Modification of the Delves Variation Principle

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A variation principle, similar to the DELVES principle, is given for the (real) wave function itself. The principle does not give a bound. The relationship between both principles is discussed. — After proper generalization a variation principle for arbitrary probability amplitudes (or generalized FOURIER coefficients) is obtained.

1. Introduction

Variation principles for the bound state wave function $\psi_0(\boldsymbol{r})$ of the SCHRÖDINGER equation

$$H\psi_0 = E_0\psi_0 \tag{1.1}$$

have been given previously by BIEDENHARN and BLATT [1], and by DELVES [2]. The variation principle of BIEDENHARN and BLATT requires trial functions for a complete set of eigenfunctions and is therefore of a rather complicated nature. DELVES succeeded in reducing the number of trial functions to two, $\psi_{0\mathrm{T}}(\boldsymbol{r})$ and $\psi_{1\mathrm{T}}(\boldsymbol{r})$, but his principle determines only the square of the wave function. Moreover, since his variation functional $[\psi_0^*\psi_0]$ is not positiv definite, difficulties may arise in practice as soon as $[\psi_0^*\psi_0]$ turnes out to be negativ for certain values of $\boldsymbol{r}$.

It is the purpose of this paper to show how these difficulties can be removed by a proper modification of the DELVES principle. A principle for ψ_0 itself instead of $|\psi_0|^2$ is given showing a close similarity with the original principle. This similarity, however, becomes less dominant, if the new principle is generalized to a wider class of physical quantities. For then it turns out that the principle – unlike the DELVES case – permits the calculation of probability amplitudes rather than of mean values (sect. 5). As in the paper of DELVES the considerations hold for an arbitrary number of dimensions in the configuration space, with $\boldsymbol{r}$ comprising all variables in the wave function.

2. Modification of the Delves Principle

We restrict ourselves to real HAMILTONians H, so that ψ can be assumed to be real. DELVES considers the equations [3]

$$(H(\boldsymbol{r}') - E_0)\,\psi_0(\boldsymbol{r}') = 0\,,\ \int \psi_0^2(\boldsymbol{r}')\,\mathrm{d}\boldsymbol{r}' = 1\,, \tag{2.1}$$

$$(H(\boldsymbol{r}') - E_0)\,\psi_1(\boldsymbol{r}', \boldsymbol{r}) = (\lambda - \delta(\boldsymbol{r}' - \boldsymbol{r}))\,\psi_0(\boldsymbol{r}') \tag{2.2}$$

where λ is a constant in $\boldsymbol{r}'$. On multiplying (2.2) on the left by $\psi_0(\boldsymbol{r}')$ and integrating we find

$$\lambda = \lambda(\boldsymbol{r}) = \psi_0^2(\boldsymbol{r}). \tag{2.3}$$

Now according to DELVES, independent variation of ψ_0 and ψ_1 in the functional

$$[\psi_0^2] = \psi_0^2(\boldsymbol{r}) + 2\int \psi_0(H - E_0)\,\psi_1\,\mathrm{d}\boldsymbol{r}' \tag{2.4}$$

subject to the normalization (2.1) yields eqs. (2.1), and (2.2) as the EULER–LAGRANGE equations while, conversely, fulfilment of these equations makes the variation of $[\psi_0^2]$ zero, and $[\psi_0^2] = \psi_0^2(\boldsymbol{r})$. Hence (2.4) is a variation principle which determines the square of the wave function to second order,

$$\begin{aligned}\psi_0^2(\boldsymbol{r}) &= \psi_{0\mathrm{T}}^2(\boldsymbol{r}) + 2\int \psi_{0\mathrm{T}}(H - E_0)\,\psi_{1\mathrm{T}}\,\mathrm{d}\boldsymbol{r}' \\ &\quad + O(\varepsilon_0^2, \varepsilon_0\varepsilon_1) \\ &= [\psi_0^2]_{\mathrm{T}} + O(\varepsilon_0^2, \varepsilon_0\varepsilon_1)\end{aligned} \tag{2.5}$$

if the trial functions $\psi_{0\mathrm{T}}$ and $\psi_{1\mathrm{T}}$ are of accuracy ε_0 and ε_1.

In a region where $\psi_{0\mathrm{T}}(\boldsymbol{r})$ is small, $[\psi_0^2]_{\mathrm{T}}$ may well become negative. We therefore look for a way to linearize the expression on the right of (2.4). First we note that equation (2.2) together with (2.3) can be written as

$$\begin{aligned}(H(\boldsymbol{r}') - E_0)\,\psi_1(\boldsymbol{r}', \boldsymbol{r}) &= (\psi_0^2(\boldsymbol{r}) - \delta(\boldsymbol{r}' - \boldsymbol{r}))\psi_0(\boldsymbol{r}') \\ &= \psi_0(\boldsymbol{r})(\psi_0(\boldsymbol{r}')\,\psi_0(\boldsymbol{r}) - \delta(\boldsymbol{r}' - \boldsymbol{r}))\,,\end{aligned} \tag{2.6}$$

where we have made use of

$$f(\boldsymbol{r}')\,\delta(\boldsymbol{r}' - \boldsymbol{r}) = f(\boldsymbol{r})\,\delta(\boldsymbol{r}' - \boldsymbol{r}) \tag{2.7}$$

[1] L. C. BIEDENHARN and J. M. BLATT, Phys. Rev. **93**, 230 [1954].
[2] L. M. DELVES, Nucl. Phys. **41**, 497 [1963].
[3] Notations are slightly changed.

for arbitrary $f(\boldsymbol{r})$. Hence the function

$$\bar{\psi}_1(\boldsymbol{r}', \boldsymbol{r}) = \psi_1(\boldsymbol{r}', \boldsymbol{r})/\psi_0(\boldsymbol{r}) \tag{2.8}$$

satisfies

$$(H(\boldsymbol{r}') - E_0)\,\bar{\psi}_1(\boldsymbol{r}', \boldsymbol{r}) = \psi_0(\boldsymbol{r}')\,\psi_0(\boldsymbol{r}) - \delta(\boldsymbol{r}' - \boldsymbol{r}), \tag{2.9}$$

and (2.4) takes the form

$$\begin{aligned}[\psi_0^2] &= \psi_0^2(\boldsymbol{r}) + 2\,\psi_0(\boldsymbol{r}) \int \psi_0(H - E_0)\,\bar{\psi}_1\,\mathrm{d}\boldsymbol{r}' \\ &= \psi_0^2(\boldsymbol{r}) + 2\,\psi_0(\boldsymbol{r})\,F(\psi_0, \bar{\psi}_1)\end{aligned} \tag{2.10}$$

where we have introduced F for abbreviation. Eq. (2.10) suggests a quadratic completion

$$[\psi_0^2] = (\psi_0(\boldsymbol{r}) + F(\psi_0, \bar{\psi}_1))^2 - F^2(\psi_0, \bar{\psi}_1). \tag{2.11}$$

Now since $F(\psi_0, \bar{\psi}_1)$ vanishes for the solution of (2.1) we have

$$\psi_0(\boldsymbol{r}) + F(\psi_0, \bar{\psi}_1) = [\psi_0], \tag{2.12}$$

and this further suggests that we should try the quadratic expression

$$[\psi_0]_{\mathrm{T}}^2 = [\psi_0^2]_{\mathrm{T}} + F^2(\psi_{0\mathrm{T}}, \bar{\psi}_{1\mathrm{T}}) \tag{2.13}$$

rather than $[\psi_0^2]$ as a variation functional for $\psi_0^2[\boldsymbol{r})$.

Indeed,

$$\delta\{[\psi_0]^2\} = \delta[\psi_0^2] + 2\,F(\psi_0, \bar{\psi}_1)\,\delta F(\psi_0, \bar{\psi}_1) = 0 \tag{2.14}$$

if ψ_0 and $\bar{\psi}_1$ satisfy (2.1) and (2.9). Moreover, since

$$\delta\{[\psi_0]^2\} = 2[\psi_0]\,\delta[\psi_0], \tag{2.15}$$

it follows immediately (apart from the case $[\psi_0] = 0$) that even

$$\delta[\psi_0] = 0\,. \tag{2.16}$$

Consequently, we are lead to consider the "linear" functional

$$[\psi_0]_{\mathrm{T}} = \psi_{0\mathrm{T}}(\boldsymbol{r}) + F(\psi_{0\mathrm{T}}, \bar{\psi}_{1\mathrm{T}}). \tag{2.17}$$

Conversely to (2.16), on varying ψ_0 and $\bar{\psi}_1$ in (2.12) independently, subject to the normalization (2.1), we obtain again the eqs. (2.1), (2.9). The latter can be reduced to (2.2) by means of the substitution (2.8). Hence

$$\begin{aligned}\psi_0(\boldsymbol{r}) &= \psi_{0\mathrm{T}}(\boldsymbol{r}) + \int \psi_{0\mathrm{T}}(H - E_0)\,\bar{\psi}_{1\mathrm{T}}\,\mathrm{d}\boldsymbol{r}' \\ &\quad + O(\varepsilon_0^2, \varepsilon_0\,\varepsilon_1) \\ &= [\psi_0]_{\mathrm{T}} + O(\varepsilon_0^2, \varepsilon_0\,\varepsilon_1)\end{aligned} \tag{2.18}$$

is a variation principle for the wave function itself. In the case of arbitrary variations it leads essentially to the same EULER–LAGRANGE equations as (2.5). Neither principle gives a bound.

The energy E_0 can be removed from (2.18) quite analogous as in the DELVES case by introducing the additional orthogonality condition

$$\int \psi_0\,\bar{\psi}_1\,\mathrm{d}\boldsymbol{r}' = 0 \tag{2.19}$$

which is readily proved by applying the method of LAGRANGian multiplicators. Both principles exhibit a variety of other similarities. For example, writing in (2.18)

$$\psi_{0\mathrm{T}}(\boldsymbol{r}) = \int \psi_{0\mathrm{T}}(\boldsymbol{r}')\,\delta(\boldsymbol{r}' - \boldsymbol{r})\,\mathrm{d}\boldsymbol{r}' \tag{2.20}$$

and substituting for $\delta(\boldsymbol{r}' - \boldsymbol{r})$ the corresponding lower dimensional delta function of a subspace S', yields a variation principle for the function $\int \psi_0\,\mathrm{d}S$ of the remaining coordinates.

3. Comparison of the two Principles

As we have seen, arbitrary variations in both principles lead to the same EULER–LAGRANGE equations provided the functions $\psi_{1\mathrm{T}}$ and $\bar{\psi}_{1\mathrm{T}}$ obey the relation

$$\psi_{1\mathrm{T}} = \bar{\psi}_{1\mathrm{T}} \cdot \psi_0(\boldsymbol{r}) \tag{3.1}$$

where ψ_0 is the *exact* bound state solution of (1.1). Now the question arises whether this close relationship between (2.5) and (2.18) will be maintained if given analytical forms containing a number of parameters α_i are used, and the parameters varied until stationarity is reached. The answer depends on the choice of normalization, or more accurate, of "relative" normalization, between $\psi_{1\mathrm{T}}$ and $\bar{\psi}_{1\mathrm{T}}$. Here relative normalization means a relation of the type (3.1). For in general the stationary values $\alpha_i^{(\mathrm{s})}(\boldsymbol{r})$ of the parameters in both principles will coincide only if the condition

$$\psi_{1\mathrm{T}}(\boldsymbol{r}', \alpha_i) = \bar{\psi}_{1\mathrm{T}}(\boldsymbol{r}', \alpha_i)\,\psi_{0\mathrm{T}}(\boldsymbol{r}, \alpha_i^{(\mathrm{s})}(\boldsymbol{r})) \tag{3.2}$$

is satisfied for the given analytical forms. Eq. (3.2) clearly reflects the above relation (3.1) as a limit, since

$$\psi_{0\mathrm{T}}(\boldsymbol{r}, \alpha_i^{(\mathrm{s})}(\boldsymbol{r})) \to \psi_0(\boldsymbol{r}) \tag{3.3}$$

for sufficiently flexible trial functions $\psi_{0\mathrm{T}}$ and $\psi_{1\mathrm{T}}$. To verify (3.2) we compare the two stationarity conditions:

$$\text{(A)}\qquad \frac{\partial}{\partial \alpha_j}\left\{2\int \psi_{0T}(\alpha_i)\,(H-E_0)\,\psi_{1T}(\alpha_i)\,d\boldsymbol{r}' + \psi_{0T}^2(\boldsymbol{r},\alpha_i)\right\} = 0\,, \quad (j=1,2,\ldots) \tag{3.4}$$

$$\text{(B)}\qquad \frac{\partial}{\partial \alpha_j}\left\{\int \psi_{0T}(\alpha_i)\,(H-E_0)\,\bar{\psi}_{1T}(\alpha_i)\,d\boldsymbol{r}' + \psi_{0T}(\boldsymbol{r},\alpha_i)\right\} = 0\,.$$

Using (3.2) we find

$$\text{(A)}\qquad \psi_{0T}(\boldsymbol{r},\alpha_i^{(s)}(\boldsymbol{r}))\cdot\frac{\partial}{\partial\alpha_j}\int\psi_{0T}(\alpha_i)\,(H-E_0)\,\bar{\psi}_{1T}(\alpha_i)\,d\boldsymbol{r}' + \psi_{0T}(\boldsymbol{r},\alpha_i)\cdot\frac{\partial}{\partial\alpha_j}\psi_{0T}(\boldsymbol{r},\alpha_i) = 0\,, \quad (j=1,2,\ldots) \tag{3.5}$$

$$\text{(B)}\qquad \frac{\partial}{\partial\alpha_j}\int\psi_{0T}(\alpha_i)\,(H-E_0)\,\bar{\psi}_{1T}(\alpha_i)\,d\boldsymbol{r}' + \frac{\partial}{\partial\alpha_j}\psi_{0T}(\boldsymbol{r},\alpha_i) = 0\,.$$

Now assume that (A) in (3.5) determines the parameters $\alpha_i = \alpha_i^{(s)}(\boldsymbol{r})$ as used in (3.2). Since $\psi_{0T}(\boldsymbol{r},\alpha_i)$ does not vanish identically, (A) then reduces to a set of equations of form (B), hence (A) and (B) have equal solutions $\alpha_i^{(s)}(\boldsymbol{r})$.

Take, for example, the one-dimensional case. Following DELVES, the "absolute" normalization for $\bar{\psi}_{1T}$ may be established by the discontinuity of slope in the function $\bar{\psi}_1(x)$. From (2.9) we obtain

$$\left.\frac{d\bar{\psi}_{1T}}{dx'}\right|_{x+\varepsilon} - \left.\frac{d\bar{\psi}_{1T}}{dx'}\right|_{x-\varepsilon} = 1\,, \tag{3.6}$$

and consequently, (3.2) requires [4]

$$\left.\frac{d\psi_{1T}}{dx'}\right|_{x+\varepsilon} - \left.\frac{d\psi_{1T}}{dx'}\right|_{x-\varepsilon} = \psi_{0T}(x,\alpha_i^{(s)}(x)) \tag{3.7}$$

if coincidence of the parameter values in both principles is desired. For the slightly different choice

$$\left.\frac{d\psi_{1T}}{dx'}\right|_{x+\varepsilon} - \left.\frac{d\psi_{1T}}{dx'}\right|_{x-\varepsilon} = \psi_{0T}(x,\alpha_i) \tag{3.8}$$

where the α_i take part in the variation, the stationary values $\alpha_i^{(s)}$ are no longer equal.

The choice (3.2) is of some interest because it allows to derive from (2.11), (2.12) and (2.17) the following simple relation between the variationally calculated quantities of both principles:

$$\begin{aligned}[\psi_0^2]_{ST} &= [\psi_0]_{ST}^2 - F^2(\psi_{0T},\bar{\psi}_{1T})\\ &= [\psi_0]_{ST}^2 - ([\psi_0]_{ST}-\psi_{0ST})^2\\ &= \psi_{0ST}(2[\psi_0]_{ST}-\psi_{0ST})\,.\end{aligned} \tag{3.9}$$

[Here ψ_{0ST} stands for $\psi_{0T}(\boldsymbol{r},\alpha_i^{(s)}(\boldsymbol{r}))$ etc.]

Hence
$$[\psi_0^2]_{ST} \leqq [\psi_0]_{ST}^2. \tag{3.10}$$

Now assume that the exact wave function has one or several zeros $\boldsymbol{r}_k$ (excited state). If the inserted analytical forms ψ_{0T} and ψ_{1T} are not too poor they will be flexible enough to bring about a $[\psi_0]_{ST}$ with zeros $\hat{\boldsymbol{r}}_k$ in the vicinity of the exact zeros. Moreover, ψ_{0ST} itself will have zeros which to some degree can be related to the exact ψ_0. In general [5], however, the zeros of $[\psi_0]_{ST}$ and ψ_{0ST} will not coincide, so that we have

$$\begin{aligned}F_{ST}|_{r=\hat{r}_k} &= \{[\psi_0]_{ST}-\psi_{0ST}\}_{r=\hat{r}_k} \neq 0\,,\\ \{[\psi_0]_{ST}\}_{r=\hat{r}_k} &= 0.\end{aligned} \tag{3.11}$$

For such a situation we may conclude from (3.9) that

$$\{[\psi_0^2]_{ST}\}_{r=\hat{r}_k} < 0 \tag{3.12}$$

i. e. no real value of the wave function can be derived. Since $\hat{\boldsymbol{r}}_k$ approximates the exact $\boldsymbol{r}_k$, the DELVES variation principle with the above choice (3.2) of normalization, as a rule, does not permit the calculation of the zeros of a bound state. The typical behaviour of $[\psi_0^2]_{ST}$ near a zero $\hat{\boldsymbol{r}}_k$ is shown in Fig. 1. Obviously, the function $[\psi_0]_{ST}$ interpolates the values of $\pm([\psi_0^2]_{ST})^{1/2}$ in the vicinity of the region PQ. A quite similar situation may occur

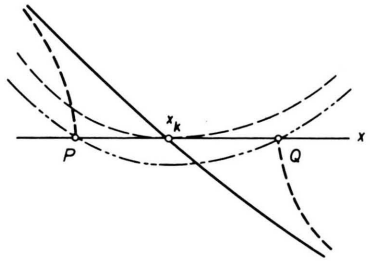

Fig. 1. Behaviour of the variation functionals in the vicinity of a zero x_k. Solid curve $[\psi_0]_{ST}$; dashed curve $[\psi_0]_{ST}^2$; heavy dashed curve $\pm\sqrt{[\psi_0^2]_{ST}}$; dot-and-dash curve $[\psi_0^2]_{ST}$.

[4] DELVES uses sometimes $-\psi_{1T}$ instead of ψ_{1T}, hence the opposite sign in his eq. (4.3).

[5] For special analytical forms of ψ_{0T} and $\bar{\psi}_{1T}$ it is possible to make F_{ST} vanish identically for arbitrary $\boldsymbol{r}$, so that $[\psi_0^2]_{ST} = [\psi_0]_{S}^2$.

cur with the "zero" at $r = \infty$. Since the variation principles (2.5) and (2.18) do not "conserve" the normalization of ψ_{0T}, the functions $[\psi_0]^2_{ST}$ and $[\psi_0^2]_{ST}$ must be re-normalized, and relation (3.9) clearly breaks down for the normalized functions. But since all functions are altered only by positive factors, the qualitative behaviour according to Fig. 1 remains unchanged.

4. Generalization: Variation Principle for Probability Amplitudes [6]

So far we have only cosidered a special case of the DELVES variation principle, namely the principle for the square of the wave function. In general the DELVES' principle holds for the mean values of arbitrary HERMITIAN operators. Hence the question arises whether our principle (2.18) can be generalized to a wider class of physical quantities. This is, in fact, the case. These quantities however, turn out not to be mean values but probability amplitudes (or generalized FOURIER coefficients). This is in agreement with the fact that the wave function itself is a probability amplitude, namely that of a state vector with respect to the eigenstates of the coordinates.

To prove this we start with the equations

$$(H(\boldsymbol{r}') - E_0)\,\psi_0(\boldsymbol{r}') = 0, \quad \int \psi_0^2(\boldsymbol{r}')\,\mathrm{d}\boldsymbol{r}' = 1\,, \tag{4.1}$$

$$(H(\boldsymbol{r}') - E_0)\,\overline{\psi}_1(\boldsymbol{r}', \boldsymbol{r}) = \int \lambda\,\psi_0(\boldsymbol{r}') - a(\boldsymbol{r}') \tag{4.2}$$

which are generalizations of eqs. (2.1) and (2.9) The constant now has the value

$$\lambda = \int \psi_0\, a\,\mathrm{d}\boldsymbol{r}' = \langle \psi_0 \,|\, a \rangle \tag{4.3}$$

which is the probability amplitude of the (real) bound state $|\,\psi_0\rangle$ with respect to a given arbitrary (real) state $|\,a\rangle$. It is then easily shown that

$$\begin{aligned}\langle \psi_0 \,|\, a \rangle = {} & \int \psi_{0T}\, a\,\mathrm{d}\boldsymbol{r}' + \int \psi_{0T}(H - E_0)\,\overline{\psi}_{1T}\,\mathrm{d}\boldsymbol{r}' \\ & + O(\varepsilon_0^2, \varepsilon_0\,\varepsilon_1) \\ = {} & [\langle \psi_0 \,|\, a \rangle]_T + O(\varepsilon_0^2, \varepsilon_0\,\varepsilon_1)\end{aligned} \tag{4.4}$$

is a variation principle for the (real) quantity $\langle \psi_0 \,|\, a \rangle$, provided ψ_{0T} and $\overline{\psi}_{1T}$ are varied as above. By setting $a = \delta(\boldsymbol{r} - \boldsymbol{r}')$ the principle reduces to the special case (2.18). A variation principle for the first derivatives of the wave function is obtained by the choice

$$a = \frac{\partial}{\partial x_i}\,\delta(\boldsymbol{r} - \boldsymbol{r}')\,. \tag{4.5}$$

If $a(\boldsymbol{r}')$ is a complex function variational approximations of $\langle \psi_0 \,|\, \mathrm{Re}\{a\} \rangle$ and $\langle \psi_0 \,|\, \mathrm{Im}\{a\} \rangle$ may be calculated separately from (4.4). Then

$$[\langle \psi_0 \,|\, a \rangle]_{ST} = [\langle \psi_0 \,|\, \mathrm{Re}\{a\} \rangle]_{ST} + i[\langle \psi_0 \,|\, \mathrm{Im}\{a\} \rangle]_{ST}$$

is also variational. Hence, for example, the principle allowes a point by point calculation of the FOURIER transform $\int \psi_0(\boldsymbol{r}') \exp\{(i\,\boldsymbol{k}\,\boldsymbol{r}')\,\mathrm{d}\boldsymbol{r}'\}$ of the (real) bound state $\psi_0(\boldsymbol{r})$ for arbitrary values of $\boldsymbol{k}$.

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[6] A report of this section has been given previously: K. MÜLLER, Physics Letters **11**, 238 [1964].