

Comments

Comments are short papers which criticize or correct papers of other authors previously published in the Physical Review. Each Comment should state clearly to which paper it refers and must be accompanied by a brief abstract. The same publication schedule as for regular articles is followed, and page proofs are sent to authors.

Comment on "Solution of a nonlinear Poisson's equation for the potential of impurity ions in semiconductors with a spatially variable dielectric constant by an equivalent variational method"

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Several errors in the above-mentioned paper are pointed out. In particular, an incorrect boundary condition at $r=0$ (which had been previously corrected by others) is again rectified. Finally, an alternate variational functional is presented which yields the nonlinear Poisson's equation exactly (rather than approximately).

In the above-named paper, Mohammad¹ considers a Poisson equation associated with an impurity ion potential. This differential equation for the potential $\varphi(r)$ is

$$\epsilon \left[\frac{d^2\varphi}{dr^2} + \frac{2}{r} \frac{d\varphi}{dr} \right] + \frac{d\epsilon}{dr} \frac{d\varphi}{dr} + G(\varphi) = 0, \quad (1)$$

where

$$G(\varphi) = 4\pi A [\mathcal{F}_{1/2}(\eta) - \mathcal{F}_{1/2}(\eta + e_0\varphi/kT)]. \quad (2)$$

Here $\mathcal{F}_{1/2}$ is the Fermi-Dirac integral, η is the reduced Fermi level, $\epsilon(r)$ is the spatially variable dielectric constant, and A is a constant. By approximating the $\mathcal{F}_{1/2}$ function as a polynomial, Mohammad recasts the problem into an equivalent variational principle. There are several errors which we wish to point out.

(a) The expression for L_1 [his equation (19)] should not have the multiplicative factors of "a" and "b."

(b) The expression for L_2 [his equation (20)] should involve the square of the derivative rather than the derivative of the square.

(c) The correct boundary condition for $\varphi(r)$ at $r=0$, corresponding to a proton of charge e_0 at the origin, is

$$\varphi(r) \rightarrow \frac{e_0}{\epsilon(0)r} \quad \text{for } r \rightarrow 0. \quad (3)$$

Here $\epsilon(0)$ is the value of the dielectric constant at the origin [not to be confused with ϵ_0 , which is the bulk value of the dielectric constant, i.e., $\epsilon(\infty)$]. This misconception concerning the boundary condition at the origin has appeared previously in the literature² and was subsequently corrected by Csavinszky.³

(d) Mohammad employs a sequence of changes of dependent variable. Starting with the actual potential φ , one has $\psi=r\varphi$ followed by $\Phi=\epsilon^{1/2}\psi$. When these are taken into account, the boundary condition for $\Phi(r)$ at

the origin becomes

$$\Phi(r) \rightarrow \frac{e_0}{\epsilon(0)^{1/2}} \quad \text{for } r \rightarrow 0 \quad (4)$$

and not e_0/ϵ_0 as stated in the above-mentioned paper.

(e) Next a trial function

$$\Phi(r) = Ce^{-ar} + De^{-br} \quad (5)$$

is chosen. In view of the above remarks, the correct relation between the coefficients C and D should be

$$D = \frac{e_0}{\epsilon(0)^{1/2}} - C \quad (6)$$

rather than $D=C-1$ as stated in the above-mentioned paper.

(f) Mohammad discusses the extremalization procedure, later remarking that the method is "simple." He claims that one can extremalize the functional $L(C,a,b)$ with respect to C to obtain $C(a,b)$. Yet the original L is a polynomial of order 10 in C . To extremalize it would require finding the roots of a ninth-order polynomial. He proposes that one choose b and then determine whether the two a values from the $\partial L/\partial a=0$ and $\partial L/\partial b=0$ extremalization equations agree with each other. We raise the point that all of this must be done *numerically* for each pair of values (a,b) . Using his suggested increments ($\Delta a = \Delta b = 0.0001$) and assuming that a and b are of the order unity (he does not give any units for these values), one can estimate $10^4 \times 10^4 = 10^8$ numerical integrations for each value of C . Thus his suggestion for implementing the method would be computationally impractical. Of course there are better search procedures available for carrying out the extremalization.

Finally, one might also question why Mohammad first approximates the $\mathcal{F}_{1/2}$ function in the differential equa-

tion and then concocts a variational principle to reproduce this approximated equation. A more logical procedure would be to first find an exact variational principle and then make what approximations are deemed convenient for implementing it. To this end, we offer the following variational principle *pro bono*:

$$\delta L[\varphi]=0, \quad (7)$$

$$L[\varphi]=\int_{r=0}^{r=r_0} F\left[\varphi, \frac{d\varphi}{dr}, r\right] dr; \quad (8)$$

where

$$F\left[\varphi, \frac{d\varphi}{dr}, r\right]=\frac{1}{2}\epsilon r^2\left[\frac{d\varphi}{dr}\right]^2+\frac{1}{3}r^3G(\varphi)\left[\frac{d\varphi}{dr}\right]. \quad (9)$$

Direct substitution of this into the Euler-Lagrange equation yields Eq. (1). This variational principle, Eqs. (7)–(9), is similar to one proposed previously by Brownstein⁴ but is perhaps even simpler in that it involves only the \mathcal{F}_j function of order $j=\frac{1}{2}$ rather than $j=\frac{3}{2}$ as in Ref. 4. One could now make any suitable approximation (e.g., a polynomial fit) to the $\mathcal{F}_{1/2}$ function in G ; however, an ordinary table look-up plus interpolation might be the most expedient procedure to follow.

¹S. N. Mohammad, Phys. Rev. B **46**, 13 152 (1992).

²P. Csavinszky, Phys. Rev. B **14**, 1649 (1976).

³P. Csavinszky, Int. J. Quantum Chem. **13**, 221 (1978).

⁴K. R. Brownstein, Phys. Rev. B **22**, 2131 (1980).