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MATHEMATICS

Analytic Solutions to Nonlinear Boundary Value Problems

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1. INTRODUCTION

The time-dependent Schrödinger equation

$$i\hbar\frac{\partial\psi}{\partial t} = H\psi, \quad H = -\frac{\hbar^2}{2m}\Delta\psi + W(x,t)\psi,$$

admits the separation

$$\psi(x,t) = e^{\frac{Et}{i\hbar}}\psi(x)$$

of variables x and t even in the case of the nonlinear nonlocal potential $W(x, t)$

$$W(x,t) = U(x) + \int\limits_y K[x, y, |\psi(y,t)|]dy.$$

Seeking a stationary solution $\psi(x)$ leads to the following boundary value problem with nonlinear nonlocal potential:

$$-\frac{\hbar^2}{2m}\Delta\psi + W(x)\psi = E\psi,$$

$$W(x) = U(x) + \int\limits_y K[x, y, |\psi(y)|]dy.$$

In applications, Schrödinger equations of the "polaron type," i.e., Bogolyubov–Pekar equations in which the dependence of the potential on the sought function have the simplest form

$$W(x) = U(x) + \int\limits_y K(x,y)\psi^2(y)dy,$$

often arise.

2. STATEMENT OF THE PROBLEM

This paper is concerned with constructing analytic solutions to the one-dimensional Schrödinger equation

$$-\psi'' + W(x)\psi = E\psi,$$

$$W(x) = U(x) + \int\limits_{-\infty}^{+\infty} K(x,y)\psi^2(y)dy.$$

The basic assumption is that the kernel $K(x, y)$ is replaced by its three-term Galerkin approximation

$$K(x,y) = a(x)b(y) + a_1(x)b_1(y) + a_2(x)b_2(y).$$

The standard procedure for decreasing the order, which dates back to d'Alambert's works, yields the following system of two first-order equations:

$$\psi'(x) = -z\psi, \quad z' - z^2 + W = E.$$

In the linear case, the second equation (in z) does not contain ψ and is solved independently; then, the solution ψ is written in the form

$$\psi(x) = C\exp\{-Z(x)\}, \quad Z'(x) = z.$$

In the case under consideration, this procedure gives the following integro-differential equation for the function z:

$$z'(x) - z^2(x) + U(x)$$

$$+ C^2\int\limits_{-\infty}^{+\infty} K(x,y)\exp\{-2Z(y)\}dy = E.$$

3. ANALYTIC SOLUTIONS

We seek the solution z in the form

$$z(x) = p(x) + \alpha q(x), \quad Z(y) = P(y) + \alpha Q(y),$$

where the functions $P(x)$ and $Q(x)$ are antiderivatives of the functions $p(x)$ and $q(x)$; i.e., $P'(y) = p(y)$ and $Q'(y) = q(y)$. Substituting this into the equation and separating the variables x and α, we obtain the following four relations for functions in the variable x and three relations for functions in the parameter α:

$$p'(x) - p^2(x) + U(x) = A, \quad a(x) = 1,$$

$$a_1(x) = q'(x) - 2p(x)q(x), \quad a_2(x) = q^2(x);$$

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$$C^2 \int_{-\infty}^{+\infty} b(y)\exp\{-2Z(y,\alpha)\}dy + A = E,$$

$$C^2 \int_{-\infty}^{+\infty} b_1(y)\exp\{-2Z(y,\alpha)\}dy + \alpha = 0,$$

$$C^2 \int_{-\infty}^{+\infty} b_2(y)\exp\{-2Z(y,\alpha)\}dy - \alpha^2 = 0.$$

The integrals converge if $P(y)$ tends to plus infinity sufficiently rapidly, meaning more rapidly than $Q(y)$. The formulas for the functions $a_i(x)$ and $U(x)$ give a "functional parametrization" of the class of Bogolyubov–Pekar equations. This class is determined by the seven functions

$$U(x),\ a(x),\ a_1(x),\ a_2(x);\quad b(y),\ b_1(y),\ b_2(y),$$

which are expressed via five functions and one number:

$$A;\quad p(x),\ q(x);\quad b(y),\ b_1(y),\ b_2(y).$$

The Bogolyubov–Pekar equation on this "five-dimensional" (determined by five independent functions) variety have the analytic solutions

$$\psi(x) = C\exp\{-P(x) - \alpha Q(x)\}.$$

Eliminating C and E from the system of equations for the sought parameters E, C, and α, we obtain a resolvent $R(\alpha)$, which determines an equation for the parameter α:

$$R(\alpha) = 0.$$

The definition of the resolvent is fairly complicated; namely, it is the integral

$$R(\alpha) \equiv \int_{-\infty}^{+\infty} [b_2(y) + \alpha b_1(y)] \times \exp\{-2P(y) - 2\alpha Q(y)\}dy.$$

The equation $R(\alpha) = 0$ is an analogue of the characteristic ("secular") equation for linear systems. In the finite-dimensional case, $R(\alpha) = D(\alpha)$ is merely a polynomial, and the number of its roots coincides with its degree. In the case under consideration, $R(\alpha)$ can have an infinite set of roots. If we solve this equation $R(\alpha) = 0$, then, for each root α, the parameters C and E are evaluated by the formulas

$$C^2 = \frac{\alpha^2}{\int_{-\infty}^{+\infty} b_2(y)\exp\{-2P(y) - 2\alpha Q(y)\}dy},$$

$$E = A + C^2 \int_{-\infty}^{+\infty} b(y)\exp\{-2P(y) - 2\alpha Q(y)\}dy.$$

4. ISO-SYSTEMS

In the linear case, where $K(x, y) \equiv 0$, the value E can be interpreted as the total energy. In the general case, it can have a completely different physical (or chemical) meaning. However, mathematically, this is always the constant of separation of the space and time variables.

The formula for E implies that, if $b(y) = 0$, then the system is "isoenergetic," because we then have $E \equiv A$ for any α.

5. CONTINUUM OF SOLUTIONS

The qualitative difference between integro-differential equations and ordinary differential equations is clearly seen in the following very interesting special case.

Suppose that the integrand in the expression for the resolvent $R(\alpha)$, which is

$$R(\alpha) \equiv \int_{-\infty}^{+\infty} [b_2(y) + \alpha b_1(y)] \times \exp\{-2P(y) - 2\alpha Q(y)\}dy$$

is the total derivative with respect to the variable y:

$$R(\alpha) = \int_{-\infty}^{+\infty} d[L(y)\exp\{-2P(y) - 2\alpha Q(y)\}].$$

In this case, the integral can be evaluated explicitly:

$$R(\alpha) = [L(y)\exp\{-2P(y) - 2\alpha Q(y)\}]_{y=-\infty}^{y=+\infty},$$

and the resolvent $R(\alpha)$ is identically (for all α) equal to zero:

$$R(\alpha) \equiv 0.$$

Thus, a Bogolyubov–Pekar equation can have not only an infinite set of solution, but also a continuum of solutions (in the example under consideration, they form a one-parameter set). This remarkable fact follows from the identity

$$[b_2(y) + \beta b_1(y)]\exp\{-2P(y) - 2\alpha Q(y)\}dy \equiv d[L(y)\exp\{-2P(y) - 2\alpha Q(y)\}].$$

This identity makes it possible to express two functions $b_1(y)$ and $b_2(y)$ through one (arbitrary) function $L(y)$:

$$b_1(y) = -2L(y)q(y),$$
$$b_2(y) = -2L(y)p(y) + L'(y).$$

In these formulas, $p(y)$ and $q(y)$ are the functions introduced above as $p(x)$ and $q(x)$. Thus, we take one arbitrary number and four arbitrary functions

$$A; \quad P(x), Q(x); \quad b(y), L(y)$$

and determine the seven elements of the Bogolyubov–Pekar equation:

$$U(x) = A + p^2(x) - p'(x), \quad a(x) = 1,$$

$$a_1(x) = q'(x) - 2p(x)q(x), \quad a_2(x) = q^2(x),$$

$$b(y) = b(y), \quad b_1(y) = -2L(y)q(y),$$

$$b_2(y) = -2L(y)p(y) + L'(y).$$

For any α, this equation has the solution

$$\psi(x) = C\exp\{-P(x) - \alpha Q(x)\}.$$

Here,

$$C^2 = \frac{\alpha^2}{\int_{-\infty}^{+\infty} b_2(y)\exp\{-2P(y) - 2\alpha Q(y)\}dy}.$$

6. THE NEIGHBORHOOD OF THE PLANCK–SCHRÖDINGER OSCILLATOR

It is useful to consider the following important special case:

$$A = 1; \quad P(x) = \frac{x^2}{2}, \quad Q(x) = -x;$$

$$b(y) = 0, \quad L(y) = -\varepsilon y.$$

Simple evaluations give

$$U(x) = x^2, \quad K(x, y) = -\varepsilon(1 + 4xy - 2y^2),$$

$$C^2 = \frac{\alpha^2}{\varepsilon\int_{-\infty}^{+\infty} (2y^2 - 1)\exp\{-y^2 - 2\alpha y\}dy},$$

$$\psi(x) = C\exp\left\{-\frac{x^2}{2} - \alpha x\right\}.$$

The complete solution consists of the following two lines in the plane α, C: either $\alpha = 0$ and C is arbitrary (as in the linear case $\varepsilon = 0$) or α is arbitrary and $C^2 = \frac{1}{\varepsilon\sqrt{\pi}}e^{-\alpha^2}$. The following parametrization of the solution is more evident:

$$\psi(x) = B\exp\left\{-\frac{1}{2}(x - \alpha)^2\right\},$$

It shows explicitly the shift (along the x-axis) symmetry of the solution found. In this parametrization, the complete solution consists of two perpendicular lines in the plane α, B: either B is arbitrary and $\alpha = 0$ or α is arbitrary and $B^2 = \frac{1}{\varepsilon\sqrt{\pi}}$.

7. CONCLUSIONS

We have found analytic solutions to the polaron-type Schrödinger equation

$$-\frac{\hbar^2}{2m}\Delta\psi + W(x)\psi = E\psi,$$

i.e., the Bogolyubov–Pekar equation in which the dependence of the potential on the sought function has the simplest form

$$W(x) = U(x) + \int_y K(x, y)\psi^2(y)dy,$$

and the kernel is the three-term Galerkin approximation

$$K(x, y) = a(x)b(y) + a_1(x)b_1(y) + a_2(x)b_2(y).$$

(i) An equation having analytic solutions is determined by the functions A; $p(x)$, $q(x)$, $b(y)$, $b_1(y)$, $b_2(y)$.

$U(x) = A - p'(x) + p^2(x)$,

$a(x) = 1$,

$a_1(x) = q'(x) - 2p(x)q(x)$,

$a_2(x) = q^2(x)$,

$K(x, y) = a(x)b(y) + a_1(x)b_1(y) + a_2(x)b_2(y)$.

To construct a solution, it is necessary to find the antiderivatives $P(x)$ and $Q(x)$ of the functions $p(x)$ and $q(x)$, respectively:

$$P'(y) = p(y), \quad Q'(y) = q(y).$$

First, we construct the resolvent

$$R(\alpha) \equiv \int_{-\infty}^{+\infty} [b_2(y) + \alpha b_1(y)]$$

$$\times \exp\{-2P(y) - 2\alpha Q(y)\}dy.$$

Next, we find the parameter α from the equation

$$R(\alpha) = 0$$

and obtain the solution in the form

$$\psi(x) = C\exp\{-P(x) - \alpha Q(x)\},$$

where

$$C^2 = \frac{\alpha^2}{\int_{-\infty}^{+\infty} b_2(y)\exp\{-2P(y) - 2\alpha Q(y)\}dy},$$

$$E = A + C^2 \int_{-\infty}^{+\infty} b(y)\exp\{-2P(y) - 2\alpha Q(y)\}dy.$$

(ii) An important special feature of nonlinear nonlocal Schrödinger equations is the possibility of the existence of an one-parameter family of solutions. This set arises if we impose additional conditions on the functions of the variable y:

$$b_1(y) = -2L(y)q(y),$$
$$b_2(y) = -2L(y)p(y) + L'(y).$$

In this case, the resolvent is identically equal to zero, i.e.,

$$R(\alpha) \equiv 0$$

and any value of the parameter α gives a solution to the Schrödinger equation.

(iii) **A neighborhood of the Planck–Schrödinger oscillator.** The equation

$$-\psi'' + W(x)\psi = \psi,$$
$$W(x) = x^2 - \varepsilon \int_{-\infty}^{+\infty} (1 + 4xy - 2y^2)\psi^2(y)dy$$

has the one-parameter family of solutions

$$\psi(x) = B\exp\left\{-\frac{1}{2}(x-\alpha)^2\right\}.$$

This family of solutions is invariant with respect to shifts along the x-axis. The complete solution consists of two perpendicular lines in the plane α, B: either B is arbitrary and $\alpha = 0$ or α is arbitrary and $B^2 = \frac{1}{\varepsilon\sqrt{\pi}}$.

The second line tends to infinity as the perturbation approaches zero. This is a quite unexpected result admitting the following paradoxical interpretation: the ordinary differential equations correspond to infinite singular points in the class of nonlinear integro-differential equations.