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LETTER

Steady-state Current Density Represented by a Velocity Vector Potential in an Inhomogeneous Electron Fluid in a Magnetic Field

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For a steady-state current density $J(r)$, the continuity equation reduces to div $J = 0$. In analogy with the description of a magnetic field **B** by a vector potential **A,** we propose to describe **J(r)** by a velocity vector potential **V(r).** Naturally, as with **A, V** is arbitrary to within the addition of the gradient of any scalar. The utility of $V(r)$ is illustrated by constructing it for a model of independent harmonically confined electrons in a constant magnetic field. The **r** dependence of **V(r)** is shown in this model to be completely determined by an equilibrium property, namely the Slater sum $Z(r, \beta)$. By explicit construction of the velocity vector potential for an inhomogeneous electron fluid in the regime of weak magnetic field plus semiclassical mechanics, it is demonstrated that a nonequilibrium property, namely current density, is linked directly with the equilibrium Slater sum for somewhat more general axially symmetric potentials than the purely harmonic form.

KEY WORDS: Velocity vector potential, current, magnetic field.

In a previous study¹, we have calculated the current density $J(r)$ for independent harmonically confined electrons in a constant magnetic field. The conclusion from that work is that a steady current is induced by a magnetic field on the nonuniform charge distribution characterizing this model of an inhomogeneous electron fluid.

Motivated by this conclusion, we wish here to propose the use of a velocity vector potential **V(r)** to describe any steady-state current density **J(r).** For such a steady-state situation, the usual continuity equation relating div **J(r)** to the time-derivative of the density reduces to

$$
\text{div } \mathbf{J}(\mathbf{r}) = 0. \tag{1}
$$

We then work in complete analogy with the introduction of a vector potential **A**

characterizing a magnetic field **B.** This latter quantity satisfies the Maxwell equation

$$
\text{div } \mathbf{B} = 0,\tag{2}
$$

allowing **B** to be written in the form

$$
\mathbf{B} = \text{curl } \mathbf{A}.\tag{3}
$$

Thus, we shall define the velocity vector potential **V(r)** introduced above by

$$
\mathbf{J}(\mathbf{r}) = \text{curl } \mathbf{V}(\mathbf{r}) \tag{4}
$$

which automatically satisfies Eq. (1). Just as with **A** introduced in Eq. **(3), V(r)** defined through Eq. (4) is arbitrary to within the addition of the gradient of any scalar.

To illustrate the usefulness of **V(r),** let us return to the model of Ref. *[l].* There, the current density **J** has the form

$$
\mathbf{J} = J_x \mathbf{i} + J_y \mathbf{j} \tag{5}
$$

with **i** and **j** the usual Cartesian unit vectors in the **x** and *y* directions, respectively. One then finds

$$
J_x = -y[\phi(\beta) - \phi(\beta, k = 0)]Z(\mathbf{r}, \beta),\tag{6}
$$

with an analogous expression for J_y . In Eq. (6), $Z(r, \beta)$ is the Slater sum, *k* is the force constant of the harmonic potential, while $\phi(\beta)$ is the phase factor entering the off-diagonal Slater sum, which is the so-called canonical density matrix.

It is now a fairly straight matter to construct a particular **V(r)** from **Eq.** (4) which will reproduce the current density in **Eq. (6).** We take

$$
V = (0, 0, V_z) \tag{7}
$$

and then find

$$
V_z(\mathbf{r}) = \frac{\left[\phi(\beta) - \phi(\beta, k = 0)\right]}{8h(\beta)} Z(\mathbf{r}, \beta), \tag{8}
$$

where $h(\beta)$ is the "nonhomogeneity factor" appearing in the model Slater sum:

$$
Z(\mathbf{r}, \beta) = f(\beta) \exp\left[-4(x^2 + y^2)h(\beta)\right].\tag{9}
$$

What seems to us remarkable is that, in this particular model, the entire spatial dependence of $V_z(\mathbf{r})$ is contained in the Slater sum $Z(\mathbf{r}, \beta)$. In turn, through Eq. (4),

this "equilibrium" quantity determines the spatial shape of the current density **J(r).** In the above model, the Slater sum $Z(r, \beta)$ is simply a Gaussian in the (x, y) plane.

Prompted by the above exactly soluble model, we next enquire whether the link exposed between a nonequilibrium property $J(r, \beta)$ and the Slater sum $Z(r, \beta)$ is robust enough to survive a generalization of the harmonic oscillator axially symmetric potential $\frac{1}{2}k(x^2 + y^2)$ to $\mathcal{V}(x^2 + y^2)$. Below we denote by \mathcal{V}' the first derivative of $\mathscr V$ with respect to its argument $(x^2 + y^2)$. Instead of now specifying the form of $\mathscr V$, we shall explicitly construct the velocity vector potential in the regime of weak magnetic fields plus semiclassical mechanics. The latter constraint imposes conditions on the smallness of higher derivatives than *Y'* of the potential.

Our starting point^{2,3} is the result for the current density $J(r, \beta)$ in this weak field semiclassical regime:

$$
\mathbf{J}(\mathbf{r}, \beta) = -\frac{\beta^2}{6} C_0(\beta) \exp\left[-\beta \mathcal{V}(\mathbf{r})\right] \mathbf{B} \times \nabla \mathcal{V},\tag{10}
$$

where $C_0(\beta)$ is the partition function for free electrons.

Writing again $J = \text{curl } V$, it is straightforward to verify that

$$
V = (0, 0, V_z), \tag{11}
$$

where

$$
V_z = \frac{\beta B}{12} C_0(\beta) \exp(-\beta \mathcal{V}).
$$
 (12)

 J_x and J_y then follow in terms of $y\mathscr{V}'$ and $x\mathscr{V}'$, respectively, as in Eq. (10). It will be noted that, *as is* the case in the exactly soluble model of axially symmetric harmonic confinement and arbitrary field strength *B,* the velocity potential **V** is determined completely in its spatial dependence by the Slater sum $Z(r, \beta)$, which now has the semiclassical, field-independent form $C_0(\beta)$ exp $[-\beta \mathcal{V}(r)]$.

In summary, we introduce here the concept of a velocity vector potential **V(r)** to characterize a steady-state current density **J(r).** As with the usual vector **potential** $A(r)$ describing a magnetic field $B(r)$, $V(r)$ is arbitrary to within the addition of the gradient of any scalar. For the model of independent, harmonically confined electrons in a constant magnetic field, a form of **V(r)** is derived. Remarkably, **V(r)** in its entire **r** dependence is then characterized by the Slater sum $Z(r, \beta)$ in this model. Thus the spatial shape of the current density $J(r)$ is completely specified by the "equilibrium" Slater sum in this case of an inhomogeneous electron fluid in a magnetic field.

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References

- **1. G. R. Freeman and N. H. March,** *Phys. Rev. A* **45, 6879 (1992).**
- **2. R. A. Harris and J. A. Cina,** *J. Chern. Phys.* **79, 1381 (1983).**
- **3. C. Amovilli and** N. **H. March,** *Phys. Rev. A* **43, 2528 (1991).**