Coupling of Nonlocal Potentials to Electromagnetic Fields

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Nonlocal Hamiltonians, in particular those employing nonlocal pseudopotentials, are used widely in *ab initio* calculations of material properties. The nonlocality stems from the elimination of undesired or irrelevant degrees of freedom, e.g. core electronic states. To date, attempts to find the coupling of nonlocal systems to external electromagnetic fields have been heuristic or limited to weak or long wavelength fields.

We present (and outline the derivation of) an exact, gauge-invariant, closed-form expression for the coupling of *arbitrary* electromagnetic fields to electronic systems with nonlocal potentials. Aside from justifying and illuminating the various forms of coupling used to date, the result is of essential value for systematic computation of linear and especially nonlinear response functions, and our result provides the explicit mathematical starting points required for these calculations. We will discuss the importance of the gauge-invariance and nonlocality for the following examples: calculation of optical spectra, magnetic susceptibilities, and the response of electrons subject to magnetic fields to external probing fields.