Quantum theory of particle motion in a rapidly oscillating field

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We show that the motion of a particle of mass m in a high-frequency time-dependent potential $V(\vec{x})=v(\vec{x})\cos(\Omega t)$ is governed by a Schrödinger equation with time-independent effective potential $V_{\text{eff}}(\vec{x})=\vec{\nabla}v(\vec{x})\cdot\vec{\nabla}v(\vec{x})/4m\Omega^2$. The validity of this approximation and an exact formal solution based on the Wigner function are discussed for the case in which $v(\vec{x})$ is quadratic.

An early treatment of particle motion in a rapidly oscillating field was given by Kapitsa within the framework of classical mechanics.[1] This was followed by the more detailed classical treatments of Gaponov and Miller,[2] of Landau and Lifschitz,[3] and of Weibel and Clark.[4] The central result of this work is that a particle of mass m subject to a high-frequency force

$$\vec{F}(\vec{x},t)=\vec{f}(\vec{x})\cos(\Omega t) \tag{1}$$

moves as if acted upon by the time-independent effective potential

$$V_{\text{eff}}(\vec{x})=\frac{\vec{f}(\vec{x})\cdot\vec{f}(\vec{x})}{4m\Omega^2}\ , \tag{2}$$

it being assumed here that $\vec{f}$ is derivable from a potential. As a result, a charged particle can be trapped at a minimum of the effective potential in a radio-frequency field (Paul trap),[5] whereas there is no point of stable equilibrium in an electrostatic field.

In recent years this effect has been used to trap a few or even single ions for the ultimate purpose of high-resolution spectroscopy and its application to the measurement of time.[6] The ions in the rf trap are cooled by means of laser radiation to eliminate first- and second-order Doppler shifts and to ensure stable trapping. In the theoretical analysis of the cooling process, the ion motion must be treated quantum mechanically.[7] It seems to have been taken for granted that this may be done by using the effective potential (2) in the Schrödinger equation for ion motion, even though this potential was derived classically. To our knowledge this plausible surmise has not been justified. In view of the potential importance of this technology for spectroscopy and time keeping, we felt that a fully quantum-mechanical derivation of the effective potential would be worthwhile. The derivation, which turns out to be surprisingly simple, is given below.

In the applied potential

$$V(\vec{x},t)=v(\vec{x})\cos(\Omega t)\ , \tag{3}$$

the motion of a particle is governed by Schrödinger's equation

$$i\hbar\frac{\partial}{\partial t}\psi=-\frac{\hbar^2}{2m}\nabla^2\psi+v(\vec{x})\cos(\Omega t)\psi\ . \tag{4}$$

If Ω is a high frequency, the potential has little effect on the particle motion because it averages to zero over the short time interval $2\pi/\Omega$. Nevertheless, the potential does have a small secular effect which we calculate as follows.

Suppose that only the potential-energy term were present on the right-hand side of (4). Then the solution of this equation would be

$$\psi(\vec{x},t)=\psi(\vec{x},0)\exp[-iv(\vec{x})\sin(\Omega t)/\hbar\Omega]\ . \tag{5}$$

This shows that the dominant effect of the potential is to add an oscillating phase factor to the wave function ψ. It is natural, therefore, to look for a solution to Eq. (4) of the form

$$\psi(\vec{x},t)=\phi(\vec{x},t)\exp[-iv(\vec{x})\sin(\Omega t)/\hbar\Omega]\ . \tag{6}$$

The important point for a subsequent approximation is that, because the dominant effect of the oscillating potential is already contained in the phase factor, $\phi(\vec{x},t)$ may be treated as a slowly varying function of time. Note also that in the position probability density

$$P(\vec{x},t)=|\psi(\vec{x},t)|^2=|\phi(\vec{x},t)|^2\ , \tag{7}$$

$\phi(\vec{x},t)$ plays the role of a wave function in position space.

On substituting (6) into (4) we obtain the equation of motion for ϕ:

$$i\hbar\frac{\partial}{\partial t}\phi=-\frac{\hbar^2}{2m}\nabla^2\phi+\frac{\vec{\nabla}v\cdot\vec{\nabla}v}{2m\Omega^2}\phi\sin^2(\Omega t)+\frac{i\hbar}{m\Omega}(\vec{\nabla}v\cdot\vec{\nabla}\phi+\tfrac{1}{2}\nabla^2v\phi)\sin(\Omega t)\ . \tag{8}$$

In this equation the coefficients of $\sin(\Omega t)$ and $\sin^2(\Omega t)$ are slowly varying functions of time, and so an average of these terms over the short time interval $2\pi/\Omega$ replaces $\sin(\Omega t)$ and $\sin^2(\Omega t)$ by their average values of 0 and $\frac{1}{2}$, respectively. Alternatively, one may write $\frac{1}{2}[1-\cos(2\Omega t)]$ for $\sin^2(\Omega t)$ in (8) and simply discard terms that oscillate rapidly with average value zero (rotating-wave approximation). In either case there results an ordinary Schrödinger equation for $\phi(\vec{x},t)$,

$$i\hbar\frac{\partial}{\partial t}\phi=-\frac{\hbar^2}{2m}\nabla^2\phi+V_{\text{eff}}(\vec{x})\phi\ , \tag{9}$$

with an effective time-independent potential energy

$$V_{\text{eff}}(\vec{x})=\frac{\vec{\nabla}v(\vec{x})\cdot\vec{\nabla}v(\vec{x})}{4m\Omega^2} . \tag{10}$$

This is equivalent to the classical result (3), since the force (1) is the negative gradient of the potential (3), and hence $\vec{f}=-\vec{\nabla}v$.

To better understand the conditions under which the effective-potential approximation is valid, we look more closely at a case of one-dimensional motion with

$$V(x,t)=\tfrac{1}{2}Kx^2\cos(\Omega t) . \tag{11}$$

This is the form of potential along each of the principle axes of a quadrupole trap, with the constant k being positive for two of the axes and negative for the third. According to (10), the effective potential is that of an harmonic oscillator, $V_{\text{eff}}=m\omega_0^2x^2/2$, with natural frequency $\omega_0=K/\sqrt{2}m\Omega$. The general solution of the oscillator equation

$$i\hbar\frac{\partial}{\partial t}\phi=-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\phi+\tfrac{1}{2}m\omega_0^2x^2\phi \tag{12}$$

is, of course, easy to write down in terms of the oscillator eigenstates $u_n(x)$ and eigenvalues $E_n=\hbar\omega_0(n+\frac{1}{2})$:

$$\phi(x,t)=\sum_{n=0}^{\infty}c_nu_n(x)e^{-iE_nt/\hbar-i\theta_n} . \tag{13}$$

With the coefficients c_n and phases θ_n constant, (13) is a solution of (12). But with time-dependent coefficients $c_n(t)$ and $\theta_n(t)=E_n\sin(\Omega t)/4\hbar\Omega$, (13) is a solution of the exact equation for $\phi(x,t)$, namely,

$$i\hbar\frac{\partial}{\partial t}\phi=-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\phi+\tfrac{1}{2}m\omega_0^2x^2\phi+\tfrac{1}{2}m\omega_0^2x^2\cos(2\Omega t)\phi$$
$$+2^{1/2}i\hbar\omega_0x\sin(\Omega t)\frac{\partial}{\partial x}\phi , \tag{14}$$

provide the coefficients c_n satisfy

$$\dot{c}_n=\omega_0\sqrt{(n+1)(n+2)}g(t)c_{n+2}e^{-i\alpha(t)}$$
$$-\omega_0\sqrt{n(n-1)}g^*(t)c_{n-2}e^{i\alpha(t)} , \tag{15}$$

in which

$$\alpha(t)=2\omega_0[t-\sin(\Omega t)/4\Omega] , \tag{16}$$

$$g(t)=2^{1/2}\sin(\Omega t)+\tfrac{1}{4}i\cos(2\Omega t) . \tag{17}$$

The arbitrary phases $\theta_n(t)$ were chosen so there would be no "diagonal terms," i.e., terms containing c_n, on the right-hand side of (15). Clearly equation (15) describe transitions between the eigenstates of the effective potential, and the strength of these transitions measures the failure of the effective-potential approximation, for there would be no transitions if the effective potential were exact. Notice that Eq. (15) couples alternate levels, i.e., the selection rule is $n\rightarrow n\pm2$. This means that the populations in even- and odd-numbered levels do not mix, and if the particle starts out in the ground state ($n=0$), the odd-numbered levels remain unoccupied for all time.

Because the perturbing terms in (14) have frequencies Ω and 2Ω, one expects strong transitions to occur when one of these frequencies equals the allowed transition frequency $2\omega_0$ ($=2^{1/2}K/m\Omega$), i.e., when $\Omega=\Omega_0$ or $\Omega=\Omega^0/\sqrt{2}$ where

$$\Omega_0=(2^{1/2}K/m)^{1/2} . \tag{18}$$

Although these two resonances do indeed occur, they are by no means the only ones. Starting with the particle in the ground state, Eq. (15) yields, in the first order of time-dependent perturbation theory, the expression

$$c_2(t)=-\omega_0\int_0^t dt'[\sin(\Omega t')-2^{-3/2}i\cos(2\Omega t')]$$
$$\times e^{2i\omega_0[t'-\sin(\Omega t')/4\Omega]} \tag{19}$$

for the amplitude to be in state 2. Upon expanding the exponential of the trigonometric function in terms of Bessel functions,

$$e^{-i\omega_0\sin(\Omega t)/2\Omega}=\sum_{k=-\infty}^{\infty}J_k(\omega_0/2\Omega)e^{-ik\Omega t} , \tag{20}$$

and performing the integration over time, one finds resonances corresponding to all multi-quantum excitations of the transition $0\rightarrow2$. That is to say, for any positive integer r, there is a resonance at $r\Omega=2\omega_0=2^{1/2}K/m\Omega$. Thus the resonant frequencies are

$$\Omega_r=\Omega_0/\sqrt{r} . \tag{21}$$

These resonances are clearly visible in Fig. 1 where the time-averaged probability $P_2=|c_2(t)|^2$ is plotted against Ω/Ω_0. Generally speaking, the resonances must be avoided if stable trapping is desired. So when we speak of a "high-frequency" field we mean one whose frequency Ω is much larger than Ω_0. It is interesting that the same resonances occur in the classical treatment of this problem. The classical equation of motion is the Mathieu equation

$$m\frac{d^2}{dt^2}X+K\cos(\Omega t)X=0 , \tag{22}$$

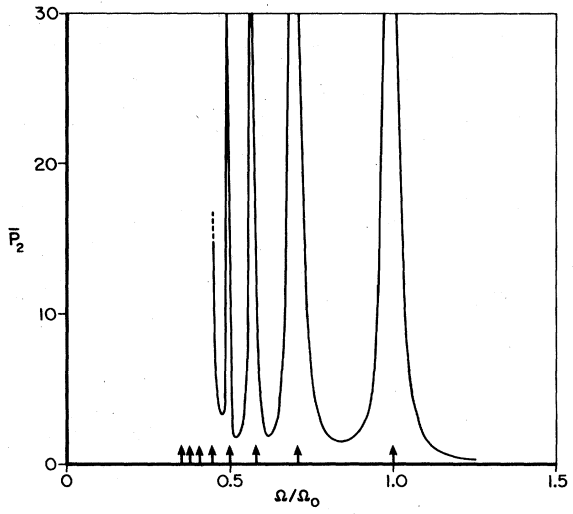

FIG. 1. Time average of first-order excitation probability to state $n=2$. Resonances occur at applied-field frequencies $\Omega=r^{-1/2}\Omega_0$, where $r=1,2,3,\ldots$ and $\Omega_0=2^{1/4}(K/m)^{1/2}$. The location of some of the resonances is indicated by arrows.

and the frequencies (21) are the parametric resonances of this equation.[5] Actually, the above results of the first-order perturbation theory are accurate only if $\bar{P}_2 \ll 1$. This occurs where $\Omega \gg \Omega_0$, in which case

$$\bar{P}_2 \propto \left[\frac{\Omega_0}{\Omega}\right]^4 . \tag{23}$$

Thus the excitation probability decreases quite rapidly with increasing frequency, and the accuracy of the effective-potential approximation improves accordingly.

It is possible to write down an exact quantum-mechanical solution for the motion of a particle in potential (11) in terms of the solution to the corresponding classical problem. This formal solution, which is based on Wigner's function, provides considerable insight into the nature of the quantum-mechanical motion. The Wigner function $f(x,p)$ is derived from the wave function $\psi(x)$ by means of the integral formula[8]

$$f(x,p)=\frac{1}{2\pi\hbar}\int ds\, \psi(x+\tfrac{1}{2}s)\psi^*(x-\tfrac{1}{2}s)e^{-ips/\hbar} . \tag{24}$$

The integral of $f(x,p)$ over momentum p is the position probability density $|\psi(x)|^2$, and the integral over position x is the correct probability density for momentum. Thus $f(x,p)$ has the properties of a phase-space distribution function, except that it is not always positive definite. Moreover, the Wigner function contains precisely the same information as the density matrix $\rho(x_1,x_2)=\psi(x_1)\psi^*(x_2)$ from which it is derived by a type of Fourier transform. Hence $f(x,p)$ provides a complete description of the state of the particle. From the Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\psi=-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi+\tfrac{1}{2}Kx^2\cos(\Omega t)\psi , \tag{25}$$

the equation of motion for $f(x,p)$ is readily derived. The result

$$\frac{\partial}{\partial t}f+\frac{p}{m}\frac{\partial}{\partial x}f=Kx\cos(\Omega t)\frac{\partial}{\partial p}f , \tag{26}$$

is identical to the classical Liouville equation for particle motion in potential (11), and it is this fact that allows the quantum-mechanical solution to be expressed in terms of the classical one.

The Liouville equation describes the motion of an ensemble of points in phase space, each of which moves in accordance with Hamilton's equations. In the present case, the Hamiltonian is

$$H=\frac{p^2}{2m}+\tfrac{1}{2}Kx^2\cos(\Omega t) , \tag{27}$$

and Hamilton's equations read

$$\frac{dx}{dt}=\frac{p}{m} , \tag{28a}$$

$$\frac{dp}{dt}=-Kx\cos(\Omega t) . \tag{28b}$$

These combine to give the Mathieu equation of motion (22). We shall assume that the classical equations of motion have been completely solved, and that we know the position x and momentum p at time t for any initial conditions (x_0,p_0) at time $t=0$:

$$\begin{aligned} x&=x(x_0,p_0,t) ,\\ p&=p(x_0,p_0,t) . \end{aligned} \tag{29}$$

There always exists a unique inverse to these equations,

$$\begin{aligned} x_0&=x_0(x,p,t) ,\\ p_0&=p_0(x,p,t) , \end{aligned} \tag{30}$$

which expresses the initial position and momentum in terms of the present values of these variables. We further assume that this inverse is known. [It may be obtained directly by solving Hamilton's equation backward in time from the "initial" point (x,p) at time t to the "final" point (x_0,p_0) at time $t=0$.] Because the Mathieu equation (22) is invariant under time reversal, the solution x_0 in (30) is a Mathieu function and p_0 is the negative time derivative of this function multiplied by the mass. Now Liouville's theorem states that the density $f(x,p,t)$ does not change with time at a point (x,p) that moves in accordance with Hamilton's equations.[9] Hence $f(x,p,t)=f(x_0,p_0,0)$, where (x,p) and (x_0,p_0) are related by (29) or (30). Therefore, if $f_0(x,p)$ is an arbitrary initial Wigner function, the solution of Eq. (26) reads

$$f(x,p,t)=f_0(x_0(x,p,t),p_0(x,p,t)) , \tag{31}$$

and the quantum-mechanical problem has been reduced to that of solving the classical Mathieu equation (22). This result makes it clear why the resonances of the Schrödinger equation (25) are the same as those of the Mathieu equation (22). Since this particular form of Mathieu's equation has been studied extensively elsewhere,[5] we shall not pursue this topic further, except to note that, for a high-frequency field ($\Omega \gg \Omega_0$), the solutions of the Mathieu equation are bounded. In view of the above relation between the classical and quantum motions, this means that there is nothing in the quantum-mechanical formulation of the problem that spoils the stable trapping which is predicted classically.

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