Addendum to "Variational principle for Poisson's equation for an impurity ion in a medium with spatially variable dielectric constant"

K. R. Brownstein
Department of Physics and Astronomy, University of Maine, Orono, Maine 04469
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In the above-named paper, a variational principle was proposed to solve the problem of calculating the potential due to an impurity ion. This variational principle included the heretofore neglected $\vec{\nabla}K$ term, where K is the spatially variable dielectric constant. This approach was still approximate, in that only the linearized theory (charge density ρ linear in the potential ϕ) was treated. In this note, the treatment is extended to include the nonlinear case exactly into an equivalent variational principle.

Poisson's equation for the potential ϕ of a charged donor ion is[1]

$$\vec{\nabla}\cdot(K\vec{\nabla}\phi)+4\pi\rho=0\,, \tag{1}$$

where the effective dielectric constant is a function of the distance to the ion site $K=K(r)$. The charge density ρ is itself a function of the potential ϕ,

$$\rho=C[\mathfrak{F}_{1/2}(\eta_\nu)-\mathfrak{F}_{1/2}(\eta_\nu+e_0\phi/k_BT)]\,, \tag{2}$$

where the constant C is given by

$$C=2e_0(2\pi m^*k_BT)^{3/2}h^{-3}\,. \tag{3}$$

Here η_ν is the reduced Fermi level, m^* is an effective mass, $\mathfrak{F}_{1/2}$ is a Fermi-Dirac integral,

$$\mathfrak{F}_k(z)=\frac{1}{k!}\int_0^\infty\frac{x^k dx}{e^{x-z}+1}\,, \tag{4}$$

and the remaining symbols have their usual meaning.

Several variational principles have recently been formulated to solve approximately Eq. (1). Csavinszky[1] first neglected the $\vec{\nabla}K$ term in (1) and linearized (2) with respect to ϕ. Later, Csavinszky[2] treated the nonlinear case by a power-series expansion of Eq. (2) while still neglecting the $\vec{\nabla}K$ term. Brownstein[3] showed how to incorporate the $\vec{\nabla}K$ term into the linear case. Treating the $\vec{\nabla}K$ term in a manner similar to that in Ref. 3, Csavinszky[4] included the $\vec{\nabla}K$ term into the nonlinear case [again, by power-series expansion of Eq. (2)].

The purpose of this note is to present a variational principle which includes the $\vec{\nabla}K$ term and treats the nonlinear case exactly (rather than by power-series expansion). This variational principle is

$$\delta\int F(\phi,\vec{\nabla}\phi,\vec{r})dV=0\,, \tag{5a}$$

where

$$F=\tfrac{1}{2}K\vec{\nabla}\phi\cdot\vec{\nabla}\phi-4\pi C \times[\phi\mathfrak{F}_{1/2}(\eta_\nu)-(k_BT/e_0)\mathfrak{F}_{3/2}(\eta_\nu+e_0\phi/k_BT)]\,. \tag{5b}$$

With the aid of the identity

$$\frac{d}{dz}\mathfrak{F}_k(z)=\mathfrak{F}_{k-1}(z)\,, \tag{6}$$

one sees that the Euler-Lagrange equation applied to (5b) yields (1). In closing, we note that the case of a tensor dielectric constant could easily be accommodated into the formalism by using $\frac{1}{2}\vec{\nabla}\phi\cdot\vec{\mathrm{K}}\cdot\vec{\nabla}\phi$ as the first term in Eq. (5b).

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[1] P. Csavinszky, Phys. Rev. B 14, 1649 (1976).
[2] P. Csavinszky, Phys. Rev. B 17, 3177 (1978). For an erratum see *ibid.* 18, 2966 (1978).
[3] K. R. Brownstein, Phys. Rev. B 15, 5073 (1977).
[4] P. Csavinszky, Phys. Rev. B 20, 4372 (1979).

