Action

Consider

$$A(\vec{c}) \equiv \int \left(\nabla\Phi(\vec{x},\vec{c}) \bullet \nabla\Phi(\vec{x},\vec{c})/2 \right) d\tau \qquad (1.1)$$

Take the partial with respect to c_i

$$\frac{\partial A(\vec{c})}{\partial c_i} \equiv \int \left(\nabla\Phi(\vec{x},\vec{c}) \bullet \frac{\partial \nabla\Phi(\vec{x},\vec{c})}{\partial c_i} \right) d\tau \qquad (1.2)$$

Interchange the derivative order – usually O.K.

$$\frac{\partial A(\vec{c})}{\partial c_i} \equiv \int \left(\nabla\Phi(\vec{x},\vec{c}) \bullet \frac{\nabla \partial\Phi(\vec{x},\vec{c})}{\partial c_i} \right) d\tau \qquad (1.3)$$

Assume that changes in c_i do not effect the boundary conditions, That is assume that On the boundary $\frac{\partial \Phi}{\partial c_i} = 0$ and then integrate by parts to find

$$\frac{\partial A(\vec{c})}{\partial c_i} \equiv \int \left(\left(-\nabla^2\Phi(\vec{x},\vec{c}) \right) \frac{\partial\Phi(\vec{x},\vec{c})}{\partial c_i} \right) d\tau \qquad (1.4)$$

If A is a minimum the partial in (1.4) is zero or for a complete set of c's

$$\nabla^2\Phi(\vec{x},\vec{c}) = 0 \qquad (1.5)$$

This is Laplace's equation for the potential inside a conductor.

This shows that if this potential is written as a function of a vector **c,** minimizing (1.1) with respect to the constants in **c** is equivalent to solving Laplace's equation.

Action ➔Poisson's equation

The action that gives rise to Poisson's equation contains an extra term

$$A(\vec{c}) \equiv \int \left(\nabla\Phi(\vec{x},\vec{c}) \bullet \nabla\Phi(\vec{x},\vec{c})/2 - (e/\varepsilon_0) n(\vec{x}) \Phi(\vec{x},\vec{c}) \right) d\tau \qquad (2.1)$$

Again set the derivative with respect to c_i equal to zero

$$\frac{\partial A(\vec{c})}{\partial c_i} = \int \left(\nabla\Phi(\vec{x},\vec{c}) \bullet \frac{\partial \nabla\Phi(\vec{x},\vec{c})}{\partial c_i} - (e/\varepsilon_0) n(\vec{x}) \frac{\partial\Phi(\vec{x},\vec{c})}{\partial c_i} \right) d\tau = 0 \qquad (2.2)$$

Integrate the first term in **(2.2)** by parts assuming that $\left. \frac{\partial \nabla\Phi(\vec{x},\vec{c})}{\partial c_k} \right)_{\vec{x}\to Surface} = 0$ to find

$$\frac{\partial A(\vec{c})}{\partial c_k} = \int \left(-\nabla^2\Phi(\vec{x},\vec{c}) - (e/\varepsilon_0) n(\vec{x}) \right) \frac{\partial\Phi(\vec{x},\vec{c})}{\partial c_k} d\tau = 0 \qquad (2.3)$$

This is zero for arbitrary values of $\frac{\partial \nabla\Phi(\vec{x},\vec{c})}{\partial c_k}$ if and only if

$$\nabla^2\Phi(\vec{x},\vec{c}) = -(e/\varepsilon_0) n(\vec{x}) \qquad (2.4)$$

Poisson's equation can be solved with a sufficiently flexible $\Phi(\mathbf{x},\mathbf{c})$ – satisfying the boundary conditions by simply finding the **c** for which **(2.1)** is a minimum.

Action for Electron Density in a 1d system

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$$n_e(\Phi) = \alpha \exp(\beta e \Phi) \qquad (3.1)$$

Charge neutrality requires

$$\int n_i d\tau = \alpha \int \exp(\beta e \Phi) d\tau \qquad (3.2)$$

Or

$$\alpha = \int n_i d\tau / \int \exp(\beta e \Phi) d\tau \qquad (3.3)$$

The correct Φ minimizes an action defined by

$$A = \int (\nabla\Phi \bullet \nabla\Phi / 2 - (e/e_0) n_i \Phi) d\tau + (1/(e_0\beta)(\int n_i d\tau)\log(\int \exp(\beta e \Phi) d\tau) \quad (3.4)$$

The forms for Φ are restricted to those which satisfy the boundary conditions. The derivative of the last term with respect to c_i is

$$(1/(e_0\beta)) \frac{\int n_i d\tau}{\int \exp(\beta e \Phi) d\tau} \int \beta e \exp(\beta e \Phi) \frac{\partial \Phi}{\partial c_i} d\tau \qquad (3.5)$$

Or

$$(e/e_0) \int \alpha \exp(\beta e \Phi) \frac{\partial \Phi}{\partial c_i} d\tau \qquad (3.6)$$

So that with the usual integration by parts

$$\frac{\partial A}{\partial c_i} = 0 = \int \left(-\nabla^2 \Phi - (e/e_0)\left(n_i - n_e(\Phi)\right)\right) \frac{\partial \Phi}{\partial c_i} d\tau \qquad (3.7)$$

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Energy

The ground state energy is always less than

$$E(\vec{c}) = \frac{\int \left(\nabla\Psi^*(\vec{x},\vec{c}) \bullet \nabla\Psi(\vec{x},\vec{c})/2 + V\Psi^2(\vec{x},\vec{c}) \right) d\tau}{\int \Psi^2(\vec{x},\vec{c}) d\tau} \qquad \mathbf{(4.1)}$$

The derivative with respect to c contains a term from the denominator

$$\frac{\partial E(\vec{c})}{\partial c_i} = \frac{\int \left(\frac{1}{2} \nabla \frac{\partial \Psi^*(\vec{x},\vec{c})}{\partial c_i} \bullet \nabla\Psi(\vec{x},\vec{c}) + \frac{\partial \Psi^*(\vec{x},\vec{c})}{\partial c_i} V \Psi(\vec{x},\vec{c}) \right) d\tau - E \int \frac{\partial \Psi^*(\vec{x},\vec{c})}{\partial c_i} \Psi(

With the usual integration by parts

$$\frac{\partial E(\vec{c})}{\partial c_i}=\frac{\int \frac{\partial \Psi^*(\vec{x},\vec{c})}{\partial c_i}\left(-\frac{\nabla^2\Psi(\vec{x},\vec{c})}{2}+(V-E)\Psi(\vec{x},\vec{c})\right)d\tau+c.c.}{\int \Psi^2(\vec{x},\vec{c})\,d\tau} \quad \textbf{(4.3)}$$

And in **(4.3)** we recognize the Schroedinger equation in the parenthesis that need to be zero. The integral in **(4.1)** is multi-3dimensional but with an intense three d character.
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Variance

The Schroedinger equation can also be solved by minimizing the error coefficient in the Monte-Carlo estimate of <H>.

$$\chi^2(\vec{c})=\frac{\int \frac{\left(\Psi(\vec{x},\vec{c})H\Psi(\vec{x},\vec{c})-<H>\Psi^2(\vec{x},\vec{c})\right)^2}{w(\vec{x})}d\tau}{\left(\int \Psi^2(\vec{x},\vec{c})\,d\tau\right)^2} \quad \textbf{(4.4)}$$

This differs from minimizing the action by the presence of w(x)?? and by the fact that the minimum is now zero rather than <H>. In multi-dimensional situations, using Monte Carlo selection guided by w(x), this becomes

$$\chi^2(\vec{c})=\frac{\sum_{i=1}^{N}\frac{\left(\Psi(\vec{x}_i,\vec{c})H\Psi(\vec{x}_i,\vec{c})-<H>\Psi^2(\vec{x}_i,\vec{c})\right)^2}{w^2(\vec{x}_i)}}{\left(\sum_{i=1}^{N}\frac{\Psi^2(\vec{x}_i,\vec{c})}{w(x_i)}\right)^2} \quad \textbf{(4.5)}$$

In curve fitting the variance is defined as

$$\chi^2(\vec{c})=\iiint_V\left(\frac{f(\vec{r})-f_A(\vec{r},\vec{c})}{\varepsilon(\vec{r})}\right)^2$$

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