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Improvement on the STLS Approach and its Application to the Spin Fully-Polarized Low-Density Electron Gas YASUTAMI TAKADA, ISSP, Univ. of Tokyo, KANAKO YOSHIZAWA, Dept. of Physics, Sophia Univ. — Four decades ago, Singwi, Tosi, Land, and Sjölander (STLS) proposed a theory that treats the local-field factor $G(q)$ and the static structure factor $S(q)$ in a self-consistent fashion. Because of its simplicity in practical calculations and reasonably good results for the correlation energy, this STLS framework has been recognized as a powerful theoretical tool to study short-range correlation beyond the RPA. At the same time, however, it has been realized that the STLS scheme has several shortcomings; among others, it does not satisfy the Pauli principle as exemplified by the fact that the on-top parallel-spin pair distribution function $g_{\uparrow\uparrow}(0)$ becomes negative. In view of this situation, we propose an improved STLS approach in which a special procedure is added to the original STLS framework in order to impose the Pauli principle. This new scheme is successfully applied to the spin-fully polarized electron gas with the electron density parameter r_s ranging from 1 to 100 to find that the correlation energy obtained by quantum Monte Carlo simulations is reproduced very accurately, along with satisfying $g_{\uparrow\uparrow}(0) = 0$ and the non- negativity condition $g_{\uparrow\uparrow}(r) \geq 0$. Implications of our results will be given in the context of the contribution to the density functional theory as well as to the spin structure of the Wigner-lattice state.

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