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MATHEMATICS

The Bogolyubov–Pekar Polaron: Three-Dimensional Solutions

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INTRODUCTION

The Bogolyubov–Pekar polaron is described by the Schrödinger equation

$$-\Delta\psi + W\psi = E\psi$$

with an integral potential nonlinear in $\psi(X)$:

$$W(X) = U(X) + \int_Y K(X, Y)\psi^2(Y)dY.$$

The solution to this equation that corresponds to the ground state can be sought in the form

$$\psi(X) = C\exp\{-Z(X)\}.$$

Calculating the Laplacian

$$\Delta\psi = [-\Delta Z + (\nabla Z)^2]\psi,$$

substituting it into the equation, and canceling out $e^{-Z(X)}$, we obtain

$$\Delta Z - [\nabla Z]^2 + U(X)$$

$$+ C^2\int_Y K(X, Y)\exp\{-2Z(Y)\}dY = E.$$

Consider the special case where the kernel 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 exponent of the exponential can then be represented as

$$Z(X) = P(X) + \alpha Q(X).$$

In what follows, the argument X is omitted from $P(X)$ and $Q(X)$. The equation takes the form

$$\Delta P - (\nabla P)^2 + U + \alpha(\Delta Q - 2\nabla P\nabla Q) - \alpha^2[\nabla Q]^2$$

$$+ C^2\int_Y K(X, Y)\exp\{-2Z(Y)\}dY = E.$$

This equation admits a separation of the variables X and α that depends on an arbitrary constant A. The following four equalities arise for functions of X:

$$U = (\nabla P)^2 - \Delta P + A, \quad a(X) = 1,$$

$$a_1(X) = \Delta Q - 2\nabla P\nabla Q, \quad a_2(X) = [\nabla Q]^2.$$

They define the external field potential $U(X)$ and the functions $a(X)$, $a_1(X)$, and $a_2(X)$ involved in the interaction kernel $K(X, Y)$. The functions $b(Y)$, $b_1(Y)$, and $b_2(Y)$ remain arbitrary.

We also have three equations for the parameters α, C, and E:

$$C^2\int_Y b_1(Y)\exp\{-2Z(Y)\}dY = -\alpha,$$

$$C^2\int_Y b_2(Y)\exp\{-2Z(Y)\}dY = \alpha^2,$$

$$E = A + C^2\int_Y b(Y)\exp\{-2Z(Y)\}dY.$$

Eliminating C from the first two equations gives an equation for α alone:

$$\int_Y [b_2(Y) + \alpha b_1(Y)]\exp\{-2Z(Y)\}dY = 0.$$

The left-hand side of this equation is naturally called the resolvent

$$R(\alpha) \equiv \int_Y [b_2(Y) + \alpha b_1(Y)]\exp\{-2Z(Y)\}dY.$$

After solving the equation $R(\alpha) = 0$ for α, C and E are explicitly determined by the relations

$$C^2 = \frac{\alpha^2}{\int_Y b_2(Y)\exp\{-2Z(Y)\}dY},$$

$$E = A + C^2\int_Y b(Y)\exp\{-2Z(Y)\}dY.$$

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ISOSYSTEMS

In the linear case (when $K(x, y) \equiv 0$), E has the meaning of total energy. In the general case, E may have an entirely different physical (or chemical) meaning. Mathematically, however, this is always a separation constant for spatial and temporal variables. The three-dimensional solutions include a subset of isoenergetic solutions. In this respect, they are entirely analogous to one-dimensional and spherically symmetric solutions. Indeed, consider the special case

$$b(y) = 0.$$

The formula for the "energy" E,

$$E = A + C^2\int_Y b(Y)\exp\{-2Z(Y)\}dY$$

implies that

$$E \equiv A$$

for any α. Hence, the system is isoenergetic.

HIDDEN SYMMETRY

The resolvent depends essentially on $b_1(Y)$ and $b_2(Y)$. These functions can be chosen so that the resolvent becomes identically zero:

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

Such a choice can be made as based on the well-known Ostrogradsky formula

$$\iiint_\Omega \left(\frac{\partial K_1}{\partial y_1} + \frac{\partial K_2}{\partial y_2} + \frac{\partial K_3}{\partial y_3}\right)dy_1dy_2dy_3$$

$$= \iint_\Sigma K_1dy_2dy_3 + K_2dy_3dy_1 + K_3dy_1dy_2.$$

In all calculations of this section, we certainly imply that

$$Y = (y_1, y_2, y_3).$$

Define the functions $K_i(Y)$ as

$$K_1(Y) = A_1(Y)e^{-2Z(Y)}, \quad K_2(Y) = A_2(Y)e^{-2Z(Y)},$$

$$K_3(Y) = A_3(Y)e^{-2Z(Y)}.$$

All of them vanish at infinity, because they contain the factor $e^{-2Z(Y)}$. Therefore, the Ostrogradsky formula can be written as

$$\iiint_Y \left(\frac{\partial K_1}{\partial y_1} + \frac{\partial K_2}{\partial y_2} + \frac{\partial K_3}{\partial y_3}\right)dy_1dy_2dy_3 = 0.$$

The first term in the integrand is found to be

$$\frac{\partial K_1}{\partial y_1} = \left[\frac{\partial A_1}{\partial y_1} - 2A_1\left(\frac{\partial P}{\partial y_1} + \alpha\frac{\partial Q}{\partial y_1}\right)\right]e^{-2Z(Y)}.$$

Calculating and summing the other two terms, we obtain the total divergence

$$\frac{\partial K_1}{\partial y_1} + \frac{\partial K_2}{\partial y_2} + \frac{\partial K_3}{\partial y_3} = [b_2(Y) + \alpha b_1(Y)]\exp\{-2Z(Y)\}.$$

Thus, $b(Y)$ remains arbitrary, while $b_1(Y)$ and $b_2(Y)$ are expressed in terms of the new arbitrary functions $A_1(Y)$, $A_2(Y)$, and $A_3(Y)$ by the formulas

$$b_2(Y) = \frac{\partial A_1}{\partial y_1} + \frac{\partial A_2}{\partial y_2} + \frac{\partial A_3}{\partial y_3} - 2\left(A_1\frac{\partial P}{\partial y_1} + A_2\frac{\partial P}{\partial y_2} + A_3\frac{\partial P}{\partial y_3}\right),$$

$$b_1(Y) = -2\left(A_1\frac{\partial Q}{\partial y_1} + A_2\frac{\partial Q}{\partial y_2} + A_3\frac{\partial Q}{\partial y_3}\right).$$

CONCLUSIONS

The Bogolyubov–Pekar equation admits three-dimensional analytical solutions of the form

$$\psi(X) = Ce^{-P(X) - \alpha Q(X)},$$

if the external field potential $U(X)$ and the functions $a(X)$, $a_1(X)$, and $a_2(X)$ in the interaction kernel $K(X, Y) = a(X)b(Y) + a_1(X)b_1(Y) + a_2(X)b_2(Y)$ are expressed in terms of the given solution by the formulas

$$U = (\nabla P)^2 - \Delta P + A, \quad a(X) = 1,$$

$$a_1(X) = \Delta Q - 2\nabla P\nabla Q, \quad a_2(X) = [\nabla Q]^2.$$

The parameter α is determined by the condition that the resolvent vanishes:

$$R(\alpha) = \int_Y [b_2(Y) + \alpha b_1(Y)]\exp\{-2Z(Y)\}dY = 0.$$

If, additionally, $b_1(Y)$ and $b_2(Y)$ are expressed in terms of the new arbitrary functions

$$A_1(Y), \quad A_2(Y), \quad A_3(Y)$$

by the formulas

$$b_2(Y) = \frac{\partial A_1}{\partial y_1} + \frac{\partial A_2}{\partial y_2} + \frac{\partial A_3}{\partial y_3} - 2\left(A_1\frac{\partial P}{\partial y_1} + A_2\frac{\partial P}{\partial y_2} + A_3\frac{\partial P}{\partial y_3}\right),$$

$$b_1(Y) = -2\left(A_1\frac{\partial Q}{\partial y_1} + A_2\frac{\partial Q}{\partial y_2} + A_3\frac{\partial Q}{\partial y_3}\right),$$

then the resolvent is identically zero:

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

and we obtain a one-parameter family of solutions

$$\psi(X) = Ce^{-P(X) - \alpha Q(X)}$$

of an equation involving no parameters. It should be noted that this class of three-dimensional solutions is wider than the class of corresponding one-dimensional and spherically symmetric solutions [1]. The main difference between these classes is that, in the former case, $b_1(Y)$ and $b_2(Y)$ can be defined in terms of three arbitrary functions

$$A_1(Y), \quad A_2(Y), \quad A_3Y$$

while for one-dimensional and spherically symmetric solutions, $b_1(Y)$ and $b_2(Y)$ are defined only by two functions.

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