



The perturbation theory of matrix mechanics based on its canonical transformations

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ABSTRACT

We elucidate that the canonical transformations of matrix mechanics are just the transformations of different representations of the standard quantum mechanics, reproduce the non-degenerate, degenerate and time-dependent perturbation theory in three men's paper, we solve the mystery of time-dependent perturbation theory of matrix mechanics. The Kramers' dispersion formula from time-dependent perturbation theory of matrix mechanics is also derived from that of wave mechanics.

Introduction

A logically consistent exposition of matrix mechanics is given by the three men's paper by Born, Heisenberg and Jordan [1], which is difficult to be understood as one is more familiar with the standard quantum mechanics based on Schrödinger's wave mechanics. For instance, the diagonal energy spectra can be obtained from the canonical transformations S of the Hamiltonian such that $q = Sq_0S^{-1}$, $p = Sp_0S^{-1}$, $W = SH(p_0, q_0)S^{-1}$. The nondegenerate and degenerate perturbation theories based on canonical transformations are formally performed, these procedures are easily understood. However, for time-dependent perturbation theory, 'Simple considerations show that for this case the perturbation formulae ensue from those cited earlier on replacing every term $H_0S^{(r)} - S^{(r)}H_0$ of the form by $H_0S^{(r)} - S^{(r)}H_0 - i\hbar \frac{dS^{(r)}}{dt}$ '. The argument of time-dependent perturbation theory puzzles many, of course, the three men's paper still attracts many, as matrix mechanics is proved to be equivalent to wave mechanics [2,3]. F. Casas expresses the time-dependent perturbation theory of three men's paper in modern quantum mechanics language and employs it to reproduce the standard perturbation theory formulated in the interaction picture [4]. It does not seem that Casas provides the clear senses of the canonical transformations. In this paper we illustrate the canonical transformations from the standard quantum mechanics and reproduce the non-degenerate, degenerate and time-dependent perturbation theory in three men's paper based on canonical transformations. Not only is the crucial Kramers' dispersion formula derived from time-dependent perturbation theory of matrix mechanics, but also the dispersion

formula is derived from that of wave mechanics.

Canonical transformations are transformations of different representations

The complete relations of two different representations or two different basis in energy representation are given by

$$\sum_n |n\rangle\langle n| = I, \quad \sum_\alpha |\alpha\rangle\langle\alpha| = I \quad (1)$$

where I is the unit matrix. Schrödinger's equation in α representation reads

$$i\hbar \frac{\partial \langle\alpha|\psi\rangle}{\partial t} = \sum_\beta \langle\alpha|H|\beta\rangle \langle\beta|\psi\rangle \quad (2)$$

The Hamiltonian in α representation may not be diagonal. Supposing that the Hamiltonian in n representation is diagonal, now we transform Schrödinger's equation from α representation to n representation. Inserting the complete relation Eq. (1) into Eq. (2) we obtain

$$i\hbar \sum_n \frac{\partial (\langle\alpha|n\rangle \langle n|\psi\rangle)}{\partial t} = \sum_{n,\beta} \langle\alpha|H|\beta\rangle \langle\beta|n\rangle \langle n|\psi\rangle \quad (3)$$

Multiplying Eq. (3) by $\langle n''|\alpha\rangle$ from the left side and summing over α , we have

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$$i\hbar \sum_{n,\alpha} \langle n'' | \alpha \rangle \frac{\partial \langle \alpha | n \rangle \langle n | \psi \rangle}{\partial t} = i\hbar \sum_{n,\alpha} \left(\langle n'' | \alpha \rangle \frac{\partial \langle \alpha | n \rangle}{\partial t} \langle n | \psi \rangle + \langle n'' | \alpha \rangle \langle \alpha | n \rangle \frac{\partial \langle n | \psi \rangle}{\partial t} \right) = \sum_{n,\alpha,\beta} \langle n'' | \alpha \rangle \langle \alpha | H | \beta \rangle \langle \beta | n \rangle \langle n | \psi \rangle \quad (4)$$

Eq. (4) is further simplified

$$i\hbar \frac{\partial \langle n'' | \psi \rangle}{\partial t} = \sum_{n,\alpha,\beta} \langle n'' | \alpha \rangle \langle \alpha | H | \beta \rangle \langle \beta | n \rangle \langle n | \psi \rangle - i\hbar \sum_{n,\alpha} \langle n'' | \alpha \rangle \frac{\partial \langle \alpha | n \rangle}{\partial t} \langle n | \psi \rangle \quad (5)$$

Denoting the matrix elements of representation transformation $S_{\beta n}^{-1} = S_{\beta n}^+$, $S_{n' \alpha} = \langle n' | \alpha \rangle$, the matrix element of Hamiltonian in α representation $H_{\alpha\beta} = \langle \alpha | H | \beta \rangle$, Eq. (5) is rewritten as

$$i\hbar \frac{\partial \langle n'' | \psi \rangle}{\partial t} = \sum_{n,\alpha,\beta} S_{n'' \alpha} H_{\alpha\beta} S_{\beta n}^{-1} \langle n | \psi \rangle - i\hbar \sum_{n,\alpha} S_{n'' \alpha} \frac{\partial S_{\alpha n}^{-1}}{\partial t} \langle n | \psi \rangle \quad (6)$$

The Hamiltonian in n representation is diagonal, that is

$$H^{(0)} = W^{(0)} \quad (14a)$$

$$S^{(1)} H^{(0)} - H^{(0)} S^{(1)} + H^{(1)} = W^{(1)} \quad (14b)$$

$$S^{(2)} H^{(0)} - H^{(0)} S^{(2)} + (H^{(0)} S^{(1)} - S^{(1)} H^{(0)}) S^{(1)} + S^{(1)} H^{(1)} - H^{(1)} S^{(1)} + H^{(2)} = W^{(2)} \quad (14c)$$

$$i\hbar \frac{\partial \langle n'' | \psi \rangle}{\partial t} = \sum_n \langle n'' | H | n \rangle \langle n | \psi \rangle = \sum_n W \delta_{n'' n} \langle n | \psi \rangle \quad (7)$$

The right side hands of Eq. (6) and Eq. (7) are equal, we have

$$\sum_n W \delta_{n'' n} \langle n | \psi \rangle = \sum_{n,\alpha,\beta} S_{n'' \alpha} H_{\alpha\beta} S_{\beta n}^{-1} \langle n | \psi \rangle - i\hbar \sum_{n,\alpha} S_{n'' \alpha} \frac{\partial S_{\alpha n}^{-1}}{\partial t} \langle n | \psi \rangle \quad (8)$$

It should be the same for the matrices acting on the n component of $|\psi\rangle$, i.e. $\langle n | \psi \rangle$, so we have the canonical transformations of three men's paper,

$$W = SHS^{-1} - i\hbar S \frac{\partial S^{-1}}{\partial t} = SHS^{-1} + i\hbar \frac{\partial S}{\partial t} S^{-1} \quad (9)$$

The second step of Eq. (9) is based on the fact $SS^{-1} = I$. As the left hand side W of Eq. (9) is time-independent, if the Hamiltonian in the right hand is time-dependent or time-independent, then the canonical transformation S should be time-dependent or time-independent, respectively.

$$\begin{aligned} W_{nn}^{(2)} &= [S^{(2)} H^{(0)} - H^{(0)} S^{(2)} + (H^{(0)} S^{(1)} - S^{(1)} H^{(0)}) S^{(1)} + S^{(1)} H^{(1)} - H^{(1)} S^{(1)} + H^{(2)}]_{nn} \\ &= [S^{(2)} H^{(0)} - H^{(0)} S^{(2)} + (H^{(1)} - W^{(1)}) S^{(1)} + S^{(1)} H^{(1)} - H^{(1)} S^{(1)} + H^{(2)}]_{nn} \\ &= \sum_i \left(S_{ni}^{(2)} H_{in}^{(0)} - H_{ni}^{(0)} S_{in}^{(2)} - W_{ni}^{(1)} S_{in}^{(1)} + S_{ni}^{(1)} H_{in}^{(1)} \right) + H_{nn}^{(2)} \\ &= \sum_i \left(S_{ni}^{(2)} H_{nn}^{(0)} \delta_{in} - H_{nn}^{(0)} \delta_{in} S_{in}^{(2)} - W_{nn}^{(1)} \delta_{in} S_{in}^{(1)} + S_{ni}^{(1)} H_{in}^{(1)} \right) + H_{nn}^{(2)} = \sum_i \left(S_{ni}^{(1)} H_{in}^{(1)} \right) + H_{nn}^{(2)} \\ &= H_{nn}^{(2)} + \sum_i \left(S_{ni}^{(1)} H_{in}^{(1)} \right) = H_{nn}^{(2)} + \sum_i \frac{H_{ni}^{(1)} H_{in}^{(1)}}{W_{nn}^{(0)} - W_{ii}^{(0)}} \end{aligned} \quad (18)$$

Nondegenerate and degenerate perturbation theory

The perturbation theory based on the canonical transformation is straightforward from Eq. (9). The Hamiltonian of a system is time-independent and is given by

$$H = H^{(0)} + \lambda H^{(1)} + \lambda^2 H^{(2)} + \dots \quad (10)$$

The diagonal energy spectra reads

$$W = W^{(0)} + \lambda W^{(1)} + \lambda^2 W^{(2)} + \dots \quad (11)$$

where λ is a parameter, $H^{(0)}$ is solved, that is $H^{(0)} = W^{(0)}$. S is also time-independent. Setting

$$S = I + \lambda S^{(1)} + \lambda^2 S^{(2)} + \dots \quad (12)$$

from the relation $SS^{-1} = I$, we obtain

$$S^{-1} = I - \lambda S^{(1)} + \lambda^2 (S^{(1)2} - S^{(2)}) + \dots \quad (13)$$

Inserting Eq. (10), Eq. (11), Eq. (12) and Eq. (13) into Eq. (9), to the second order approximation, we have

From Eq. (14a) we know that $H^{(0)}$ is diagonal. The first order energy is the diagonal matrix element of Eq. (14b)

$$W_{nn}^{(1)} = H_{nn}^{(1)} + \sum_i \left(S_{ni}^{(1)} H_{in}^{(0)} - H_{ni}^{(0)} S_{in}^{(1)} \right) = H_{nn}^{(1)} + S_{nn}^{(1)} (H_{nn}^{(0)} - H_{nn}^{(0)}) = H_{nn}^{(1)} \quad (15)$$

The off-diagonal matrix element of Eq. (14b) should be zero,

$$0 = W_{nm}^{(1)} = H_{nm}^{(1)} + \sum_i \left(S_{ni}^{(1)} H_{im}^{(0)} - H_{ni}^{(0)} S_{im}^{(1)} \right) = H_{nm}^{(1)} + S_{nm}^{(1)} (H_{mm}^{(0)} - H_{mm}^{(0)}) \quad (16)$$

From Eq. (16) we have the first order matrix element of canonical transformation.

$$S_{nm}^{(1)} = \frac{H_{nm}^{(1)}}{H_{nn}^{(0)} - H_{mm}^{(0)}} = \frac{H_{nm}^{(1)}}{W_{nn}^{(0)} - W_{mm}^{(0)}} \quad (17)$$

The first order approximation of $SS^{-1} = I$ is $I + \lambda(S^{(1)} + S^{-1(1)}) = I$, from which the diagonal matrix element $S_{nn}^{(1)}$ should be zero i.e. $S_{nn}^{(1)} = 0$. The second order energy is the diagonal matrix element of Eq. (14c), that is

The prime on the summation indicates that the term $i = n$ is excluded. The off-diagonal matrix element of Eq. (14c) is

$$\begin{aligned} 0 = W_{nm}^{(2)} &= \sum_i \left(S_{ni}^{(2)} H_{im}^{(0)} - H_{ni}^{(0)} S_{im}^{(2)} - W_{ni}^{(1)} S_{im}^{(1)} + S_{ni}^{(1)} H_{im}^{(1)} \right) + H_{nm}^{(2)} \\ &= \sum_i \left(S_{ni}^{(2)} H_{nm}^{(0)} \delta_{im} - H_{nm}^{(0)} \delta_{in} S_{im}^{(2)} - W_{ni}^{(1)} \delta_{in} S_{im}^{(1)} + S_{ni}^{(1)} H_{im}^{(1)} \right) + H_{nm}^{(2)} \\ &= S_{nm}^{(2)} (W_{nm}^{(0)} - W_{nn}^{(0)}) - W_{nm}^{(1)} S_{nm}^{(1)} + \sum_i \left(S_{ni}^{(1)} H_{im}^{(1)} \right) + H_{nm}^{(2)} \end{aligned} \quad (19)$$

From Eq. (19) we get

$$S_{nm}^{(2)} = \frac{H_{nm}^{(2)}}{W_{nm}^{(0)} - W_{mm}^{(0)}} - \frac{H_{nm}^{(1)} H_{nm}^{(1)}}{(W_{nn}^{(0)} - W_{mm}^{(0)})^2} + \sum_i \frac{H_{ni}^{(1)} H_{im}^{(1)}}{(W_{nn}^{(0)} - W_{ii}^{(0)})(W_{mm}^{(0)} - W_{mm}^{(0)})} \quad (20)$$

The prime on the summation indicates that the term $i = n$ is excluded.

The Hamiltonian and diagonal energy of degenerate system are the same to Eq. (10), Eq. (11), we have the diagonalization without perturbation interaction

$$IW_n^{(0)} = S^{(0)} H^{(0)} S^{(0)-1} \quad (21)$$

where the left hand side of Eq. (21) is a constant matrix and $S^{(0)} S^{(0)-1} = S^{(0)-1} S^{(0)} = I$. The canonical transformation is such that

$$S = S^{(0)} (I + \lambda S^{(1)} + \lambda^2 S^{(2)} + \dots) \quad (22)$$

and then

$$S^{-1} = (I - \lambda S^{(1)} + \lambda^2 (S^{(1)2} - S^{(2)}) + \dots) S^{(0)-1} \quad (23)$$

Inserting Eq. (10), Eq. (11), Eq. (21), Eq. (22) and Eq. (23) into Eq. (9), to the second order approximation, we have

$$S^{(0)} H^{(0)} S^{(0)-1} = W^{(0)} = IW_n^{(0)} \quad (24a)$$

$$S^{(0)} S^{(1)} H^{(0)} S^{(0)-1} - S^{(0)} H^{(0)} S^{(1)} S^{(0)-1} + S^{(0)} H^{(1)} S^{(0)-1} = W^{(1)} \quad (24b)$$

$$\begin{aligned} S^{(0)} S^{(2)} H^{(0)} S^{(0)-1} + S^{(0)} H^{(0)} (S^{(1)2} - S^{(2)}) S^{(0)-1} + S^{(0)} H^{(2)} S^{(0)-1} \\ - S^{(0)} H^{(1)} S^{(1)} S^{(0)-1} + S^{(0)} S^{(1)} H^{(1)} S^{(0)-1} - S^{(0)} S^{(1)} H^{(0)} S^{(1)} S^{(0)-1} = W^{(2)} \end{aligned} \quad (24c)$$

We only calculate the first order perturbation energy. Because of a constant matrix Eq. (24a), Eq. (24b) becomes

$$\begin{aligned} S^{(0)} S^{(1)} S^{(0)-1} S^{(0)} H^{(0)} S^{(0)-1} - S^{(0)} H^{(0)} S^{(0)-1} S^{(0)} S^{(1)} S^{(0)-1} + S^{(0)} H^{(1)} S^{(0)-1} \\ = (S^{(0)} S^{(1)} S^{(0)-1}) (IW_n^{(0)}) - (IW_n^{(0)}) (S^{(0)} S^{(1)} S^{(0)-1}) + S^{(0)} H^{(1)} S^{(0)-1} \\ = S^{(0)} H^{(1)} S^{(0)-1} = W^{(1)} \end{aligned} \quad (25)$$

Eq. (25) is the first order perturbation approximation of the degenerate system. Recalling that $S^{(0)}$ is the transformation of various bases in energy representation, we can re-combine the zeroth order wave function into a set of new basis and diagonalize the first order Hamiltonian $H^{(1)}$ to get the first order energy $W^{(1)}$ by solving the secular equation $\det(H_{ij}^{(1)} - W^{(1)} \delta_{ij}) = 0$.

Time-dependent perturbation theory and Kramers' dispersion formula

Without loss of generality, we consider the periodic time-dependent perturbation closely connected to transition of a quantum system. The equations of canonical transformations are the same to Eq. (10), Eq. (11), Eq. (12) and Eq. (13). However, time enters explicitly into $H^{(1)}$, $H^{(2)}$... but not into $H^{(0)}$, the canonical transformation S should be time-dependent. Inserting Eq. (10), Eq. (11), Eq. (12) and Eq. (13) into Eq.

(9), to the second order approximation, we have

$$H^{(0)} = W^{(0)} \quad (26a)$$

$$H^{(1)} - \left(H^{(0)} S^{(1)} - S^{(1)} H^{(0)} - i\hbar \frac{\partial S^{(1)}}{\partial t} \right) = W^{(1)} \quad (26b)$$

$$\begin{aligned} \left(H^{(0)} S^{(1)} - S^{(1)} H^{(0)} - i\hbar \frac{\partial S^{(1)}}{\partial t} \right) S^{(1)} - \left(H^{(0)} S^{(2)} - S^{(2)} H^{(0)} \right. \\ \left. - i\hbar \frac{\partial S^{(2)}}{\partial t} \right) + S^{(1)} H^{(1)} - H^{(1)} S^{(1)} + H^{(2)} \\ = W^{(2)} \end{aligned} \quad (26c)$$

The argument in three men's paper is verified, that is, we replace the terms $H_0 S^{(r)} - S^{(r)} H_0$ in Eq. (14b) and Eq. (14c) by $H_0 S^{(r)} - S^{(r)} H_0 - i\hbar \frac{\partial S^{(r)}}{\partial t}$, we obtain the Eq. (26b) and Eq. (26c). Setting $H^{(1)} = Eeq^{(0)} \cos(2\pi\nu_0 t) = \frac{Eeq^{(0)}}{2} (e^{i2\pi\nu_0 t} + e^{-i2\pi\nu_0 t})$ for the periodic time-dependent perturbation, then we have its matrix elements for positive frequency and negative frequency, respectively,

$$H_{nm,1}^{(1)} = \frac{Ee}{2} q_{nm}^{(0)} e^{i2\pi\nu_0 t}, H_{nm,-1}^{(1)} = \frac{Ee}{2} q_{nm}^{(0)} e^{-i2\pi\nu_0 t} \quad (27)$$

We take the off-diagonal matrix element of Eq. (26b), then obtain the first order approximation of the canonical transformation.

$$\begin{aligned} 0 = W_{nm}^{(1)} = H_{nm}^{(1)} + \sum_i \left(S_{ni}^{(1)} H_{im}^{(0)} - H_{ni}^{(0)} S_{im}^{(1)} \right) + i\hbar \frac{\partial S_{nm}^{(1)}}{\partial t} \\ = H_{nm}^{(1)} + \sum_i \left(S_{ni}^{(1)} H_{nm}^{(0)} \delta_{im} - H_{ni}^{(0)} \delta_{in} S_{im}^{(1)} \right) + i\hbar \frac{\partial S_{nm}^{(1)}}{\partial t} \\ = i\hbar \frac{\partial S_{nm}^{(1)}}{\partial t} + H_{nm}^{(1)} + S_{nm}^{(1)} (H_{nm}^{(0)} - H_{nn}^{(0)}) = i\hbar \frac{\partial S_{nm}^{(1)}}{\partial t} + H_{nm}^{(1)} - S_{nm}^{(1)} \nu_{nm}^{(0)} \end{aligned} \quad (28)$$

It follows from Eq. (27) and Eq. (28) that

$$S_{nm,1}^{(1)} = \frac{Ee}{2\hbar} \frac{q_{nm}^{(0)}}{\nu_{nm}^{(0)} + \nu_0} e^{i2\pi\nu_0 t}, S_{nm,-1}^{(1)} = \frac{Ee}{2\hbar} \frac{q_{nm}^{(0)}}{\nu_{nm}^{(0)} - \nu_0} e^{-i2\pi\nu_0 t} \quad (29)$$

The first order displacement matrix is

$$\begin{aligned} q = S q^{(0)} S^{-1} = (1 + \lambda S^{(1)}) q^{(0)} (1 - \lambda S^{(1)}) = q^{(0)} + \lambda (S^{(1)} q^{(0)} - q^{(0)} S^{(1)}) \\ = q^{(0)} + q^{(1)} \end{aligned} \quad (30)$$

From Eq. (29) and Eq. (30) we obtain

$$\begin{aligned} q_{nm,1}^{(1)} = \sum_i \left(S_{ni}^{(1)} q_{im}^{(0)} - q_{ni}^{(0)} S_{im}^{(1)} \right) = \frac{e^{i2\pi\nu_0 t} Ee}{2\hbar} \sum_i \left(\frac{q_{ni}^{(0)} q_{im}^{(0)}}{\nu_{ni}^{(0)} + \nu_0} - \frac{q_{ni}^{(0)} q_{im}^{(0)}}{\nu_{im}^{(0)} + \nu_0} \right), \\ q_{nm,-1}^{(1)} = \sum_i \left(S_{ni}^{(1)} q_{im}^{(0)} - q_{ni}^{(0)} S_{im}^{(1)} \right) = \frac{e^{-i2\pi\nu_0 t} Ee}{2\hbar} \sum_i \left(\frac{q_{ni}^{(0)} q_{im}^{(0)}}{\nu_{ni}^{(0)} - \nu_0} - \frac{q_{ni}^{(0)} q_{im}^{(0)}}{\nu_{im}^{(0)} - \nu_0} \right) \end{aligned} \quad (31)$$

Eq. (31) agree with the formulae obtained from Kramers' dispersion theory. Actually, it follows from $n = m$ and Eq. (31) that

$$q_{nn,1}^{(1)} = \frac{e^{i2\pi\nu_0 t} Ee}{h} \sum_i \frac{q_{ni}^{(0)} q_{in}^{(0)} \nu_{ni}^{(0)}}{\nu_{ni}^{(0)2} - \nu_0^2}, q_{nn,-1}^{(1)} = \frac{e^{-i2\pi\nu_0 t} Ee}{h} \sum_i \frac{q_{ni}^{(0)} q_{in}^{(0)} \nu_{ni}^{(0)}}{\nu_{ni}^{(0)2} - \nu_0^2} \quad (32)$$

The atomic polarization induced by light is written as

$$\begin{aligned} P = -e \left(q_{n,1}^{(1)} + q_{n,-1}^{(1)} \right) = \frac{-2e^2 E \cos(2\pi\nu_0 t)}{h} \sum_i \frac{q_{ni}^{(0)} q_{in}^{(0)} \nu_{ni}^{(0)}}{\nu_{ni}^{(0)2} - \nu_0^2} \\ = \frac{2e^2 E \cos(2\pi\nu_0 t)}{h} \left(\sum_{i(>n)} \frac{|q_{ni}^{(0)}|^2 \nu_{in}^{(0)}}{\nu_{in}^{(0)2} - \nu_0^2} - \sum_{i'(<n)} \frac{|q_{ni'}^{(0)}|^2 \nu_{ni'}^{(0)}}{\nu_{ni'}^{(0)2} - \nu_0^2} \right) \end{aligned} \quad (33)$$

which is our familiar Kramers' dispersion formula for positive

frequency. The terms for $i = n, i' = n$ in Eq. (33) disappears because of the fact $-eq_{nn}^{(0)} = 0$.

The calculation of transition probability in matrix mechanics is straightforward. For the harmonic perturbation case, see Eq. (27), the atomic polarization induced by light is written in Einstein's spontaneous emission coefficients form as [5]

$$P = \frac{3c^3 E_0 \cos(2\pi\nu_0 t)}{32\pi^4} \left[\sum_{i(i>n)} \frac{A_n^i}{\nu_{in}^{(0)2} (\nu_{in}^{(0)2} - \nu_0^2)} - \sum_{i'(i'<n)} \frac{A_{i'}^n}{\nu_{n i'}^{(0)2} (\nu_{n i'}^{(0)2} - \nu_0^2)} \right] \quad (34)$$

Comparing Eq. (34) to Eq. (33), we obtain Einstein's spontaneous emission coefficient A_n^i for the transition $i \rightarrow n$

$$A_n^i = \frac{4(2\pi)^4 \nu_{in}^{(0)3} e^2 |q_{in}^{(0)}|^2}{3hc^3} \quad (35)$$

Einstein's stimulated emission coefficient B_n^i is given by

$$B_n^i = \frac{A_n^i}{8\pi h \nu_{in}^{(0)3} / c^3} = \frac{(2\pi)^3 e^2 |q_{in}^{(0)}|^2}{3h^2} \quad (36)$$

The transition rate, i.e. transition probability per unit time, is obtained

$$R_{i \rightarrow n} = \frac{-dN_i}{dt \cdot N_i} = B_n^i \cdot 2\pi\rho(\omega_{in}^{(0)}) = \frac{4\pi^2 e^2 |q_{in}^{(0)}|^2 \rho(\omega_{in}^{(0)})}{3h^2} \quad (37)$$

in which N_i is the number of atoms in excited state i , $\rho(\omega_{in}^{(0)})$ is the energy density of the field, per unit frequency at $\omega_{in}^{(0)}$. The transition probability for $i \rightarrow n$ is

$$P_{i \rightarrow n} = \frac{-dN_i}{N_i} = R_{i \rightarrow n} \cdot t = \frac{4\pi^2 e^2 |q_{in}^{(0)}|^2 \rho(\omega_{in}^{(0)})}{3h^2} t \quad (38)$$

The transition rate, Eq. (37), and transition probability, Eq. (38), agree with that calculated by wave mechanics [6].

Kramers' dispersion formula Eq. (33) is also derived from wave mechanics. An atom interacting with a light obeys Schrödinger equation

$$i\hbar\partial_t \psi = (H_0 + \lambda H_1) \psi \quad (39)$$

where the interaction term is $H_1 = eq^{(0)} E \cos(\omega_0 t) = eE q^{(0)} (e^{i\omega_0 t} + e^{-i\omega_0 t})/2$ and the unperturbed eigenstate equation is $H_0(\phi_n e^{-ie_n t/\hbar}) = \varepsilon_n(\phi_n e^{-ie_n t/\hbar})$. The wave function in Eq. (39) can be expanded to the eigen states [6]

$$\psi = \sum_i a_i \phi_i e^{-ie_i t/\hbar} \quad (40)$$

Substituting Eq. (40) into Eq. (39), we have the equation of the coefficient a_i

$$i\hbar \frac{da_k}{dt} = \sum_i \lambda H_{1ki} a_i e^{i\omega_{ki}^{(0)} t} \quad (41)$$

with the interaction matrix element $H_{1ki} = \int \phi_k^* H_1 \phi_i d\tau$ and the Bohr frequent condition $\omega_{ki}^{(0)} = (\varepsilon_k - \varepsilon_i)/\hbar$. To the first order approximation $a_k(t) = a_k^{(0)}(t) + \lambda a_k^{(1)}(t)$, Eq. (41) becomes the two equation.

$$\begin{cases} i\hbar \frac{da_k^{(0)}}{dt} = 0 \\ i\hbar \frac{da_k^{(1)}}{dt} = \sum_i H_{1ki} a_i^{(0)} e^{i\omega_{ki}^{(0)} t} \end{cases} \quad (42)$$

Assuming the initial state of the atom is $\phi_n e^{-ie_n t/\hbar}$, that is $a_k^{(0)}(t) = \delta_{kn}$,

we obtain the solutions of Eq. (42)

$$a_k^{(1)}(t) = \frac{eE q_{kn}^{(0)}}{2\hbar} \left(\frac{1 - e^{i(\omega_{kn}^{(0)} + \omega_0)t}}{\omega_{kn}^{(0)} + \omega_0} + \frac{1 - e^{i(\omega_{kn}^{(0)} - \omega_0)t}}{\omega_{kn}^{(0)} - \omega_0} \right) \quad (43)$$

with the position matrix element $q_{kn}^{(0)} = \int \phi_k^* q^{(0)} \phi_n d\tau$. The wave function of the atom follows from Eq. (40) that

$$\psi = \phi_n e^{-ie_n t/\hbar} + \sum_i \lambda a_i^{(1)} \phi_i e^{-ie_i t/\hbar} \quad (44)$$

The term $i = n$ in Eq. (44) is excluded, as the position matrix element in $a_i^{(1)}$ is zero, i.e., $q_{nn}^{(0)} = 0$. To the first order approximation, the polarization of the atom is given by

$$\begin{aligned} P &= \int \psi^* (-eq^{(0)}) \psi d\tau = -e \left(\sum_i q_{ni}^{(0)} a_i^{(1)} e^{i\omega_{ni}^{(0)} t} + \sum_i q_{in}^{(0)} a_i^{(1)*} e^{i\omega_{in}^{(0)} t} \right) \\ &= \frac{e^2 E \cos(\omega_0 t)}{\hbar} \left(\sum_i |q_{in}^{(0)}|^2 \omega_{in}^{(0)} - \sum_i |q_{ni}^{(0)}|^2 \omega_{ni}^{(0)} \right) \end{aligned} \quad (45)$$

The primes on the summations indicate that the two terms $i = n, i' = n$ are excluded. Eq. (45) for positive and negative frequency is just Eq. (33) of Kramers' dispersion formula for positive frequency. In the process we drop the noncoherent terms $\frac{eE q_{in}^{(0)}}{2\hbar} \left(\frac{1}{\omega_{kn}^{(0)} - \omega_0} + \frac{1}{\omega_{kn}^{(0)} + \omega_0} \right)$ in Eq. (43), as these two terms do not reflect the interaction of atom with light.

Conclusion

In this paper we illustrate that the canonical transformations in three men's paper are nothing but the transformations of different representations, and reproduce the perturbation theory based on canonical transformations. Performing the canonical transformations in matrix mechanics is a natural thing, then the perturbation theory ensues. However, the time-dependent perturbation theory based on the canonical transformation needs extraordinary intuitions. The authors of three men's paper are outstanding. The time-dependent perturbation theory is employed to derive Kramers' dispersion formula, which is also investigated from wave mechanics. Why are the canonical transformations performed? Because the solutions of Heisenberg's equation of motion can be reduced to the procedure: the canonical transformation S is determined such that $p = Sp_0 S^{-1}$ and $q = Sq_0 S^{-1}$, then function $SH(p_0, q_0, t) S^{-1} - i\hbar S \frac{dS^{-1}}{dt} = W$ becomes a diagonal matrix. From the canonical transformations we not only obtain the energy spectra of quantum system, but also get the canonical transformation matrices. The process of canonical transformations is akin to that of solving Schrödinger's equation, both the energy eigen values and the corresponding eigen wave functions are simultaneously determined.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

No data was used for the research described in the article.

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