Perturbation Theory for the One Dimensional Quantum Mechanical Problem and the Lagrange Method

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IN this note the unknown regular solution is represented as the sum, Eq. (1), of two solutions (regular and irregular) with variable coefficients of the unperturbed problem. This representation is unique, and simple equations are obtained for the coefficients by the application of the well-known auxiliary Lagrange condition, Eq. (2) :

$$\varphi_a(r) = c_a(r)\varphi_{0a}(r) + c_b(r)\varphi_{0b}(r), \qquad (1)$$

$$\dot{\varphi} = c_a\dot{\varphi}_{0a} + c_b\dot{\varphi}_{0b}, \qquad (2)$$

where $\dot{\varphi} = d\ \ /dr$. All the functions, including $c_a(r)$ and $c_b(r)$, depend only on the one independent variable r. The proposed method yields unknown expressions for the energy change in the discrete spectrum in a first approximation and for the scattering phase change in the continuous spectrum. The method provides extremely descriptive equations for the change in the wave function itself due to the perturbation. In the case of the discrete spectrum, moreover, a curious equation in the form of a double integral is obtained for the energy change in second order. Let us examine the spherically symmetrical problem of the quantum mechanics of a single particle; after separating the angular variables and introducing $\varphi = r\psi$, where ψ is the wave function, the problem for a definite value for the momentum l is reduced to an equation having the form

$$-(\hbar^2/2m)\ddot{\varphi} + V(r)\varphi - E\varphi = (H-E)\varphi = 0. \qquad (3)$$

Here $V(r)$ also includes, besides the potential, the centrifugal potential $\hbar^2 l(l+1)/2mr^2$.
Equations of second order have two linearly independent solutions. One of them can be selected in such a way that when r is small, then $\varphi_a \sim r^{l+1}$ (regular solution). The second solution φ_b behaves (for small r) as $\varphi_b \sim r^{-l}$. When $E > 0$, φ_a and φ_b behave (at large r) as $\cos(r\sqrt{2mE/\hbar}+\alpha)$, and it is possible to select $\alpha_b = \varphi_b + \pi/2$. Actually the second solution satisifes the equation everywhere, except at $r=0$. The solution of any physical problem is subject to the condition of regularity, i.e., it must be composed of regular functions of the same type as φ_a.

A problem posed in theperturbation theory is to find a φ_a type of solution for a potential $V(r)$ such that $V(r) = V_0(r) + v(r)$, where $v(r)$ is small and the equation for $V_0(r)$ is solved.

Let us substitute Eq. (1) and (2) in Eq. (3). We first examine the case of the continuous spectrum. Since all the functions of φ_{aE}, φ_{0aE}, φ_{obE} apply to the same value for E, we omit the index for E. We bear in mind that c_a and c_b are functions of r. In an elementary way, we obtain

$$\dot{c}_a = -(2v/D)(c_a\varphi_{0a}\varphi_{0b} + c_b\varphi_{0b}^2); \qquad (4)$$

$$\dot{c}_b = (2v/D)(c_a\varphi_{0a}^2 + c_b\varphi_{0a}\varphi_{0b}),$$

$$D = (\hbar^2/m)(\varphi_{0a}\dot{\varphi}_{0b} - \varphi_{0b}\dot{\varphi}_{0a}). \qquad (5)$$

Inasmuch as φ_{oa} and φ_{ob} satisfy the same type of equation as Eq. (3), D does not depend on r.

In order to arrive at the regular solution of the perturbation problem we assume $c_b(0) = 0$ and (correct to the last normalization change) $c_a(0)=1$. In the first order in v we obtain

$$c_a(r) = 1 - \frac{2}{D}\int_0^r v\varphi_{0a}\varphi_{0b}\,dr; \qquad (6)$$

$$c_b(r) = \frac{2}{D}\int_0^r v\varphi_{0a}^2\,dr.$$

Equations (4) are exact. In order for succeeding approximations to differ only slightly from the first approximation, Eq. (6), the well-known condition $\int vr\,dr \ll \hbar^2/2m$ must be satisfied, the smallness of v is not restrictive and the smallness of $\int vr^2\,dr$ is not sufficient. [This condition is obtained by requiring that the second term in expression $c(r)$ in Eq. (6) be small].

When $r < R$, let $v=$ const and let the asymptotic expressions φ_{oa} and φ_{ob} still be valid. Then we have

$c_a = 1 - k_1 v r^2; \quad c_b = k_2 v r^{2l+3};$

$$c_b \varphi_{0b} = k_3 v r^{l+3} \ll \varphi_{0a}$$

for small r, k_1, k_2 and $k_3$are constants.

In the assumed solution, the function φ_{ob}, which has an inadmissible singularity at $r = 0$, entered with coefficient c_b, which approaches zero sufficiently rapidly as $r \to 0$, so that a solution of the form of Eq. (1) is valid everywhere, including the point $r = 0$, where the correct limiting conditions must be imposed on $c_b(0)$.

In the region where v approaches zero, c_a and c_b are constant, and the stucture of the solution is vastly simpler than in the conventional perturbation theory in which the solution of the perturbation problem for a given E is presented as a sum of regular nonperturbed solutions related to all the possible proper values E', with constant (independent of r) coefficients. As is known, these coefficients even become infinite (when E' approaches E) in the conventional first approximation perturbation theory of the continuous specturm.

In particle scattering theory the cross section and phases of scattering may be expressed by the logarithmic derivative $d \ln \varphi_a / dr$. Employing Eq. (1) and Eq. (2), we find

$$d \ln \varphi_a / dr = (c_a \dot{\varphi}_{0a} + c_b \dot{\varphi}_{0b}) / (c_a \varphi_{0a} + c_b \varphi_{0b}).$$

In the perturbation theory, when $|c_b| \ll 1$, $|1 - c_a| \ll 1$ then

$$\frac{d \ln \varphi_a}{dr} = \frac{d \ln \varphi_{0a}}{dr} + \frac{D c_b}{\varphi_{0d}^2} = \frac{d \ln \varphi_{0a}}{dr} + \frac{2}{\varphi_{0a}^2} \int v \varphi_{0a}^2 \, dr. \qquad (7)$$

This familiar relation is usually obtained by considering $\int (\varphi_{0a} H \varphi_a - \varphi_a H_0 \varphi_{0a}) \, dr$.

Let us examine the discrete spectrum. In this case we apply, simultaneously with a perturbation of the potential $V = V_0 + v$, a small (constant) perturbation to the proper value of energy $E = E_0 + \Delta$. If in the non-perturbed problem $(H_0 - E_0)\varphi_0 = 0$ then we must consider

$$(H - E)\varphi = (H_0 + v - E_0 - \Delta)\varphi = 0.$$

In Eq. (4)–(6) let us substitute $v - \Delta$ for v. The proper function of the non-perturbed problem φ_{0a}, which corresponds to E_0, is not only regular when $r = 0$ but falls exponentially when $r \to \infty$. The second linearly independent solution for the non-perturbed problem φ_{0b} grows exponentially as $r \to \infty$. In order to obtain a proper function in the perturbed problem with the correct behavior as $r \to 0$ and $r \to \infty$, it is necessary that $c_b(0) = c_b(\infty) = 0$. In first order approximation theory we obtain

$$\int_0^\infty [v(r) - \Delta] \varphi_{0a}^2 \, dr = \int_0^\infty [v(r) - \Delta] \psi_0^2 r^2 \, dr = 0;$$

$$\int v \psi_0^2 \, d\omega = \Delta \int \psi_0^2 d\omega,$$

where $d\omega$ is the volume element. In this fashion we obtain the well known equation for the energy change to first order,

$$\Delta_{\mathrm{I}} = \int v(r) \psi_0^2 \, d\omega. \qquad (8)$$

Substituting Eq. (6), which was obtained to first order, in the right component of Eq. (4) we find c_b to second order. From the condition that $c_b(\infty) = 0$ we find that the energy change to second order is

$$\Delta_{\mathrm{II}} = \Delta_{\mathrm{I}} - 4 / D \iint [v(r) - \Delta_{\mathrm{I}}] \qquad (9)$$

$$[v(\rho) - \Delta_{\mathrm{I}}] \varphi_{0a}^2(r) \varphi_{0a}(\rho) \varphi_{0b}(\rho) \, d\rho \, dr;$$

where the integral over ρ is from 0 to r, the integral over r is from 0 to ∞, and the normalization is

$$\int \varphi^2{}_{0a} \, dr = 1.$$

Equation (5), in which D = const, permits one to express φ_{0b} by φ_{0a}, thus

$$\varphi_{0b}(\tau) = -D \varphi_{0a}(\tau) \int^\tau [\varphi_{0a}(x)]^{-2} \, dx.$$

The results in Eq. (7) and Eq. (8), in which φ_{0b} does not enter, obviously are not specific to the Lagrange method and can be easily obtained by other means. The same cannot be said of Eq. (9), where φ_{ob} has entered in a clear fashion.

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Internal Bremsstrahlung in Electric Monopole $0^+ \to 0^+$ Nuclear Transitions

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AN electric monopole transition from an excited 0^+ nuclear state to a ground state which also has a zero spin and positive parity will in all probability be accompanied by the formation of conversion electrons or electron-positron pairs. At the same time, both the conversion electron and the components of the pair may emit γ quanta of a continuous spectrum with an upper boundary equal respectively to $E - I$ and $E - 2\mu c^2$ (E is the total energy of the nuclear transition, I the ionization energy, and μ the rest mass of the electron). This investigation presents the results of calculations of the relative probability of internal bremsstrahlung emitted by the components of a pair in a $0^+ \to 0^+$ nuclear transition. As in Ref. 1*, where the same effect is examined in the case of ordinary conversion, the calculation is done in the Born approximation and is therefore applicable only to light nuclei.

The differential probability of internal bremsstrahlung by the emitted pair in an electric monopole transition is ($\hbar = c = 1$)

$$dw = \frac{e^6 Q_0^2}{72(2\pi)^8}\frac{d\omega}{\omega} B\delta(\varepsilon_- + \varepsilon_+ + \omega - E)\, p_- d\varepsilon_- p_+ d\varepsilon_+ d\Omega_{\mathbf{p}_-} d\Omega_{\mathbf{p}_+} d\Omega_{\mathbf{k}}, \tag{1}$$

$$\begin{aligned}B = &-\mu^2(\varepsilon_- - p_- x_-)^{-2}(\varepsilon_+\varepsilon_- + \mathbf{p}_+\mathbf{p}_- + \varepsilon_+\omega + \mathbf{k}\mathbf{p}_+ - \mu^2)\\ &- \mu^2(\varepsilon_+ - p_+x_+)^{-2}(\varepsilon_-\varepsilon_+ + \mathbf{p}_-\mathbf{p}_+ + \varepsilon_-\omega + \mathbf{k}\mathbf{p}_- - \mu^2)\\ &+ \omega(\varepsilon_+\omega + \mathbf{k}\mathbf{p}_+ + \mu^2)/(\varepsilon_- - p_-x_-) + \omega(\varepsilon_-\omega + \mathbf{k}\mathbf{p}_- + \mu^2)/(\varepsilon_+ - p_+x_+)\\ &+ 2[\varepsilon_+^2\varepsilon_-^2 + \varepsilon_-^2\, \mathbf{k}\mathbf{p}_+ + \varepsilon_+^2\, \mathbf{k}\mathbf{p}_- - \mathbf{p}_+\mathbf{p}_-(\mathbf{p}_+\mathbf{p}_- + \mathbf{k}\mathbf{p}_+ + \mathbf{k}\mathbf{p}_-)\\ &+ \mu^2(\mathbf{p}_+\mathbf{p}_- - \varepsilon_+\varepsilon_- - \omega^2)]/(\varepsilon_- - p_-(x_-)(\varepsilon_+ - p_+x_+),\end{aligned}$$

where $Q_0 = \int \Psi_f^*(\mathbf{r})\Psi_i(\mathbf{r})r^2dr$ is the matrix element of the electric monopole operator (Ψ_i and Ψ_f are the initial and final wave functions of the nucleus); $\varepsilon_-, \mathbf{p}_-; \varepsilon_+, \mathbf{p}_+, \omega, \mathbf{k}$ are the energy and momentum respectively of the electron positron, and photon; and

$$x_- = \mathbf{k}\mathbf{p}_- / \omega p_-, \quad x_+ = \mathbf{k}\mathbf{p}_+ / \omega p_+.$$

After integrating over the directions of emergence of all the particles (the nucleus is considered infinitely heavy) and over the energy of one of the components of the pair (the probability equation is symmetrical with regard to the electron and positron) we obtain

$$dw_{\pi,\gamma} = \frac{e^6 Q_0^2}{9(2\pi)^5} F(E;\ W,\ \omega)\, dW\, d\omega, \tag{2}$$

$$\begin{aligned}F(E;\ W,\ \omega) = (1/\omega)\ \{&[5W^2 + 5W\omega + 2\omega^2 - 5(E-2)W - (3E-5)\omega - 5E + 9]\\ &\times \sqrt{(W+1)^2-1}\sqrt{(E-1-W-\omega)^2-1} + \sqrt{(W+1)^2-1}\,[2W^3 + 2W^2\omega + W\omega^2\\ &- 2(2E-3)W^2 - 2(E-2)W\omega + \omega^2 + (2E^2-8E+9)W - (2E-5)\omega\\ &+ 2E^2 - 6E + 5]\ln(E-1-W-\omega+\sqrt{(E-1-W-\omega)^2-1})\\ &+ \sqrt{(E-1-W-\omega)^2-1}\,[-2W^3 - 4W^2\omega - 3W\omega^2 - \omega^3 + 2(E-3)W^2\\ &+ 2(E-4)W\omega + (E-3)\omega^2 + (4E-9)W + 2(E-2)\omega\\ &+ 3E - 5]\ln(W+1+\sqrt{(W+1)^2-1})\\ &- (1+2\omega^2)\ln(W+1+\sqrt{(W+1)^2-1})\cdot\ln(E-1-W-\omega+\sqrt{(E-1-W-\omega)^2-1})\},\end{aligned}$$

where W is the kinetic energy of the electron or positron (the energy is expressed in units of μc^2).