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Deriving Energy-Level Gap of Some Dynamic Hamiltonians in Many Particle Physics by Virtue of the Invariant Eigen-Operator Method

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Abstract By virtue of the "invariant eigen-operator" method which originates from the Heisenberg equation of motion, we derive energy-level gap of some dynamic Hamiltonians in many particle physics, which includes a Tomonaga model and spin wave model.

Keywords Invariant eigen-operator · Heisenberg equation · Tomonaga model · Many-particle

1 Introduction

Traditionally, deriving eigen-energy spectra of quantum mechanical dynamic systems [1] is to solving stationary Schrödinger equation when the corresponding Hamiltonian $\hat{H}$ does not include time explicitly, and the solution of Schrödinger equation $\hat{H}\Psi_n = E_n\Psi_n$ is usually obtained by diagonalizing $\hat{H}$ or by recasting the equation into some quantum mechanical representation (e.g. the coherent state and entangled state representations) to become some c-number differential equations. However, in many cases these differential equations are hardly analytically solved, only very limited dynamic systems can be solved exactly and analytically. A question thus emerges: Can we directly employ the Heisenberg equation to derive energy spectra of some dynamic systems in many-particle physics theory? Though the Heisenberg equation is on the same solid footing as the Schrödinger equation, the former is seldom directly employed to derive energy-level information of dynamic systems.

In this work based on the invariant eigen-operator (IEO) method set up in Refs. [2–5] we shall concisely derive the energy spectrum of some many-particle Hamiltonians which

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involve either Bose operators or Fermi operators. Through solving these models one can conclude that this method possesses the universal feature, i.e. it can be not only applied to solving some bosonic models, but also the fermionic ones. In Sect. 2 we shall briefly review the invariant eigen-operator method. In Sect. 3 we shall deal with the famous Tomonaga model [6] ($\hat{H}_1$ in (5)) which describes the one-dimensional electron gas. Usually this model was solved by reducing it to bosonic form after taking some appropriate approximation, though the original model is fermionic. We shall apply IEO method to the approximated Tomonaga model to derive this system's energy-level gap. In Sect. 4 and Sect. 5 we apply the IEO method to the electron–electron interacting Hamiltonian $\hat{H}_2$, and electron–phonon interacting Hamiltonian $\hat{H}_3$ respectively. As one can see shortly later, the IEO method significantly simplifies the energy-gap calculations.

2 The Invariant Eigen-Operator Method

Let us recall the original idea of Schrödinger quantization scheme, he took the identification $i\frac{d}{dt} \longleftrightarrow \hat{H}$, so $i\frac{d}{dt}$ is named the Schrödinger operator in many references. Similarly, we have $(i\frac{d}{dt})^n \longleftrightarrow \hat{H}^n$, now we set up an equation for an operator $\hat{O}_e$,

$$\left(i\frac{d}{dt}\right)^n \hat{O}_e = \lambda \hat{O}_e \tag{1}$$

when $n = 1$, it looks like in form to $i\frac{d}{dt}\psi = \hat{H}\psi$. Thus we call (1) as n-order invariant eigen-operator equation, and λ is the corresponding 'eigenvalue'. Using the Heisenberg equation of motion

$$i\frac{d}{dt}\hat{O}_e = \big[\hat{O}_e, \hat{H}\big], \quad \hbar = 1, \tag{2}$$

we can write (1) as

$$\left(i\frac{d}{dt}\right)^n \hat{O}_e = \big[\ldots\big[\big[\hat{O}_e, \hat{H}\big], \hat{H}\big]\ldots, \hat{H}\big] = \lambda \hat{O}_e. \tag{3}$$

If we can find such an $\hat{O}_e$ that satisfies (3) we can say that $\sqrt[n]{\lambda}$ is the energy-level gap. To clarify this point of view, we take $n = 2$ in (3), and assuming $|\psi_a\rangle$, $|\psi_b\rangle$ are two adjacent stationary eigen-states of Hamiltonian $\hat{H}$ with eigen-values E_a, E_b, then we have

$$\begin{aligned}\langle\psi_a|\left(i\frac{d}{dt}\right)^2 \hat{O}_e|\psi_b\rangle &= \langle\psi_a|\big[\big[\hat{O}_e, \hat{H}\big], \hat{H}\big]|\psi_b\rangle = (E_b - E_a)^2\langle\psi_a|\hat{O}_e|\psi_b\rangle \\ &= \lambda\langle\psi_a|\hat{O}_e|\psi_b\rangle.\end{aligned} \tag{4}$$

Since $\langle\psi_a|\hat{O}_e|\psi_b\rangle$ is a nonzero matrix element, the energy gap between $|\psi_a\rangle$ and $|\psi_b\rangle$ is $E_a - E_b = \sqrt{\lambda}$. Generally speaking, due to $(i\frac{d}{dt})^n \longleftrightarrow \hat{H}^n$, we can judge that $\sqrt[n]{\lambda}$ is one of the energy-gap. Therefore, once the 'invariant eigen-operator' $\hat{O}_e$ is found, some information about energy eigenvalues can be obtained. This method is quite concise and effective and may be applicable to many situations in many particle physics.

3 Searching for Energy-Gap of the Tomonaga Model by IEO Method

The Hamiltonian describing an one-dimensional interacting electron gas (the length of the system is L) by Tomonaga [5] has the following initial form

$$\hat{H}_1 = v_F \sum_{k\sigma} |k| \hat{C}^{\dagger}_{k\sigma} \hat{C}_{k\sigma} + \frac{1}{2L} \sum_{k} V_k \hat{\rho}(k) \hat{\rho}(-k), \tag{5}$$

where $\hat{C}_{k\sigma}$ is the Fermi operator, the density operator is

$$\hat{\rho}(k) = \sum_{p,\sigma} \hat{C}^{\dagger}_{p-k/2,\sigma} \hat{C}_{p+k/2,\sigma}, \tag{6}$$

and v_F denotes the Fermi velocity of the particles, the index $\sigma = \pm 1$ denote for spin $\uparrow$ and $\downarrow$ respectively, and V_k figures the electron-eletron interaction term. Basing on the momentum p above or below zero, $\hat{\rho}(k)$ may be devided into two terms: $\hat{\rho}(k) = \hat{\rho}_1(k) + \hat{\rho}_2(k)$, where

$$\begin{aligned} \hat{\rho}_1(k) &= \sum_{p>0,\sigma} \hat{C}^{\dagger}_{p-k/2,\sigma} C_{p+k/2,\sigma}, \\ \hat{\rho}_2(k) &= \sum_{p<0,\sigma} \hat{C}^{\dagger}_{p-k/2,\sigma} C_{p+k/2,\sigma}. \end{aligned} \tag{7}$$

After making some approximations (in which the important one is assumimg that the excitations of the electron gas are exactly bosons), i.e. expressing the density operators in terms of the bosonic creation and destruction operators ($[\hat{b}_k, \hat{b}^{\dagger}_{k'}] = \delta_{kk'}$)

$$\begin{aligned} \hat{\rho}_1(k) &= \hat{b}_k \left(\frac{kL}{\pi}\right)^{\frac{1}{2}}, \qquad \hat{\rho}_1(-k) = \hat{b}^{\dagger}_k \left(\frac{kL}{\pi}\right)^{\frac{1}{2}}, \\ \hat{\rho}_2(k) &= \hat{b}^{\dagger}_{-k} \left(\frac{kL}{\pi}\right)^{\frac{1}{2}}, \qquad \hat{\rho}_2(-k) = \hat{b}_{-k} \left(\frac{kL}{\pi}\right)^{\frac{1}{2}}, \end{aligned} \tag{8}$$

the one-dimensional electron gas can be recast into the boson Hamiltonian

$$\hat{H}_1 = \sum_{k} \omega_k \hat{b}^{\dagger}_k \hat{b}_k + \sum_{k} \bar{V}_k \left(\hat{b}_k + \hat{b}^{\dagger}_{-k}\right)\left(\hat{b}^{\dagger}_k + \hat{b}_{-k}\right), \tag{9}$$

where $\bar{V}_k = \frac{|k| V_k}{2\pi}$.

We now derive invariant eigen-operators $\hat{O}_e$ for $\hat{H}_1$. Without loss the generality we assume that $\hat{O}_e$ is

$$\hat{O}_e = m\hat{b}_k + n\hat{b}^{\dagger}_k + l\hat{b}_{-k} + p\hat{b}^{\dagger}_{-k}. \tag{10}$$

where m, n, l and p are four ordinary coefficients undetermined.

Using the Heisenberg equation we obtain a series of commutation relations

$$\begin{aligned} \left[\hat{b}_k, \hat{H}_1\right] &= \omega_k \hat{b}_k + \bar{V}_k \hat{b}_k + \bar{V}_k \hat{b}^{\dagger}_{-k}, \\ \left[\hat{b}^{\dagger}_k, \hat{H}_1\right] &= -\omega_k \hat{b}^{\dagger}_k - \bar{V}_k \hat{b}^{\dagger}_k - \bar{V}_k \hat{b}_{-k}, \end{aligned} \tag{11}$$

$$\left[\hat{b}_{-k}, \hat{H}_1\right] = \bar{V}_k \hat{b}_k^\dagger + \bar{V}_k \hat{b}_{-k},$$
$$\left[\hat{b}_{-k}^\dagger, \hat{H}_1\right] = -\bar{V}_k \hat{b}_k - \bar{V}_k \hat{b}_{-k}^\dagger.$$

It then follows from (2) and (11) that

$$\begin{aligned}\left[\hat{O}_e, \hat{H}_1\right] &= \left(m\omega_k + m\bar{V}_k - p\bar{V}_k\right)\hat{b}_k + \left(-n\omega_k - n\bar{V}_k + l\bar{V}_k\right)\hat{b}_k^\dagger \\ &\quad + \left(-n\bar{V}_k + l\bar{V}_k\right)\hat{b}_{-k} + \left(m\bar{V}_k - p\bar{V}_k\right)\hat{b}_{-k}^\dagger. \end{aligned} \tag{12}$$

Comparing (12) with (3) ($n = 1$) we obtain a set of linear algebraic equations

$$\begin{aligned}\left(\omega_k + \bar{V}_k - \lambda\right)m - \bar{V}_k p &= 0, \\ -\left(\omega_k + \bar{V}_k + \lambda\right)n + \bar{V}_k l &= 0, \\ -\bar{V}_k n + \left(\bar{V}_k - \lambda\right)l &= 0, \\ \bar{V}_k m - \left(\bar{V}_k + \lambda\right)p &= 0. \end{aligned} \tag{13}$$

As a linear homogeneous algebraic equations of the unknown variables m, n, l and p, the sufficient and necessary condition for existing nonzero solutions is that the coefficient determinant of the matrix is zero, i.e.

$$\det\begin{pmatrix} \omega_k + \bar{V}_k - \lambda & 0 & 0 & -\bar{V}_k \\ 0 & -\omega_k - \bar{V}_k - \lambda & \bar{V}_k & 0 \\ 0 & -\bar{V}_k & \bar{V}_k - \lambda & 0 \\ \bar{V}_k & 0 & 0 & -\bar{V}_k - \lambda \end{pmatrix} = 0, \tag{14}$$

which is

$$\lambda^2 - \frac{1}{4}\left[4\bar{V}_k\omega_k + 2\omega_k^2 \pm 2\omega_k\sqrt{\omega_k^2 + 4\bar{V}_k\omega_k}\right] = 0, \tag{15}$$

so the energy-level gap ΔE of the Hamiltonian $\hat{H}_1$ is

$$\Delta E = \lambda = \frac{1}{2}\left(\omega_k^2 + 4\bar{V}_k\omega_k\right)^{\frac{1}{2}} \pm \frac{1}{2}\omega_k. \tag{16}$$

Alternately, according to (3) for $n = 2$ case, we can further calculate

$$\begin{aligned}\left[\left[\hat{O}_e, \hat{H}_1\right], \hat{H}_1\right] &= \left(m\omega_k^2 + 2m\bar{V}_k\omega_k - p\bar{V}_k\omega_k\right)\hat{b}_k + \left(n\omega_k^2 + 2n\bar{V}_k\omega_k - l\bar{V}_k\omega_k\right)\hat{b}_k^\dagger \\ &\quad + n\bar{V}_k\omega_k\hat{b}_{-k} + m\bar{V}_k\omega_k\hat{b}_{-k}^\dagger. \end{aligned} \tag{17}$$

Letting (17) be equal to $\lambda'\hat{O}_e$, we can derive another coefficient determinant

$$\det\begin{pmatrix} \omega_k^2 + 2\bar{V}_k\omega_k - \lambda' & 0 & 0 & -\bar{V}_k\omega_k \\ 0 & \omega_k^2 + 2\bar{V}_k\omega_k - \lambda' & -\bar{V}_k\omega_k & 0 \\ 0 & \bar{V}_k\omega_k & -\lambda' & 0 \\ \bar{V}_k\omega_k & 0 & 0 & -\lambda' \end{pmatrix} = 0, \tag{18}$$

with the solution

$$\lambda' = \frac{1}{4}\left(4\bar{V}_k\omega_k + 2\omega_k^2 \pm 2\omega_k\sqrt{\omega_k^2 + 4\bar{V}_k\omega_k}\right). \tag{19}$$

Thus the energy-gap is $\Delta E = \sqrt{\lambda'} = \frac{1}{2}(\omega_k^2 + 4\bar{V}_k\omega_k)^{\frac{1}{2}} \pm \frac{1}{2}\omega_k$, which is just the same as (16). At this point we mention that the unknown constants m, n, l and p need not be solved, this is the advantage of our formalism. The above energy-gap coincides with the result in [5] gained via diagonalization method.

4 Energy-Gap of the Electron–Electron Interaction Hamiltonian Gained by IEO Method

Next we deal with a Hamiltonian model which describes the electron-electron interaction process,

$$\hat{H}_2 = \sum_{i=1}^{2}\omega_i\hat{C}_i^\dagger\hat{C}_i + k_1\big(\hat{C}_1^\dagger\hat{C}_2^\dagger + \hat{C}_2\hat{C}_1\big) + k_2\big(\hat{C}_1^\dagger\hat{C}_2 + \hat{C}_2^\dagger\hat{C}_1\big), \tag{20}$$

where $\hat{C}_i^\dagger$ and $\hat{C}_i$ $(i = 1, 2)$ denote the fermion creation and annihilation operators, respectively, and they obey the anticommutation relation $\{\hat{C}_i, \hat{C}_j^\dagger\} = \delta_{ij}$. k_1 and k_2 are two real coupling coefficients. In this Hamiltonian, the first term can be considered as the total kinetic energy of two electrons. $\hat{C}_2\hat{C}_1$ denotes the destruction of two electrons process, while $\hat{C}_1^\dagger\hat{C}_2^\dagger$ is its inverse process. $\hat{C}_1^\dagger\hat{C}_2$ indicates the process of creation of the second electron at the expense of annihilating the first electron. $\hat{C}_2^\dagger\hat{C}_1$ is its inverse process. In whole process, the system total energy is conservative, because $[\sum_{i=1}^{2}\omega_i\hat{C}_i^\dagger\hat{C}_i, \hat{C}_1^\dagger\hat{C}_2^\dagger + \hat{C}_2\hat{C}_1] = 0$, and $[\hat{C}_1^\dagger\hat{C}_2 + \hat{C}_2^\dagger\hat{C}_1, \sum_{i=1}^{2}\omega_i\hat{C}_i^\dagger\hat{C}_i] = 0$.

Using the following operator identity

$$\big[\hat{P}, \hat{D}\hat{F}\big] = \big\{\hat{P}, \hat{D}\big\}\hat{F} - \hat{D}\big\{\hat{P}, \hat{F}\big\}, \tag{21}$$

where the bracket $\{\}$ denotes anticommutation symbol, we can derive

$$\begin{aligned}
\big[\hat{C}_1, \hat{H}_2\big] &= \omega_1\hat{C}_1 + k_1\hat{C}_2^\dagger + k_2\hat{C}_2,\\
\big[\hat{C}_1^\dagger, \hat{H}_2\big] &= -\omega_1\hat{C}_1^\dagger - k_1\hat{C}_2 - k_2\hat{C}_2^\dagger,\\
\big[\hat{C}_2, \hat{H}_2\big] &= \omega_2\hat{C}_2 + k_1\hat{C}_1^\dagger + k_2\hat{C}_1,\\
\big[\hat{C}_2^\dagger, \hat{H}_2\big] &= -\omega_2\hat{C}_2^\dagger - k_1\hat{C}_1 - k_2\hat{C}_1^\dagger.
\end{aligned} \tag{22}$$

In order to search the invariant eigen-operator $\hat{O}_e$ of the Hamiltonian $\hat{H}_2$, we assume its form being

$$\hat{O}_e = \alpha\hat{C}_1 + \beta\hat{C}_1^\dagger + \mu\hat{C}_2 + \nu\hat{C}_2^\dagger, \tag{23}$$

where α, β, μ, and ν are unknown. Substituting (23) into the Heisenberg equation and comparing with (3) ($n = 1$), we can obtain a set of linear algebraic equations

$$\begin{cases} (\omega_1 - \lambda)\alpha + k_2\mu - k_1\nu = 0, \\ (-\omega_1 - \lambda)\beta + k_1\mu - k_2\nu = 0, \\ k_2\alpha - k_1\beta + (\omega_2 - \lambda)\mu = 0, \\ k_1\alpha - k_2\beta + (-\omega_2 - \lambda)\nu = 0. \end{cases} \tag{24}$$

As a linear homogeneous algebraic equations of the unknown variables α, β, μ, and ν, the sufficient and necessary condition for existing nonzero solutions is that the coefficient determinant of the matrix in (24) is zero, i.e.

$$\det \begin{pmatrix} \omega_1 - \lambda & 0 & k_2 & -k_1 \\ 0 & -\omega_1 - \lambda & k_1 & -k_2 \\ k_2 & -k_1 & \omega_2 - \lambda & 0 \\ k_1 & -k_2 & 0 & -\omega_2 - \lambda \end{pmatrix} = 0, \tag{25}$$

from which we can derive the energy-gap

$$\Delta E = \lambda = \frac{1}{\sqrt{2}} \left(-2k_1^2 + 2k_2^2 + \omega_1^2 + \omega_2^2 \pm \sqrt{\varepsilon}\right)^{\frac{1}{2}}, \tag{26}$$

where ε is a complex value

$$\varepsilon = \left[(\omega_1 + \omega_2)^2 - 4k_1^2\right](\omega_1 - \omega_2)^2 + 4k_2^2(\omega_1 + \omega_2)^2. \tag{27}$$

5 Energy-Gap of the Electron–Phonon Interaction Hamiltonian with Use of IEO Method

In this section, we tackle the electron-phonon interaction Hamiltonian [6]

$$\hat{H}_3 = \hat{C}^\dagger \hat{C} \left[\varepsilon_c + \sum_q M_q \left(\hat{a}_q + \hat{a}_q^\dagger \right) \right] + \sum_q \omega_q \hat{a}_q^\dagger \hat{a}_q, \tag{28}$$

where $\hat{a}_q^\dagger$ and $\hat{a}_q$ denote the independent boson operators of phonon creation and destruction, respectively, $\hat{C}^\dagger$ is the electron's creation operators. $\hat{H}_3$ describes an electron with energy ε_c interacting with a set of phonons with vibrating frequency ω_q. The interaction can not occur unless when the states occupied and $\hat{C}^\dagger \hat{C} = 1$.

For $\hat{H}_3$ we assume that the first invariant eigen-operator is

$$\hat{O}_{e1} = \hat{a}_q + \frac{M_q}{\omega_q} \hat{C}^\dagger \hat{C}. \tag{29}$$

Directly using the Heisenberg equation, we can deduce

$$i \frac{d}{dt} \hat{O}_{e1} = \left[\hat{O}_{e1}, \hat{H}_3 \right] = \omega_q \left(\hat{a}_q + \frac{M_q}{\omega_q} \hat{C}^\dagger \hat{C} \right) = \omega_q \hat{O}_{e1}. \tag{30}$$

Thus, we see that one of the energy-level gaps of this system is $\Delta E_1 = \omega_q$.

Secondly, we exam if the another invariant eigen-operator has the form

$$\hat{O}_{e2} = \hat{C}\exp\left[\sum_q \frac{M_q}{\omega_q}\left(\hat{a}_q^\dagger - \hat{a}_q\right)\right]. \tag{31}$$

By calculating

$$\begin{aligned} i\frac{d}{dt}\hat{O}_{e2} &= \left[\hat{O}_{e2}, \hat{H}_3\right] \\ &= \left[\hat{C}\exp\left[\sum_q \frac{M_q}{\omega_q}\left(\hat{a}_q^\dagger - \hat{a}_q\right)\right], \hat{C}^\dagger\hat{C}\left(\varepsilon_c + \sum_q M_q\left(\hat{a}_q + \hat{a}_q^\dagger\right)\right) + \sum_q \omega_q^\dagger \hat{a}_q\hat{a}_q\right] \\ &= \varepsilon_c\hat{C}\exp\left[\sum_q \frac{M_q}{\omega_q}\left(\hat{a}_q^\dagger - \hat{a}_q\right)\right] - 2\Delta C\left(\hat{C}^\dagger\hat{C} - \frac{1}{2}\right)\exp\left[\sum_q \frac{M_q}{\omega_q}\left(\hat{a}_q^\dagger - \hat{a}_q\right)\right] \end{aligned} \tag{32}$$

and taking the above mentioned condition $\hat{C}^\dagger\hat{C} = 1$ into account we see that (32) becomes

$$i\frac{d}{dt}\hat{O}_{e2} = (\varepsilon_c - \Delta)\hat{C}\exp\left[\sum_q \frac{M_q}{\omega_q}\left(\hat{a}_q^\dagger - \hat{a}_q\right)\right] = (\varepsilon_c - \Delta)\hat{O}_{e2}. \tag{33}$$

Thus $\hat{O}_{e2}$ is indeed an invariant eigen-operator. Correspondingly, another energy-gap is

$$\Delta E_2 = \varepsilon_c - \Delta = \varepsilon_c - \sum_q \frac{M_q^2}{\omega_q}. \tag{34}$$

In [6], $\hat{H}_3$ is diagonalized as $\hat{H}_3' = \hat{C}^\dagger\hat{C}(\varepsilon_c - \Delta) + \sum_q \omega_q^\dagger\hat{a}_q\hat{a}_q$ by making a complicated canonical transformation, where $\Delta = \sum_q \frac{M_q^2}{\omega_q}$ is named as the self-energy, this coincides with our conclusion. From this example, we can conclude that for the Hamiltonian $\hat{H}_3$ there exist two invariant eigen-operators (this resembles that an operator may have a few eigenstates). Consequently, there exists two set of energy spectra in this system.

In summary, by employing the IEO method, we have resolved several models in many-body physics and obtained their energy-level gaps successfully. Without doubt, its features of simpleness, directness and efficiency have been embodied fully.

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