],

$$\Psi(12\cdots ij\cdots n)=\sum_{\alpha\beta}\sum_{\substack{ij\\ j=i+1}}(-1)^{i+j}\phi_\alpha(ij)\,\psi_\beta(\bar{i}\,\bar{j}) \tag{1}$$

In equation (2), (1, 2 . . . n) represents coordinates of n-particles, α and β label all quantum numbers needed to define an infinity of states, and $\psi_\beta(\bar{i}\,\bar{j})$ is a function of all but the ith and jth coordinates. The expansion above forms a complete set and normally $\psi_\beta(\bar{i}\,\bar{j})$ would refer to all the states of the target Hamiltonian $H_T(\bar{i}\,\bar{j})$. the function Ψ is completely anti-symmetric if ϕ_α and ψ_β are anti-symmetric with respect to interchange of two adjacent coordinates.

For bound states, the equations for ϕ_α and ψ_β have been derived using the variation of total energy of the system with auxiliary conditions of orthornormality and anti-symmeterization. These are coupled sets of integro-differential equations.

For continuum states of ϕ_α, the appropriate equations are obtained by evaluating the scalar product $\left(\psi_\beta, (H-E)\,\Psi\right)=0$. The structure of the equation for the continuum states of ϕ_α is the same as the one for bound states, but now the modulation of ψ_β due to ϕ_α is neglected.

The expansion (1) provides a complete description of pairs in a state α and is an alternative to Jastrow's ansatz [4], which assumes the correlated part of the wavefunction to be state independent. One may, however, generalize the Jastrow ansatz making the correlation state dependent by multiplying the right-hand side of (1) with symmetric, correlated functions, g (ij). Thus, the generalized Jastrow function is

$$\Psi(12\cdots n) = \Sigma_{\alpha\beta}\, \Sigma_{ij}\, (-1)^{i+j}\, \phi_\alpha(ij) \prod_{k,l}\, g(il)\, g(kj)\, \psi_\beta(\bar{i}\,\bar{j}) \Pi\, g(kl) \tag{2}$$

Although equation (2) may be more convenient to deal with potentials with hard cores, its completeness property needs further investigation.

References

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