Modern Physics Letters B, Vol. 7, Nos. 29 & 30 (1993) 1941–1946

DENSITY FUNCTIONAL THEORY AND STATISTICAL GAUGE FIELDS

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Received July 1993

We consider the possibility that the exchange-correlation vector potential of density functional theory and the Chern–Simons gauge potential, used to change the statistics of particles in two dimensions, are related. By comparing the corresponding gauge invariant field strengths and their dependence on density and external magnetic field, we find no connection between these two potentials, in contrast to a recent proposal.

Since the seminal papers of Hohenberg and Kohn[1] and Kohn and Sham,[2] density functional theory has emerged as a principal tool for the study of the inhomogeneous interacting electron gas.[3] Among the many important generalizations of the original work is the current-density functional theory of Vignale and Rasolt.[4] These authors show that the exact ground state energy E, density $n(\mathbf{r})$, and current density $\mathbf{j}(\mathbf{r})$ of an interacting electron gas in the presence of applied electric and magnetic fields may be obtained from the solution of an effective single-particle problem. The inclusion of magnetic fields leads to the introduction of an exchange-correlation functional $E_{\rm xc}[n, \mathbf{j}_{\rm p}]$ of density and *paramagnetic* current density $\mathbf{j}_{\rm p}(\mathbf{r})$. For interacting electrons in the presence of an external scalar potential V and vector potential $\mathbf{A}$, both time-independent, these effective single-particle equations have the form

$$\left[\frac{1}{2m}\left(\mathbf{p} - \frac{e}{c}\,\mathbf{A}_{\rm eff}\right)^2 + V_{\rm eff}\right]\psi_\alpha = \epsilon_\alpha \psi_\alpha\,, \qquad (1)$$

where

$$\mathbf{A}_{\rm eff}(\mathbf{r}) = \mathbf{A}(\mathbf{r}) + \mathbf{A}_{\rm xc}(\mathbf{r}) \qquad (2)$$

and

$$V_{\rm eff} = V(\mathbf{r}) + e^2 \int d^3r'\, \frac{n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} + \frac{e^2}{2mc^2}\left[A^2(\mathbf{r}) - A_{\rm eff}^2(\mathbf{r})\right] + V_{\rm xc}(\mathbf{r})\,. \qquad (3)$$

PACS Nos.: 71.10.+x, 11.15.-q, 73.40.Hm, 74.20.Kk.

The exchange-correlation scalar and vector potentials,

$$V_{xc}(\mathbf{r}) \equiv \left.\frac{\delta E_{xc}[n, \mathbf{j}_p]}{\delta n(\mathbf{r})}\right|_{\mathbf{j}_p}, \tag{4}$$

$$\mathbf{A}_{xc}(\mathbf{r}) \equiv \left.\frac{c}{e}\frac{\delta E_{xc}[n, \mathbf{j}_p]}{\delta \mathbf{j}_p(\mathbf{r})}\right|_{n}, \tag{5}$$

account for the effects of exchange and correlation in these otherwise Hartree-like equations. The ground state density n and paramagnetic or canonical current density $\mathbf{j}_p$ for N electrons are given by

$$n = \sum_{\alpha} |\psi_\alpha|^2 \tag{6}$$

and

$$\mathbf{j}_p = \sum_{\alpha} \frac{\hbar}{2mi}\left[\psi_\alpha^* \nabla \psi_\alpha - (\nabla \psi_\alpha^*)\psi_\alpha\right], \tag{7}$$

where the summations are over the N lowest "energy" states of (1). The total gauge-invariant current density is

$$\mathbf{j} = \mathbf{j}_p + \frac{e}{mc} n\mathbf{A}. \tag{8}$$

The so-called Kohn–Sham equations (1) are to be solved self-consistently since $\mathbf{A}_{eff}$ and V_{eff} are functionals of the density (6) and the paramagnetic current (7).

Since Leinaas and Myrheim,[5] Wilczek,[6] and others[7] showed that a Chern–Simons gauge field, introduced through a singular gauge transformation, changes the statistics of particles confined to two space dimensions, the technique of introducing this so-called *statistical* gauge field has been common in the analysis of two-dimensional correlated electron systems. Statistical gauge fields have been used in theories of high-temperature superconductivity for compounds with planar structure,[7,8] in the studies of off-diagonal long-range order in the fractional quantum Hall effect[9] and in the construction of low-energy effective field theories of the quantum Hall effect.[9,10]

In a recent paper,[11] Dharma-Wardana has made the intriguing proposal that the Chern–Simons gauge potential, appearing in the standard Landau–Ginzburg effective field theory of the quantum Hall effect, may be interpreted as an exchange-correlation vector potential for a two-dimensional interacting electron system. If this proposal is correct, it would provide an example of *dynamically generated* statistical gauge fields, where interactions change the statistics of the constituent particles. For the study of two-dimensional strongly correlated electron systems, this possibility is certainly an interesting one.

We have also considered this question, and have arrived at the opposite conclusion, for the reasons summarized in this note. We do not prove that Dharma-Wardana's proposal is an impossibility, but rather, we consider two-dimensional