Self-consistent potential for a two-level atom in a standing-wave field

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It is shown that the effects of a standing electromagnetic wave of cosinusoidal form on a neutral two-level atom can be represented by an effective static potential, which is obtained by a local unitary transformation to dress the atom by the field. The form of the effective potential is obtained self-consistently by minimizing fluctuations of the atomic kinetic energy induced by the locality of the dressing transformation. Moreover this effective potential is shown to depend on the atom-field detuning and on the field intensity, and to exhibit discontinuities in some ranges of these parameters. The band structure which characterizes the eigenvalue spectrum of the dressed Hamiltonian is discussed in the spirit of the tight-binding approximation, and the fluctuations of the kinetic energy near resonance are shown to induce splitting of the bands; a physical interpretation of the atomic dynamics associated with these splittings is presented. Off resonance the fluctuations are shown to induce exchange of real photons and variations of the atomic kinetic energy. The results are compared with those of previous theories, leading to an improved understanding of the dynamics of a two-level atom in a standing-wave field.

I. INTRODUCTION

The problem of the influence of external electromagnetic fields on the motion of a neutral atom or molecule has received increasing attention in recent years. The reason for this attention is related to a wealth of potentially useful applications. As an example, it is easily perceived that research on atomic beam deflection by laser radiation[1] is relevant for isotope separation and selective excitation of atoms and molecules, while trapping and cooling of neutral atoms by strong radiation fields[2] might prove essential for ultrahigh-resolution spectroscopy of individual atoms or molecules. In connection with the above experiments, theoretical models have been devised and investigated. According to these models the atoms have usually been represented by two-level point systems of finite mass M, while the electromagnetic field has generally been taken in the form of a classical traveling[3,4,6] or standing[4-9] monochromatic wave. The case of the time-dependent frequency of the classical wave[6] and the effects of thermal[6] and nonmonochromatic[7] fields have also been studied to some extent. In most of these treatments the role of spontaneous emission on atomic dynamics has also been considered, and it has been shown to lead to different dynamical regimes which can be distinguished on the basis of the duration of the atom-laser interaction as compared to the spontaneous emission time.[1,10,11] In most of the cases theoretically investigated, reduction of the problem to essentially one dimension has been found feasible and useful. The theoretical situation, also in connection with the experiments, has recently been discussed in a review article[12] whose set of references summarizes in a remarkably complete way previous work on the subject.

This paper is devoted to an investigation of the one-dimensional dynamics of a two-level atom in the field of a sinusoidal standing wave in absence of spontaneous emission. The simplest Hamiltonian to represent this model (with $\hbar=1$) is[5]

$$\begin{aligned}&\mathscr{H}=\frac{1}{2M}p^2+\mathscr{H}_0\,;\\&\mathscr{H}_0=\omega\alpha^\dagger\alpha+\omega_0 S_z+\epsilon(\alpha S_+ +\alpha^\dagger S_-)\,,\end{aligned}\tag{1.1}$$

where $p=-i\partial/\partial x$ is the linear momentum of the atomic center of mass, ω is the frequency of the standing wave, ω_0 is the frequency corresponding to the internal atomic energy, and

$$\epsilon=\epsilon_0\cos Qx\tag{1.2}$$

is the atom-field coupling constant, whose cosine form is directly related to the spatial variation along

x of the amplitude of the electric component of the standing-wave field of wave vector Q. We shall take $0 \leq x \leq L$. Furthermore, the operators in (1.1) are creation and annihilation operators pertaining to the field mode, and the S operators are the usual pseudospin atomic operators $S=\frac{1}{2}$. The relevant commutation relations are

$$[\alpha,\alpha^\dagger]=1, \quad [S_+,S_-]=2S_z ,$$
$$[S_z,S_+]=S_+ .$$

The Hamiltonian (1.1), in its semiclassical version,[4,6–10] has been used as a basis for previous treatments of the atomic dynamics, e.g., in connection with the already-mentioned problem of atomic deflection. In some of these treatments,[6–8] the idea has been more or less explicitly introduced that the forces exerted by the field on the atom can be represented by a local effective potential $V(x)$ which depends on the internal state of the atom itself and on the detuning $\omega_0-\omega$. The advantages of this point of view are obvious, since one can then immediately use the results of the familiar theory of the motion of a point particle in an external potential and thereby reduce the problem to a purely mechanical one. Some difficulties related to the definition of the effective potential in the neighborhood of $\omega_0 \sim \omega$ have arisen, however, since as $\omega_0-\omega$ tends to zero the near-resonance potential rather unexpectedly does not seem to convert into the resonant potential.[8] A treatment which does not suffer this drawback is the exact Floquet-Lyapounov theory, which does not make use of the effective-potential concept and which leads to a band structure of the atomic center-of-mass eigenvalue.[9,10,12] The mathematical complications of this theory, however, tend to obscure somewhat the physical meaning of the off-resonance results,[9,10] some of which display curious features such as a splitting of the bands which is detuning-dependent and which vanishes on resonance for $\omega_0=\omega$. The aim of this paper is to investigate the possibility of using an effective potential to describe the effects of a standing-wave electromagnetic field on a two-level atom and the limits of this concept. We also wish to inquire as to the shape of this potential in relation to the amplitude of the local elastic field and to the detuning $\omega_0-\omega$. We shall see that this investigation also clarifies some of the points which remain rather obscure in the physics of the results of the Floquet-Lyapounov theory.

We also remark that, contrary to most previous theories, the electromagnetic field in (1.1) is fully quantized, although most of the plausible experimental situations admittedly refer to strong fields which can be treated classically. We shall see that this quantization, while it introduces no complications in the treatment, increases its generality since it extends the theory to cover cases of relatively weak fields.

II. THE DRESSED ATOM

Perhaps the most natural way of introducing an effective potential is through diagonalization of $\mathscr{H}_0$ in (1.1) with respect to the internal atomic coordinates. A most useful tool for this purpose is the unitary dressing operator

$$T=\exp[-\theta(4\mathscr{N})^{-1/2}(\alpha S_+ - \alpha^\dagger S_-)] ;$$
$$\mathscr{N}=\alpha^\dagger\alpha+S_z+\tfrac{1}{2} , \tag{2.1}$$

which we have introduced previously in connection with various problems of atom-field interaction.[5,13] In the present case the dependence of θ on the atomic position through the x dependence of ϵ in (1.2) evidences the local character of T. Transforming $\mathscr{H}_0$ by (2.1), we obtain the equivalent Hamiltonian

$$\begin{aligned}\tilde{\mathscr{H}}_0 &\equiv T^{-1}\mathscr{H}_0 T \\ &= \omega(\mathscr{N}-\tfrac{1}{2}) \\ &\quad +[(\omega_0-\omega)\cos\theta+\omega_1\sin\theta]S_z ,\end{aligned} \tag{2.2}$$

provided we choose

$$\theta=\arctan\frac{\omega_1}{\omega_0-\omega}; \quad \omega_1=2\epsilon\mathscr{N}^{1/2} . \tag{2.3}$$

It should be noted that ω_1 and θ are not c numbers in (2.2) and (2.3), but this difficulty can be easily overcome since $\mathscr{N}$ is a constant of motion and commutes with T; therefore we may limit our considerations to a subspace of the total Hilbert space characterized by a single eigenvalue of $\mathscr{N}$, and within this subspace we may interpret θ, ω_1, and $\mathscr{N}$ as c numbers. A more serious point, however, is that θ, as given by (2.3), is a multivalued function of the two variables ω_1 and $\omega_0-\omega$, which may be represented as double-helix surfaces on the ω_1, $\omega_0-\omega$ plane. The two helices are shifted by π with respect to each other along the θ direction and the step of each helix is 2π, as represented in Fig. 1. To obtain a single-valued function, which is necessary

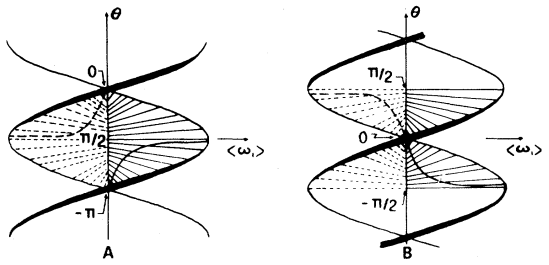

FIG. 1. The portions of the double helix surface on which θ is a one-valued function of $\omega_0-\omega$ and $\langle\omega_1\rangle$ according to the choice A ($-\pi<\theta\leq 0$) and B ($-\pi/2<\theta\leq\pi/2$). The $\omega_0-\omega$ axis is parallel to the line of sight. The straight lines on each portion of the double helix show the intersections of the surface with $\theta=$ const planes, while curved lines on each portion show the intersection of the surface with a $\omega_0-\omega=$const plane. The dotted parts of the double helix are seen from below and the continuous parts are seen from above.

in order to define uniquely the dressing operator T, we have to limit the variable θ to any chosen interval of amplitude π. We consider first the two possible choices $-\pi<\theta\leq 0$ (choice A) and $-\pi/2<\theta\leq\pi/2$ (choice B). With the help of Fig. 1 it is easy to check that these two cases correspond to

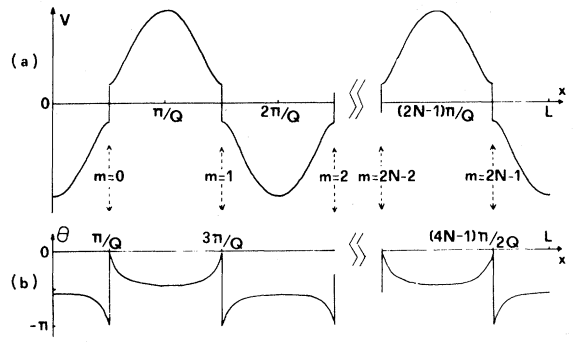

FIG. 2. (a) The potential $V_\uparrow(x)$ for $4\epsilon_0^2\mathcal{N}/(\omega_0-\omega)^2=24$ according to choice A. $V_\downarrow(x)=-V_\uparrow(x)$. (b) θ as a function of x for $4\epsilon_0\mathcal{N}/(\omega_0-\omega)^2=24(\omega_0-\omega>0)$ according to choice A. For $\omega_0-\omega<0$ the new $\theta(x)$ is given by $-\theta-\pi$.

At the discontinuous points x_m ($m=0,1,\ldots,2N-1$) the jump in $V_\uparrow$ is $|\omega_0-\omega|$ and the corresponding one in θ is π. At its extrema,

$$V_\uparrow=\pm\tfrac{1}{2}[(\omega_0-\omega)^2+4\epsilon_0^2\mathcal{N}]^{1/2}\ ,$$

while at the same points

$$\theta=-\frac{\pi}{2}\pm\arctan\frac{2\epsilon_0\mathcal{N}^{1/2}}{\omega_0-\omega}\ .$$

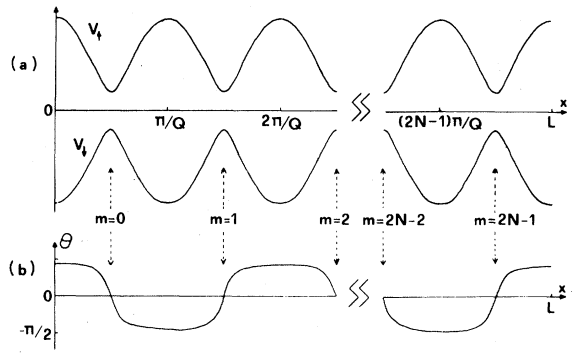

FIG. 3. (a) The potentials $V_\uparrow$ and $V_\downarrow$ for $4\epsilon_0^2\mathcal{N}/(\omega_0-\omega)^2=24$ according to choice B. (b) θ as a function of x for $4\epsilon_0^2\mathcal{N}/(\omega_0-\omega)^2=24$ according to choice B ($\omega_0-\omega>0$). For $\omega_0-\omega<0$ the new $\theta(x)$ is given by $-\theta$. In the limit $\omega_0\to\omega$, $V_{\uparrow\downarrow}$ is characterized by cusps at points x_m ($m=0,1,\ldots,2N-1$) and θ becomes discontinuous at the same points.

$$\begin{aligned} A&\begin{cases}\sin\theta=-\mathrm{sgn}(\omega_1)\omega_1/\Delta,\\ \cos\theta=-\mathrm{sgn}(\omega_1)(\omega_0-\omega)/\Delta,\end{cases}\\ B&\begin{cases}\sin\theta=\mathrm{sgn}(\omega_0-\omega)\omega_1/\Delta,\\ \cos\theta=|\omega_0-\omega|/\Delta,\end{cases}\end{aligned}\qquad(2.4)$$

where

$$\Delta=[(\omega_0-\omega)^2+4\epsilon^2\mathcal{N}]^{1/2}\ .\qquad(2.5)$$

Substituting (2.4) in (2.2), we obtain in the two cases considered

$$\begin{aligned}&(\mathrm{A})\ \tilde{\mathcal{H}}_0=\omega(\mathcal{N}-\tfrac{1}{2})-\mathrm{sgn}(\omega_1)\Delta S_z\ ,\\ &(\mathrm{B})\ \tilde{\mathcal{H}}_0=\omega(\mathcal{N}-\tfrac{1}{2})+\mathrm{sgn}(\omega_0-\omega)\Delta S_z\ ,\end{aligned}\qquad(2.6)$$

We now meet with a curious situation. In fact, calling $\theta_A(x)$ and $\theta_B(x)$ the two θ's corresponding to choices A and B, respectively, it is clear that the two Hamiltonians in (2.6) are fully equivalent, since they are are related by a canonical transformation

$$T_{\mathrm{A,B}}=\exp[-(\theta_\mathrm{A}-\theta_\mathrm{B})(4\mathcal{N})^{1/2}\times(\alpha S_+-\alpha^\dagger S_-)]\ .\qquad(2.7)$$

On the other hand, the difference between A and B in (2.6) seems far from irrelevant since the term in S_z in either Hamiltonian is going to play the role of an effective potential acting on the center of mass of the atom, due to the x dependence of ϵ which appears in Δ and in ω_1. In fact, the potential of choice A, as a function of x, has the same periodicity $2\pi/Q$ as ϵ and is characterized by discontinuities of amplitude $|\omega_0-\omega|$ wherever ϵ changes sign, that is at points

$$x_m=(2m+1)\pi/2Q \tag{2.8}$$

along the x axis, as shown in Fig. 2, while the potential of choice B, shown in Fig. 3, has periodicity of π/Q and is continuous as a function of x. Thus the two potentials are quite different. Still, the two cases considered must be equivalent in the sense that the eigenvalue distribution obtained by transforming (1.1) according to choice A and choice B must be the same. This paradox is only apparent, however, since $\mathscr{H}_0$ is only part of the complete Hamiltonian (1.1). Consequently, one should also T transform the kinetic energy term in (1.1), and the resulting Hamiltonian $\tilde{\mathscr{H}}=T^{-1}\mathscr{H}T$, if amenable to an exact treatment, gives the same eigenvalue distribution in case A as in case B. On the other hand, if an exact treatment of the total Hamiltonian is not feasible, one of the two choices A or B may be more appropriate, if it is more easily approximable than the other. We shall see that this is indeed the case and that, roughly speaking, choice A is appropriate for a treatment in the neighborhood of resonances, while far from resonance choice B provides a better starting point. We shall discuss the other infinite possible choices $-\pi+\beta<\theta\leq\beta$ $(\beta>0)$, intermediate between choices A and B, at the end of the next section.

III. SELF-CONSISTENT POTENTIAL NEAR RESONANCE

In this section we shall assume that the atom-field system is in a neighborhood of resonance where $|\omega_0-\omega|<2\epsilon_0\mathscr{N}^{1/2}$, and we shall transform by the operator T in (2.1) also the kinetic energy term in the Hamiltonian (1.1). We remark first that for any $\theta(x)$,

$$\begin{aligned}&[p,\theta]=-i\theta',[p^2,\theta]=-(2i\theta'p+\theta''),\\&[[p^2,\theta],\theta]=-[2i\theta'p+\theta'',\theta],\\&[[[p^2,\theta],\theta],\theta]=0,\end{aligned} \tag{3.1}$$

where each prime indicates a derivative with respect to x. By usual expansion techniques, we obtain

$$\begin{aligned}&T^{-1}\frac{1}{2M}p^2T=\frac{1}{2M}p^2+\mathscr{H}_2+\mathscr{H}_3,\\&\mathscr{H}_2=-\frac{1}{4M\mathscr{N}^{1/2}}(2i\theta'p+\theta'')(\alpha S_+-\alpha^\dagger S_-),\\&\mathscr{H}_3=\frac{1}{8M}[2i\theta'p+\theta'',\theta].\end{aligned} \tag{3.2}$$

From (3.2) we see that the T transformation of the kinetic energy introduces new terms $\mathscr{H}_2$ and $\mathscr{H}_3$ in the Hamiltonian. We easily realize that these two terms differ in cases A and B because of the presence of the derivatives of θ, which exhibit jumps of amplitude π along lines of the $(\omega_1,\omega_0-\omega)$ plane different in the two cases, as it is evident from Fig. 1. Thus we are led to develop the following procedure to decide the appropriateness of either choice A or B.

(i) For each choice we calculate the amplitude of the matrix elements of $\mathscr{H}_2$ and $\mathscr{H}_3$ between the eigenstates of

$$\mathscr{H}_1=\frac{1}{2M}p^2+\tilde{\mathscr{H}}_0. \tag{3.3}$$

(ii) We look for the choice according to which of these amplitudes are small enough to have a negligible influence on the eigensolutions of $\mathscr{H}_1$, and we adopt the $\mathscr{H}_1$ of this choice as a good zero-order approximation for the Hamiltonian of our system.

In this sense we may say that we are adopting a self-consistent criterion, since we choose the function $\theta(x)$ that minimizes the effects of $\mathscr{H}_2$ and $\mathscr{H}_3$ on the eigensolutions of $\mathscr{H}_1$, which in turn depend on this choice. Now $\mathscr{H}_1$ contains $\tilde{\mathscr{H}}_0$, which is essentially a pseudospin-dependent potential different for different $\theta(x)$; consequently, this minimization procedure leads to a potential which we can use as a good first approximation to represent in a self-consistent fashion the effects of the electromagnetic field on the two-level atom.

In order to apply the procedure outlined above, we shall estimate separately for the choices A and B the matrix elements of $\mathscr{H}_2$ and $\mathscr{H}_3$ between the eigenstates of $\mathscr{H}_1$. Finally, we shall comment on the other possible choices of $\theta(x)$ intermediate between A and B.

A. Choice A

From (2.6) and (3.3)

$$\mathscr{H}_1=\frac{1}{2M}p^2+\omega(\mathscr{N}-\tfrac{1}{2})-\mathrm{sgn}(\omega_1)\Delta S_z. \tag{3.4}$$

We see that $\mathscr{H}_1$ describes a particle of mass M in the pseudospin-dependent potential

$$V_{\uparrow\downarrow}(x)=\mp\tfrac{1}{2}\,\mathrm{sgn}(\cos Qx)[(\omega_0-\omega)^2+4\epsilon_0^2\mathscr{N}\cos^2Qx]^{1/2} \tag{3.5}$$

represented in Fig. 2(a). In this section, an explicit calculation of the eigenstates and eigenvalues of $\mathscr{H}_1$ is not necessary, and we shall postpone it to the next section. Here we only need to remark that (3.5) is a periodic potential which reduces to the Mathieu potential[14] for $\omega_0=\omega$. Therefore we expect the eigenfunctions of $\mathscr{H}_1$ to be of the Floquet form and to reduce to the solutions of the Mathieu equation on resonances.[15] For any detuning near resonance, we shall indicate them by

$$|r,k_\uparrow,\mathscr{N},\uparrow\rangle, |r,k_\downarrow,\mathscr{N},\downarrow\rangle ,$$

$$k=\frac{2\pi l}{Na} , \quad \left[l=-\frac{N-1}{2},\ldots,-1,0,1,\ldots,\frac{N}{2} \right] \tag{3.6}$$

where N is the number of wells in either potential $V_{\uparrow\downarrow}$, and where periodic boundary conditions have been assumed. The orbital parts $|r,k_\uparrow\rangle$, and $|r,k_\downarrow\rangle$, which refer to the motion of the atomic center of mass, are, in the x representation,

$$\begin{aligned} &\langle x\,|\,r,k_\uparrow\rangle\equiv\Psi^{\uparrow}_{r,k}(x) , \\ &\langle x\,|\,r,k_\downarrow\rangle\equiv\Psi^{\downarrow}_{r,k}(x) . \end{aligned} \tag{3.7}$$

The eigenvalues of $|r,k_\uparrow,\mathscr{N},\uparrow\rangle$ are obviously degenerate with those of $|r,k_\downarrow,\mathscr{N},\downarrow\rangle$, since $V_\uparrow$ and $V_\downarrow$ are simply shifted with respect to each other by $a/2$, and they are distributed in bands, each characterized by a value of r. Within each band k plays the usual role of wave vector.

With the help of (2.3), (2.4), and of Fig. 1(a), it is possible to convince oneself that in case A we may represent $\theta(x)$ explicitly as

$$\theta(x)=\theta_c(x)+\theta_g(x) , \tag{3.8}$$

where $\theta_c(x)$ is the usual arctan function which behaves as

$$\theta_c(x)=\begin{cases} \dfrac{2\epsilon_0\mathscr{N}^{1/2}}{\omega_0-\omega}\cos Qx-\dfrac{1}{3}\left[\dfrac{2\epsilon_0\mathscr{N}^{1/2}}{\omega_0-\omega}\cos Qx\right]^3+\dfrac{1}{5}\left[\dfrac{2\epsilon_0\mathscr{N}^{1/2}}{\omega_0-\omega}\cos Qx\right]^5-\cdots , & (\cos Qx\to 0) \\ \dfrac{\pi}{2}-\dfrac{\omega_0-\omega}{2\epsilon_0\mathscr{N}^{1/2}\cos Qx}+\dfrac{1}{3}\left[\dfrac{\omega_0-\omega}{2\epsilon_0\mathscr{N}^{1/2}\cos Qx}\right]^3-\dfrac{1}{5}\left[\dfrac{\omega_0-\omega}{2\epsilon_0\mathscr{N}^{1/2}\cos Qx}\right]^5+\cdots , & (\cos Qx\to 1) \end{cases} \tag{3.9}$$

and where

$$\theta_g(x)=-\pi H[\mathrm{sgn}(\omega_0-\omega)\cos Qx], \quad H(y)=\begin{cases} 1 & (y>0) \\ 0 & (y<0) \end{cases} . \tag{3.10}$$

Hence we find after some algebra

$$\begin{aligned} &\theta_c'(x)=-2\epsilon_0\mathscr{N}^{1/2}Q\sin(Qx)\frac{\omega_0-\omega}{(\omega_0-\omega)^2+4\epsilon_0^2\mathscr{N}\cos^2Qx} , \\ &\theta_g'(x)=\pi\,\mathrm{sgn}(\omega_0-\omega)\sum_m(-1)^m\delta(x-x_m) , \end{aligned} \tag{3.11}$$

where x_m has been defined in (2.8). It is interesting to remark that

$$\begin{aligned} \lim_{\omega_0\to\omega}\theta_c'(x)&=-\mathrm{sgn}(\omega_0-\omega)2\epsilon_0\mathscr{N}^{1/2}Q\sin(Qx)\pi\delta(2\epsilon_0\mathscr{N}^{1/2}\cos Qx) \\ &=\pi\,\mathrm{sgn}(\omega_0-\omega)\sum_m(-1)^{m+1}\delta(x-x_m)=-\theta_g'(x) . \end{aligned} \tag{3.12}$$

As for the matrix elements of $\mathscr{H}_2$, first we obtain from (3.11) and for any $f(x)$

$$\begin{aligned} \int_0^{\pi/Q}f(x)\theta_c'(x)dx&=-2\epsilon_0\mathscr{N}^{1/2}Q\int_0^{\pi/Q}f(x)\sin(Qx)\frac{\omega_0-\omega}{(\omega_0-\omega)^2+4\epsilon_0^2\mathscr{N}\cos^2Qx}dx \\ &=\int_{2\epsilon_0\mathscr{N}^{1/2}}^{-2\epsilon_0\mathscr{N}^{1/2}}f(y)\frac{\omega_0-\omega}{(\omega_0-\omega)^2+y^2}dy . \end{aligned}$$

Consequently, if $f(x)$ is sufficiently smooth and for $|\omega_0-\omega|<2\epsilon_0\mathscr{N}^{1/2}$, we have

$$\int_0^{\pi/Q} f(x)\theta_c'(x)dx \simeq -2f(\pi/2Q)\arctan\frac{2\epsilon_0\mathcal{N}^{1/2}}{\omega_0-\omega}$$

$$\simeq -f(\pi/2Q)\left[\pi\,\mathrm{sgn}(\omega_0-\omega)-\frac{\omega_0-\omega}{\epsilon_0\mathcal{N}^{1/2}}\right]. \tag{3.13}$$

In the final result of (3.13), terms nonlinear in $(\omega_0-\omega)$ have been neglected. Thus

$$\int_L f(x)\theta_c'(x)dx=\sum_{m=0}^{2N-1}\int_{m\pi/Q}^{(m+1)\pi/Q} f(x)\theta_c'(x)dx \simeq \left[\pi\,\mathrm{sgn}(\omega_0-\omega)-\frac{\omega_0-\omega}{\epsilon_0\mathcal{N}^{1/2}}\right]\sum_m(-1)^{m+1}f(x_m)\,, \tag{3.14}$$

where L is the total length of the standing wave ($0\le x\le L$) and the m integers number the discontinuities in either potential $V_{\uparrow\downarrow}$ at points x_m as shown in Fig. 2(a). Moreover, from (3.11),

$$\int_L f(x)\theta_g'(x)dx=\pi\,\mathrm{sgn}(\omega_0-\omega)\sum_m(-1)^m f(x_m)\,, \tag{3.15}$$

which together with (3.14) yields

$$\int_L f(x)\theta'(x)dx\simeq\frac{\omega_0-\omega}{\epsilon_0\mathcal{N}^{1/2}}\sum_m(-1)^m f(x_m)\,. \tag{3.16}$$

Furthermore, integrating (3.14) by parts and using the same approximations, we get

$$\int_L f(x)\theta_c''(x)dx\simeq-\left[\pi\,\mathrm{sgn}(\omega_0-\omega)-\frac{\omega_0-\omega}{\epsilon_0\mathcal{N}^{1/2}}\right]\sum_m(-1)^{m+1}f'(x_m)\,, \tag{3.17}$$

whereas integrating (3.15) by parts

$$\int_L f(x)\theta_g''(x)dx=\pi\,\mathrm{sgn}(\omega_0-\omega)\sum_m(-1)^{m+1}f'(x_m)\,. \tag{3.18}$$

From (3.17) and (3.18), we find

$$\int_L f(x)\theta''(x)dx\simeq\frac{\omega_0-\omega}{\epsilon_0\mathcal{N}^{1/2}}\sum_m(-1)^{m+1}f'(x_m)\,. \tag{3.19}$$

On the basis of (3.16) and (3.19) it easy to obtain

$$\langle r,k_\downarrow\,|\,(2i\theta'p+\theta'')\,|\,r',k'_\uparrow\rangle\simeq\frac{\omega_0-\omega}{\epsilon_0\mathcal{N}^{1/2}}J^{rk_\downarrow}_{r'k'_\uparrow},\quad J^{rk_\downarrow}_{r'k'_\uparrow}=\sum_m(-1)^m j^{rk_\downarrow}_{r'k'_\uparrow}(x_m)\,, \tag{3.20a}$$

$$\langle r,k_\uparrow\,|\,(2i\theta'p+\theta'')\,|\,r',k'_\downarrow\rangle\simeq\frac{\omega_0-\omega}{\epsilon_0\mathcal{N}^{1/2}}J^{rk_\uparrow}_{r'k'_\downarrow},\quad J^{rk_\uparrow}_{r'k'_\downarrow}=\sum_m(-1)^m j^{rk_\uparrow}_{r'k'_\downarrow}(x_m)\,, \tag{3.20b}$$

where the out of diagonal matrix elements of the density current $j_b^a(x_m)$ are given by

$$\begin{aligned} j^{rk_\downarrow}_{r'k'_\uparrow}(x_m)&=[\Psi^{\downarrow *}_{r,k}(\Psi^{\uparrow}_{r',k'})'-(\Psi^{\downarrow *}_{r,k})'\Psi^{\uparrow}_{r',k'}]_{x=x_m}\,,\\ j^{rk_\uparrow}_{r'k'_\downarrow}(x_m)&=[\Psi^{\uparrow *}_{r,k}(\Psi^{\downarrow}_{r',k'})'-(\Psi^{\uparrow *}_{r,k})'\Psi^{\downarrow}_{r',k'}]_{x=x_m}\,. \end{aligned} \tag{3.21}$$

Using (3.20), we obtain the matrix elements of $\mathscr{H}_2$ between the eigenstates (3.7) of $\mathscr{H}_1$ as

$$\langle r,k_\downarrow,\mathcal{N},\downarrow\,|\,\mathscr{H}_2\,|\,r',k'_\uparrow,\mathcal{N},\uparrow\rangle\simeq\frac{\omega_0-\omega}{4M\epsilon_0\mathcal{N}^{1/2}}J^{rk_\downarrow}_{r'k'_\uparrow}\,, \tag{3.22a}$$

$$\langle r,k_\uparrow,\mathcal{N},\uparrow\,|\,\mathscr{H}_2\,|\,r',k'_\downarrow,\mathcal{N},\downarrow\rangle\simeq=-\frac{\omega_0-\omega}{4M\epsilon_0\mathcal{N}^{1/2}}J^{rk_\uparrow}_{r',k'_\downarrow}\,. \tag{3.22b}$$

We now turn to the evaluation of the matrix elements of $\mathscr{H}_3$. From (3.1) we have

$$\langle r,k_\downarrow,\mathscr{N},\downarrow|\mathscr{H}_3|r',k'_\downarrow,\mathscr{N},\downarrow\rangle=\frac{1}{8M}\sum_{r'',k''_\downarrow}[\langle r,k_\downarrow|(2i\theta'p+\theta'')|r'',k''_\downarrow\rangle\langle r'',k''_\downarrow|\theta|r',k'_\downarrow\rangle$$
$$-\langle r,k_\downarrow|\theta|r'',k''_\downarrow\rangle\langle r'',k''_\downarrow|(2i\theta'p+\theta'')|r',k'_\downarrow\rangle]\ . \tag{3.23}$$

Now we observe that, because of (3.1), we may write

$$2i\theta'p+\theta''=[\theta,p^2]=2M[\theta,\mathscr{H}_1]\ . \tag{3.24}$$

Thus, using (3.24) in (3.23), we find after some algebra

$$\langle r,k_\downarrow,\mathscr{N},\downarrow|\mathscr{H}_3,|r',k'_\downarrow,\mathscr{N},\downarrow\rangle$$
$$=\frac{1}{4}\sum_{r'',k''_\downarrow}\{\langle r,k_\downarrow|\theta|r'',k''_\downarrow\rangle\langle r'',k''_\downarrow|\theta|r',k'_\downarrow\rangle[2E(r'',k''_\downarrow,\mathscr{N},\downarrow)-E(r,k_\downarrow,\mathscr{N},\downarrow)-E(r',k'_\downarrow,\mathscr{N},\downarrow)]\}\ , \tag{3.25}$$

where $E(\{a\})$ is the eigenvalue of $\mathscr{H}_1$ corresponding to the set $\{a\}$ of quantum numbers. An order-of-magnitude evaluation of (3.25), which should be good particularly for large fields, is easily performed, since near the bottom of each well, where presumably the wave functions of the lowest bands are concentrated, $\cos Qx\sim 1$ and $\theta(x)$ in choice A differ from $\pi/2$ only by quantities of the order of $(\omega_0-\omega)$ according to (3.9). It follows immediately that (3.25) is of the order of $(\omega_0-\omega)^2$, and must be neglected with respect to (3.22) coherently with our previous approximations.

B. Choice B

Using (2.6) and (3.3) again, we find

$$\mathscr{H}_1=\frac{1}{2M}p^2+\omega(\mathscr{N}-\tfrac{1}{2})+\mathrm{sgn}(\omega_0-\omega)\Delta S_z\ . \tag{3.26}$$

$\mathscr{H}_1$ now represents the motion of a particle of mass M in the pseudospin-dependent potential of Fig. 3(a),

$$V_{\uparrow\downarrow}(x)=\pm\tfrac{1}{2}[(\omega_0-\omega)^2+4\epsilon_0^2\mathscr{N}\cos^2Qx]^{1/2}\ . \tag{3.27}$$

Contrary to the situation originated by the previous choice, it is obvious that the orbital part of the wave functions must be very different for up and down pseudospin, at least for small $\omega_0-\omega$. Moreover, the number of wells in each potential (3.27) is now $2N$, the distance between two neighboring wells being π/Q and the total length of the chain $L=Na$ as before. We also use the same symbols $|r,k_\downarrow,\mathscr{N},\uparrow\rangle$ and $|r,k_\downarrow,\mathscr{N}\downarrow\rangle$ for the eigenkets of (3.26), although the Brillouin zone of the system is doubled, since

$$k=\frac{2\pi l}{Na}\quad(l=-N+1,\ldots,-1,0,1,\ldots,N) \tag{3.28}$$

because of the new periodicity of $V_{\uparrow\downarrow}$. The orbital part of the complete eigenkets are denoted by $|r,k_\uparrow\rangle$ and $|r,k_\downarrow\rangle$, which can be x represented as

$$\langle x|r,k_\uparrow\rangle\equiv\Phi^\uparrow_{r,k}(x),\quad\langle x|r,k_\downarrow\rangle\equiv\Phi^\downarrow_{r,k}(x)\ . \tag{3.29}$$

Using (2.3), (2.4), and Fig. 1(b), we obtain that $\theta(x)$ coincides in case B with $\theta_c(x)$ as given by (3.9). Thus we may use the main results of the previous subsection, and by neglecting terms linear in $(\omega_0-\omega)$ we find from (3.14) and (3.17)

$$\int_L f(x)\theta'(x)dx\simeq\pi\,\mathrm{sgn}(\omega_0-\omega)\sum_{m=0}^{2N-1}(-1)^{m+1}f(x_m)\ ,$$
$$\int_L f(x)\theta''(x)dx\simeq-\pi\,\mathrm{sgn}(\omega_0-\omega)\sum_m(-1)^{m+1}f'(x_m)\ . \tag{3.30}$$

We remark that the integrals in (3.30) do not vanish as $\omega_0-\omega$, whereas the corresponding integrals of choice A did. Introducing the matrix elements of the density current

$$j^{rk_\downarrow}_{r'k'_\uparrow}(x_m)=[\Phi^{\downarrow *}_{r,k}(\Phi^{\uparrow}_{r',k'})'-(\Phi^{\downarrow *}_{r,k})'\Phi^{\uparrow}_{r',k'}]_{x=x_m}\,,$$
$$j^{rk_\uparrow}_{r'k'_\downarrow}(x_m)=[\Phi^{\uparrow *}_{r,k}(\Phi^{\downarrow}_{r',k'})'-(\Phi^{\uparrow *}_{r,k})'\Phi^{\downarrow}_{r',k'}]_{x=x_m}\,, \tag{3.31}$$

and using the same expressions for J^a_b in terms of $j^a_b(x_m)$ as in (3.20), we obtain

$$\langle r,k_\downarrow\,|\,(2i\theta' p+\theta'')\,|\,r',k'_\uparrow\rangle\simeq-\pi\,\mathrm{sgn}(\omega_0-\omega)J^{rk_\downarrow}_{r'k'_\uparrow}\,,$$
$$\langle r,k_\uparrow\,|\,(2i\theta' p+\theta'')\,|\,r',k'_\downarrow\rangle\simeq-\pi\,\mathrm{sgn}(\omega_0-\omega)J^{rk_\uparrow}_{r'k'_\downarrow}\,. \tag{3.32}$$

The sought-for matrix elements of $\mathscr{H}_2$ can be immediately obtained from (3.32) as in the case of choice A. We remark that the ambiguity in the sign of the amplitude for $(\omega_0-\omega)\to\pm 0$ is without physical consequences, in view of the fact that any physical quantity, such as energy shifts or transition probabilities, should depend on the modulus of these amplitudes.

C. The intermediate choices.

We can already draw some qualitative conclusions from the foregoing analysis. First we remark that the results (3.22) and (3.25) ensure that in an appropriately small neighborhood of resonance and for choice A, the matrix elements of $\mathscr{H}_2+\mathscr{H}_3$ between the eigenstates of $\mathscr{H}_1$ are small enough to be negligible in a first approximation, so that the eigenvalue distribution of the total Hamiltonian $\mathscr{H}$ should be reasonably similar to that of $\mathscr{H}_1$ as given by (3.4). On the contrary, results (3.32) show that the matrix elements of $\mathscr{H}_2$ for choice B do not vanish on resonance so that there is no guarantee that $\mathscr{H}_2$ may be treated in this case as a small perturbation near resonance and that the eigenvalue distribution of $\tilde{\mathscr{H}}$ is approximately represented by that of $\mathscr{H}_1$ as given by (3.26); a calculation of the matrix elements of $\mathscr{H}_3$ for choice B is superfluous in view of this result concerning $\mathscr{H}_2$. Therefore we are led to conclude that the appropriate pseudospin-dependent potential for representing approximately the effects of the standing electromagnetic wave on the atoms sufficiently near resonance is the periodically discontinuous one given by (3.5) and not the continuous one given by (3.27). We remark that the periodic discontinuities of potential (3.5) are associated with the discontinuities of $\theta(x)=\theta_c(x)+\theta_g(x)$; the latter has the interesting property that in the limit $\omega_0=\omega$ the singularities in θ'_c compensate exactly those of θ'_g, as is evident from (3.12), and this cancellation effect is responsible for the vanishing of the matrix elements of $\mathscr{H}_2+\mathscr{H}_3$ in choice A and for the vanishing of the discontinuities in the effective potential. Out of resonance, due to the fact that the position of the maxima of θ'_c coincide always with the position of the singularities of θ'_g, the cancellation is only partial, leaving terms of the order of $|\omega_0-\omega|$ in the matrix elements of $\mathscr{H}_2+\mathscr{H}_3$. On the other hand, according to choice B it is $\theta(x)=\theta_c(x)$, and for $\omega_0\to\omega$ there is no cancellation of the singularities of $\theta'_c(x)$, so that the matrix elements of $\mathscr{H}_2$ remain finite in this limit.

We have now to inquire whether a choice for $\theta(x)$ intermediate between A and B, such as

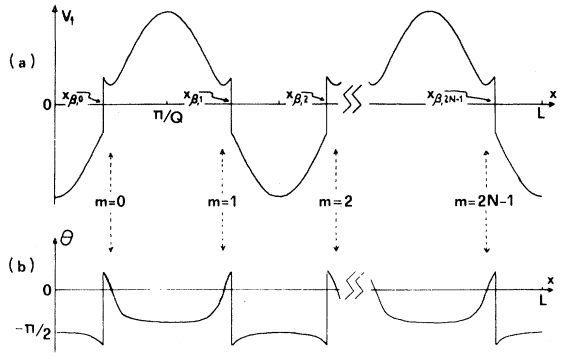

FIG. 4. (a) The potential $V_\uparrow(x)$ for $4\epsilon_0^2\mathscr{N}/(\omega_0-\omega)^2=24$ and $\omega_0-\omega>0$ according to the intermediate choice $-\pi+\beta<\theta\le\beta$ $(\beta=\pi/4)$. $V_\downarrow(x)=-V_\uparrow(x)$. (b) $\theta(x)$ for $4\epsilon_0^2\mathscr{N}/(\omega_0-\omega)^2=24$ and $\omega_0-\omega>0$ according to the intermediate choice $-\pi+\beta<\theta\le\beta$ $(\beta=\pi/4)$. The discontinuities in V and θ take place at points $x_{\beta,m}\neq x_m$. At points x_m, $\theta'(x)$ has a relative maximum or minimum and $V_\uparrow$ develops new relative minima. As β increases from 0, each point $x_{\beta,m}$ (for $\omega_0-\omega>0$) moves towards the nearest multiple of $2\pi/Q$, thereby progressively changing the potential $V_\uparrow$ of the intermediate choice into the $V_\uparrow$ potential of choice B. The transformation is complete when $\beta=\arctan[(\omega_0-\omega)/2\epsilon_0\mathscr{N}^{1/2}]$.

$-\pi+\beta<\theta\leq\beta$ ($\beta>0$) could yield matrix elements of $\mathscr{H}_2+\mathscr{H}_3$, which, near resonance, are smaller than those of choice A. In Fig. 4 we have represented the case in question for $\beta=\pi/4$ and for $V=V_\uparrow$. We see that the rather exotic potential which is obtained in this case for $\omega_0\neq\omega$ is characterized by the appearance of new relative maxima at points x_m. It is obvious that no simple way of calculating the eigenfunctions and eigenvalues of $\mathscr{H}_1$ exists in this case, contrary to those of choices A and B where we may devise, e.g., suitable versions of the tight-binding approximation. Thus we shall have to rely on qualitative considerations in order to estimate the magnitude of the matrix elements of $\mathscr{H}_2+\mathscr{H}_3$ between the eigenstates of $\mathscr{H}_1$. From Fig. 4(b) we see that the maxima of θ_c' at $x=x_m$ do not coincide with the singularities of θ_g', at least for $\omega_0\neq\omega$, which indicates that the partial cancellation of case A cannot take place. In fact, it is possible to convince oneself that in the intermediate case at hand

$$\theta_g(x)=-\pi H\{\mathrm{sgn}(\omega_0-\omega)[\cos Qx-\cos Qx_\beta]\}\ ,$$
$$\cos Qx_\beta=\frac{\omega_0-\omega}{2\epsilon_0\mathscr{N}^{1/2}}\tan\beta \tag{3.33}$$
$$\theta_g'(x)=\pi\,\mathrm{sgn}(\omega_0-\omega)\sum_m(-1)^m\delta(x-x_{\beta,m})\ ,$$

where $x_{\beta,m}$ are the points which satisfy to

$$x_{\beta,m}=\frac{1}{Q}\arccos\left[\frac{\omega_0-\omega}{2\epsilon_0\mathscr{N}^{1/2}}\tan\beta\right];\ \lim_{\beta\to0}x_{\beta,m}=x_m\ , \tag{3.34}$$

whereas $\theta_c(x)$ is still given by (3.9), $\theta_c'(x)$ having its maxima at points x_m. Thus, developing the calculations for the matrix elements of $\mathscr{H}_2$ as previously and neglecting terms linear in $|\omega_0-\omega|$, we obtain

$$\int_L f(x)\theta'(x)dx=\pi\,\mathrm{sgn}(\omega_0-\omega)\sum_m(-1)^m[f(x_{\beta,m})-f(x_m)]\ ,$$
$$\int_L f(x)\theta''(x)dx=\pi\,\mathrm{sgn}(\omega_0-\omega)\sum_m(-1)^{m+1}[f'(x_{\beta,m})-f'(x_m)]\ , \tag{3.35}$$

which show that in general the matrix elements of $\mathscr{H}_2$ may not be negligible due to the likely existence of maxima of the eigenfunctions of $\mathscr{H}_1$ at points x_m of Fig. 4; these maxima make terms such as $f(x_{\beta,m})-f(x_m)$ in (3.35) presumably large and very difficult to evaluate. In the rest of this paper we shall be content with these qualitative considerations and we shall concentrate on the extreme cases of choices A and B.

Finally, we wish to discuss briefly the physical meaning of some of the results we have obtained, and in particular the physical origin of the terms $\mathscr{H}_2+\mathscr{H}_3$ defined in (3.2). Consider first the dressing of the atomic momentum

$$T^{-1}pT=p+i(4\mathscr{N})^{-1/2}\theta'(\alpha S_+-\alpha^\dagger S_-)\ , \tag{3.36}$$

which can be obtained from (2.1) and (3.1). Expression (3.36) indicates that the dressed atomic velocity is modulated by the transitions between opposite pseudospin eigenstates of the dressed atom. Such a modulation can be understood as follows. Each change of the internal state of the dressed atom entails a change in the effective potential from $V_\uparrow$ and $V_\downarrow$ or vice versa; since the maxima of $V_\uparrow$ coincide with the minima of $V_\downarrow$ for any choice of θ, each internal transition of the dressed atom favors a displacement by a finite amount the pattern of the center-of-mass wave function whose maxima tend to coincide with the minima of the potential. This explains qualitatively the velocity modulation. Moreover, Eq. (3.36) shows that this modulation is proportional to θ', and we have seen that according to choice A the singularities in θ' tend to cancel for ω_0 sufficiently near to ω, while no such cancellation operates according to choice B. This means that choice A entails a minimization of the frequency of switching from $V_\uparrow$ to $V_\downarrow$ and vice versa: the dressed atom sees the same potential over a long span of time. The opposite is true for choice B, which in the neighborhood of $\omega_0=\omega$ entails large values of θ' at points x_m with a consequent high frequency of switching from one potential to the other. This is precisely the physical reason why the matrix elements of $\mathscr{H}_2+\mathscr{H}_3$, which arise in $T^{-1}(p^2/2M)T$ because of the presence of the second term in the right-hand side (RHS) of (3.36), are very small for choice A in the neighborhood of resonance: they describe processes of tunneling of the total system (dressed atom effective potential) between two equivalent configurations displaced

with respect to each other over a distance $\pi/Q=a/2$, and the tunneling frequency tends to zero as $\omega_0\to\omega$ because θ tends to $-\pi/2$ in this limit. On the contrary, choice B gives a $\theta(x)$ which jumps discontinuously between 0 and a high tunneling frequency. Thus choice A yields an effective potential for the atomic center of mass which is "good" in the sense that it remains the same for a long time (infinite for $\omega_0=\omega$), while the potential of choice B changes frequently between $V_\uparrow$ and $V_\downarrow$, and it should therefore not be used for a good zero-order approximation description of the atomic motion. It is also appropriate to emphasize that the discontinuities active in inducing the velocity modulation and the switching of the internal dressed configuration are those associated with $V_{\uparrow\downarrow}$, as is evident from (3.2) or (3.36); indeed, according to choice B we have for $\omega_0\sim\omega$ a continuous potential and a high frequency of switching, while the opposite is true according to choice A in the same region of detuning.

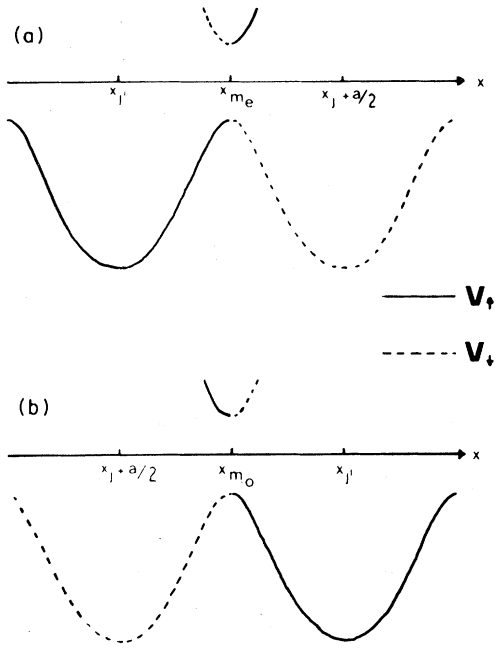

FIG. 5. The adjacent wells on either side of x_m. (a) For $m=m_e$, $x_{j'}=x_{m_e}-a/4$, $x_j+a/2=x_{m_e}+a/4$. (b) For $m=m_0$, $x_j-a/2=x_{m_0}-a/4$, $x_{j'}=x_{m_0}+a/4$.

IV. THE TIGHT-BINDING TREATMENT

We now wish to make our treatment near resonance rather more quantitative than it has been up to now. In particular, we may ask what are the limits of validity of choice A in terms of various parameters of the theory, such as the detuning $\omega_0-\omega$. In fact, we have shown that our treatment, in Sec. III, is valid for $|\omega_0-\omega|<2\epsilon_0\mathcal{N}^{1/2}$, but this is only a necessary condition, as is obvious, to make choice A more appropriate than choice B in the vicinity of $\omega_0=\omega$. We are also interested in finding the sufficient condition to establish quantitatively the region of the parameters in which choice A prevails over other choices. In order to achieve this aim it is necessary to obtain explicit expression for the matrix elements of the density current appearing in (3.22) for choice A, and for this we need the explicit form of $\Psi^{\uparrow\downarrow}_{r,k}(x)$ introduced in (3.7). One of the most simple treatments of a particle in a periodic potential can be obtained in terms of the tight-binding approximation,[16] which we shall adopt here because it is sufficient for our aims. Thus for any $|\omega_0-\omega|<2\epsilon_0\mathcal{N}^{1/2}$, we define $\Psi_r(x-x_j)$ as the localized eigenfunction belonging to the rth eigenvalue of the well whose minimum is at points $x_j=2\pi j/Q$ $(j=0,1,\ldots,N-1)$ for $V=V_\uparrow(x)$ as in Fig. 2(a), whereas $\psi_r(x-x_j-a/2)$ is the equivalent localized eigenfunction for $V_\downarrow(x)$. In terms of these localized eigenfunctions

$$\Psi^{\uparrow}_{r,k}(x)=\frac{1}{\sqrt{N}}\sum_j e^{ikx_j}\psi_r(x-x_j),\quad \Psi^{\downarrow}_{r,k}(x)=\frac{1}{\sqrt{N}}\sum_j e^{ik(x_j+a/2)}\psi_r(x-x_j-a/2)\,, \tag{4.1}$$

which are properly normalized and which we may use to calculate,

$$\begin{aligned}E(r,k_\uparrow,\mathcal{N},\uparrow)&=\langle r,k_\uparrow,\mathcal{N},\uparrow\,|\,\mathscr{H}_1\,|\,r,k_\uparrow,\mathcal{N},\uparrow\rangle=\omega(\mathcal{N}-\tfrac{1}{2})+\int_0^L\Psi^{\uparrow *}_{r,k}\left[\frac{1}{2M}p^2+V_\uparrow(x)\right]\Psi^{\uparrow}_{r,k}dx\\&\simeq\omega(\mathcal{N}-1/2)+\frac{1}{N}\sum_j\int_{-\infty}^{+\infty}\psi_r^*(x-x_j)\left[\frac{1}{2M}p^2+V_\uparrow(x)\right]\psi_r(x-x_j)dx\\&\quad+\frac{2}{N}\cos ka\sum_j\int_{-\infty}^{+\infty}\psi_r^*(x-x_j-a)\left[\frac{1}{2M}p^2+V_\uparrow(x)\right]\psi_r(x-x_j)dx\,,\end{aligned} \tag{4.2}$$

where the overlap between eigenfunctions localized in nonadjacent wells has been neglected and where translational invariance has been assumed. In the spirit of the tight-binding approximation, we introduce the local potential $V_{\uparrow}^{j}(x)$, which differs very little from $V_{\uparrow}(x)$ for $x \sim x_j$ and which we take to satisfy the localized Schrödinger equation

$$\left[\frac{1}{2M}p^2+V_{\uparrow}^{j}(x)\right]\psi_r(x-x_j)=E_r\psi_r(x-x_j)\ . \tag{4.3}$$

Using (4.3) and $V_{\uparrow}=V_{\uparrow}^{j}+(V_{\uparrow}-V_{\uparrow}^{j})$ in (4.2), we arrive at

$$E(r,k_{\uparrow},\mathcal{N},\uparrow)\simeq\omega(\mathcal{N}-\tfrac{1}{2})+E_r+\frac{1}{N}\sum_j\int_{-\infty}^{+\infty}\psi_r^*(x-x_j)[V_{\uparrow}(x)-V_{\uparrow}^{j}(x)]\psi_r(x-x_j)dx$$
$$+\frac{2}{N}\cos ka\{NE_r\beta_r+\sum_j\int_{-\infty}^{+\infty}\psi_r^*(x-x_j-a)[V_{\uparrow}(x)-V_{\uparrow}^{j}(x)]\psi_r(x-x_j)dx\ , \tag{4.4}$$

where we have put

$$\beta_r=\int_{-\infty}^{+\infty}\psi_r^*(x-x_j-a)\psi_r(x-x_j)dx\ . \tag{4.5}$$

The first integral on the RHS of (4.4) can be neglected because we assume $|\psi_r(x-x_j)|^2$ to be sharply peaked at $x=x_j$, where $V_{\uparrow}$ and $V_{\uparrow}^{j}$ practically coincide. We also assume that the product $\psi_r^*(x-x_j-a)\psi_r(x-x_j)$ is peaked at $x=x_j+a/2$, so that we may approximate

$$\int_{-\infty}^{+\infty}\psi_r^*(x-x_j-a)[V_{\uparrow}(x)-V_{\uparrow}^{j}(x)]\psi_r(x-x_j)dx\simeq\beta_r[V_{\uparrow}(x_j+a/2)-V_{\uparrow}^{j}(x_j+a/2)]\ . \tag{4.6}$$

Consequently, we obtain

$$E(r,k\mathcal{N},\uparrow)\simeq\omega(\mathcal{N}-\tfrac{1}{2})+E_r+2\beta_r[E_r+V_{\uparrow}(x_j+a/2)-V_{\uparrow}^{j}(x_j+a/2)]\cos ka\ , \tag{4.7}$$

which clearly displays the band like features of the eigenvalue distribution of $\mathscr{H}_1(\uparrow)$. The corresponding distribution for $\mathscr{H}_1(\downarrow)$ is equivalent to (4.7) as remarked at the beginning of Sec. III A. An important parameter that we wish to extract from the foregoing analysis is the bandwidth W_r of the rth band,

$$W_r\simeq|\,4\beta_r[E_r+V_{\uparrow}(x_j+a/2)-V_{\uparrow}^{j}(x_j+a/2)]\,|\ . \tag{4.8}$$

We have now to find an expression for the matrix elements (3.22) in terms of the states (4.1). The current density (3.21) contains products like

$$[\Psi_{r,k}^{\downarrow *}(\Psi_{r',k'}^{\uparrow})']_{x=x_m}=\frac{1}{N}\left[\sum_j e^{-ik(x_j+a/2)}\psi_r^*(x_m-x_j-a/2)\right]\left[\sum_{j'}e^{ik'x_{j'}}\psi_{r'}'(x_m-x_{j'})\right]. \tag{4.9}$$

Among the N^2 terms appearing in the double sum in (4.9), it is reasonable to assume that the dominant contribution should come from the product of two wave functions localized in adjacent wells, symmetrically placed about x_m. From Fig. 5(a), it is easy to see that for even $m\equiv m_e$ the above contribution to (4.9) comes from the product with $x_j+a/2=x_{m_e}+a/4$, $x_{j'}=x_{m_e}-a/4$, whereas for odd $m\equiv m_0$ it comes from the product with $x_j+a/2=x_{m_0}-a/4$, $x_{j'}=x_{m_0}+a/4$. Neglecting all other contributions which come from pairs of wells more distant from each other or from x_m, we obtain immediately

$$\begin{aligned}[\Psi_{r,k}^{\downarrow *}(\Psi_{r',k'}^{\uparrow})']_{x=x_{m_e}}&\simeq\frac{1}{N}e^{-ik(x_{m_e}+a/4)}\psi_r^*(-a/4)e^{ik'(x_{m_e}-a/4)}\psi_{r'}'(a/4)\ ,\\ [\Psi_{r,k}^{\downarrow *}(\Psi_{r',k'}^{\uparrow})']_{x=x_{m_0}}&\simeq\frac{1}{N}e^{-ik(x_{m_0}-a/4)}\psi_r^*(a/4)e^{ik'(x_{m_0}+a/4)}\psi_{r'}'(-a/4)\ .\end{aligned} \tag{4.10}$$

Using the above ideas and approximations, one eventually arrives at the following approximate expressions for the matrix elements of the density current (3.21):

$$j^{rk\downarrow}_{r'k'\uparrow}(x_{m_e})\simeq\frac{1}{N}e^{-i(k-k')x_{m_e}}e^{-i(k+k')a/4}[\psi^*_r(-a/4)\psi'_{r'}(a/4)-\psi^{*\prime}_r(-a/4)\psi_{r'}(a/4)]\,,$$
$$j^{rk\downarrow}_{r'k'\uparrow}(x_{m_0})\simeq\frac{1}{N}e^{-i(k-k')x_{m_0}}e^{i(k+k')a/4}[\psi^*_r(a/4)\psi'_{r'}(-a/4)-\psi^{*\prime}_r(a/4)\psi_{r'}(-a/4)]\,. \tag{4.11}$$

Introducing (4.11) into (3.20a), summing separately over x_{m_e} and x_{m_0}, and using

$$\sum_{m_e}e^{-i(k-k')x_{m_e}}=e^{-i(k-k')a/4}\times\sum_{j=0}^{N-1}e^{-i(k-k')x_j}=N\delta_{kk'}\,,$$
$$\sum_{m_0}e^{-i(k-k')x_{m_0}}=e^{-i(k-k')3a/4}\times\sum_{j=0}^{N-1}e^{-i(k-k')x_j}=N\delta_{kk'}\,, \tag{4.12}$$

we find

$$J^{rk\downarrow}_{r'k'\uparrow}\simeq A^{rr'}_k\delta_{kk'}\,,$$
$$A^{rr'}_k=e^{-ika/2}[\psi^*_r(-a/4)\psi'_{r'}(a/4)-\psi^{*\prime}_r(-a/4)\psi_{r'}(a/4)]$$
$$-e^{ika/2}[\psi^*_r(a/4)\psi'_{r'}(a/4)-\psi^{*\prime}_r(a/4)\psi_{r'}(-a/4)]\,. \tag{4.13}$$

As for $J^{rk\uparrow}_{r'k'\downarrow}$, it is easily seen from (3.20b) and (3.21) that it can be obtained from $J^{rk\downarrow}_{r'k'\uparrow}$ by the operations of sign change, complex conjugation, and exchange of (r,k) with (r',k'). Performing these operations on (4.13), we obtain

$$J^{rk\uparrow}_{r'k'\downarrow}\approx-A^{rr'}_k\delta_{kk'}\,, \tag{4.14}$$

substituting (4.13) and (4.14) into (3.22), we finally obtain

$$\langle r,k_\downarrow,\mathcal{N}\downarrow|\mathcal{H}_2|r',k'_\uparrow,\mathcal{N},\uparrow\rangle=\langle r,k_\uparrow,\mathcal{N},\uparrow|\mathcal{H}_2|r',k'_\downarrow,\mathcal{N},\downarrow\rangle$$
$$\simeq\frac{\omega_0-\omega}{4M\epsilon_0N^{1/2}}A^{rr'}_k\delta_{kk'}\,. \tag{4.15}$$

The selection rule evident in (4.15) is interesting, since it can be exploited in a perturbative treatment of $\mathcal{H}_2$ to simplify the calculations. In fact, (4.15) shows that $\mathcal{H}_2$ connects only states with opposite pseudospins and with the same k; consequently, if one adopts a perturbation approach and neglects the matrix elements of $\mathcal{H}_2$ with $r\neq r'$, one is led to diagonalize for each k the very simple 2×2 matrix

$$\begin{vmatrix} E(r,k_\downarrow,\mathcal{N},\downarrow & \frac{\omega_0-\omega}{4M\epsilon_0\mathcal{N}^{1/2}}A^{rr}_k \\ \frac{\omega_0-\omega}{4M\epsilon_0\mathcal{N}^{1/2}}A^{rr}_k & E(r,k_\uparrow,\mathcal{N},\uparrow) \end{vmatrix}\,, \tag{4.16}$$

where $E(r,k_\downarrow,\mathcal{N},\downarrow)=E(r,k_\uparrow,\mathcal{N},\uparrow)$, as remarked previously, and where A^{rr}_k is real. We remind the reader that the corrections of $\mathcal{H}_3$ are of the order of $(\omega_0-\omega)^2$ and must be neglected. The eigenvalues of (4.16) are simply

$$\lambda_\pm(r,k,\mathcal{N})=E(r,k_\uparrow,\mathcal{N},\uparrow)\pm\frac{\omega_0-\omega}{4M\epsilon_0\mathcal{N}^{1/2}}A^{rr}_k\,. \tag{4.17}$$

Thus the bands of $V_\uparrow$ and $V_\downarrow$, which are degenerate in zero-order because these two potentials are simply shifted by $a/2$ with respect to each other, are split off resonance by the action of $\mathcal{H}_2$. We remark that the splitting vanishes on resonance and this feature is shared with the splitting obtained by the Floquet-Lyapounov theory which we have mentioned in the Introduction.[10,12] We are, however, in a position to investigate the physical meaning of this splitting. In fact, suppose that at time $t=0$ we put the atom in a wavepacket with average position $\langle x\rangle_0$ and velocity

$$\langle V\rangle_0=\left\langle\frac{\partial E(r,k_\uparrow,\mathcal{N},\uparrow)}{\partial k_\uparrow}\right\rangle$$

in the $V_\uparrow$ potential. After a time t, neglecting dispersion and in the absence of $\mathcal{H}_2$, we still find the particle in the $V_\uparrow$ potential with velocity $\langle v\rangle_0$ at the average position $\langle x\rangle_0+\langle V\rangle_0 t$. Equation (4.17) tells us that the action of $\mathcal{H}_2$ is such as to displace periodically the particle from $V_\uparrow$ to $V_\downarrow$ with frequency $(\lambda_+-\lambda_-)$. Consequently, after time $t=(\lambda_+-\lambda_-)^{-1}$, the average position of the particle is shifted by the quantity $a/2$ with respect to the position $\langle x\rangle_0+\langle v\rangle_0 t$. This is another aspect of the velocity modulation experienced by the dressed atom and discussed at the end of Sec. III C. We are

led to conclude that the band splitting of the Floquent-Lyapounov theory is due to this velocity modulation effect.

We may now inquire more precisely than we did at the beginning of Sec. III C about the limit of validity of the self-consistent procedure that has led us to identify "the best" zero-order potential for our problem in the neighborhood of resonance as the discontinuous one of choice A defined by (3.5). We shall adopt a quantitative self-consistent criterion by requiring that the average splitting induced by $\mathscr{H}_2$ on the eigenvalues of $\mathscr{H}_1$ be smaller than the average splitting which is characteristic of the unperturbed spectrum of $\mathscr{H}_1$, as measured by the bandwidth W_r given by (4.8). In practice we shall require that

$$\langle\,|\,\lambda_+(r,k,\mathscr{N})-\lambda_-(r,k,\mathscr{N})\,|\,\rangle < W_r\ , \qquad (4.18)$$

where the average on the left-hand side (LHS) of (4.18) is taken over all possible values of k belonging to the same band r. The form of (4.18) suggests an interesting interpretation of the self-consistency criterion in terms of the velocity modulation previously discussed. In fact, the inverse of the LHS of (4.18) is proportional to the average time for an atom in the rth band to switch from the $V_\uparrow$ to the $V_\downarrow$ potential, while W_r^{-1} can be interpreted as the average time for the same atom to move over the distance between two neighboring wells in the $V_{\uparrow\downarrow}$ potential. Thus if the former is much larger than the latter, the atom during its motion through the periodic potential shall see the same potential for a long time, which is just another way to say that the potential of choice A is self-consistent enough. On the contrary, if the two sides of (4.18) are equal, the potential of the atom shall switch between $V_\uparrow$ and $V_\downarrow$ at the same rate at which it is hopping from one well to the next, and a look at Figs. 2(a) and 3(a) will clearly show that the effective potential seen by the atom in these conditions is equivalent to one of the two potentials of choice B, which is a symptom of lack of self-consistency of choice A.

In order to extract more information from (4.18), we have to specialize in a definite model for the local potential $V_\uparrow^j(x)$. A convenient choice might be

$$V_\uparrow^j(x)=-\epsilon_0\mathscr{N}^{1/2}\left[\left[1+\frac{(\omega_0-\omega)^2}{8\epsilon_0^2\mathscr{N}}\right]+\left[1-\frac{(\omega_0-\omega)^2}{8\epsilon_0\mathscr{N}}\right]\tfrac{1}{2}Q^2(x-x_j)^2\right]\ , \qquad (4.19)$$

which reduces to $V_\uparrow$ for $x\to x_j$ up to terms of order of $(x-x_j)^2$ and $(\omega_0-\omega)^2$. When using (4.19) in (4.8), however, we must remember to discard terms of the order $(\omega_0-\omega)^2$ coherently with all previous approximations. Thus we find

$$V_\uparrow(x_j+a/2)-V_\uparrow^j(x_j+a/2)\approx\tfrac{1}{2}\pi^2\epsilon_0\mathscr{N}^{1/2} \qquad (4.20)$$

and

$$E_r\approx-\epsilon_0\mathscr{N}^{1/2}+(r+\tfrac{1}{2})[(2\epsilon_0\mathscr{N}^{1/2})(Q^2/2M)]^{1/2}\ , \qquad (4.21)$$

while the $\psi_r(x-x_j)$ are the usual eigenfunctions of the harmonic oscillator of frequency

$$\Omega=[(2\epsilon_0\mathscr{N}^{1/2})(Q^2/2M)]^{1/2} \qquad (4.22)$$

in terms of which it is possible to prove that

$$\beta_r=\frac{1}{\sqrt{\pi}}\frac{1}{2^r r!}\int_{-\infty}^{+\infty}e^{-z^2/2}H_r(z)e^{-(z-\sqrt{M\Omega}a)^2}\times H_r(z-\sqrt{M\Omega}a)dz$$
$$=e^{-M\Omega a^2/4}L_r(M\Omega a^2/2)\ , \qquad (4.23)$$

where $H_r(z)$ and $L_r(z)$ are Hermite and Laguerre polynomials, respectively.[17] Within the same approximation we obtain

$$A_k^{rr}=\frac{4}{\sqrt{\pi}}\cos(ka/2)\frac{1}{2^r r!}e^{-M\Omega(a/4)^2}\times M\Omega H_r(\sqrt{M\Omega}\,a/4)\times[2rH_{r-1}(\sqrt{M\Omega}\,a/4)-\sqrt{M\Omega}\,(a/4)H_r(\sqrt{M\Omega}\,a/4)]\ . \qquad (4.24)$$

In principle, results (4.20)–(4.24) can be substituted in (4.18), which is then expressed in terms of the basic parameters of the system. In practice this is not very useful due to the complicated form of the results, and it is convenient to resort to more approximations to improve the transparency of the theory. We point out, however, that the r dependence of β_r and A_k^{rr} imply that (4.18) itself is r dependent, which opens the interesting possibility that the potential of choice A may be self-consistent for some of the bands that it originates, and not for others. To investigate this possibility, we observe that for large intensity of the standing wave it is

likely that

$$\sqrt{M\Omega}a=\sqrt{2}\pi[(2\epsilon_0\mathcal{N}^{1/2})/(Q^2/2M)]^{1/4}\equiv\sqrt{2}\pi R^{1/4}$$
$$[R=(2\epsilon_0\mathcal{N}^{1/2})/(Q^2/2M)] \quad (4.25)$$

is larger than 1 since R is the ratio between the depth of the effective potential and the recoil energy of the atom for a single absorption process. Thus for r not too large we may appropriate the orthogonal polynomials in (4.23) and (4.24) as[17]

$$L_r(z)\sim(-1)^r z^r/r!\,,\quad H_r(z)\sim(2z)^r \quad (4.26)$$

and also

$$E_r=-\epsilon_0\mathcal{N}^{1/2}[1-2(r+\tfrac{1}{2})R^{-1/2}]$$
$$\approx-\epsilon_0\mathcal{N}^{1/2}\,. \quad (4.27)$$

Because of (4.26) we obtain

$$\beta_r\sim\frac{2^r}{r!}(\sqrt{M\Omega}a/2)^{2r}\exp(-M\Omega a^2/4)\,,$$
$$\langle\,|A_k^r|\,\rangle\sim\frac{1}{\sqrt{\pi}}\frac{1}{2^{r-2}r!}\frac{1}{a^2}(\sqrt{M\Omega}a/2)^{2r+3}$$
$$\times\exp(-M\Omega a^2/16)\,. \quad (4.28)$$

With approximations (4.27) and (4.28), (4.18) can be put into the form

$$\frac{|\omega_0-\omega|}{2\epsilon_0\mathcal{N}^{1/2}}<2^{2r}(\pi/2)^{-3/2}(1+\pi^2/2)R^{1/4}$$
$$\times\exp(-3\pi^2R^{1/2}/8)\,, \quad (4.29)$$

whose surprisingly simple r dependence illustrates the fact that for large ratio of R, choice A is self-consistent for low-energy bands, provided $|\omega_0-\omega|/2\epsilon_0\mathcal{N}^{1/2}$ is small enough. Moreover, (4.25) shows that a small R corresponds to a situation in which the spread $(M\Omega)^{-1}$ of the localized ground-state wave function $\psi_0(x-x_j)$ is larger than the wavelength of the standing field, and in these conditions the tight-binding approach becomes questionable. It is likely, however, that a sizable region of intermediate values of R exists in which the tight-binding approximation is valid but the oscillations of $L_r(z)$ and $H_r(z)$ in (4.23) and (4.24) call for different self-consistent potentials in different bands. This may occur also if the approximate expression (4.29) is valid; for example, assuming $|\omega_0-\omega|/(Q^2/2M)\approx7.10^{-2}$, then (4.29) is satisfied for any band if $R=1$, whereas if $R=1.5$, (4.29) is not satisfied for the $r=0$ band.

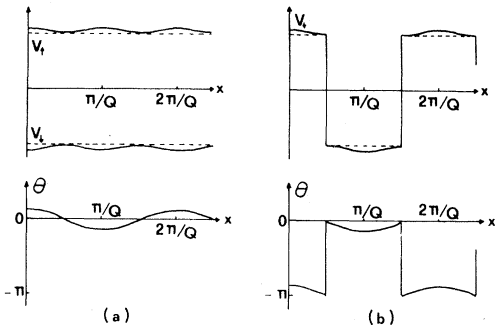

FIG. 6. (a) The potentials $V_{\uparrow\downarrow}(x)$ for $4\epsilon_0^2\mathcal{N}/(\omega_0-\omega)^2=0.2$ (continuous line) and 0 (broken line), and $\theta(x)$ for $4\epsilon_0^2\mathcal{N}/(\omega_0-\omega)^2=0.2$ according to choice B. (b) The potential $V_\downarrow(x)$ for $4\epsilon_0^2\mathcal{N}/(\omega_0-\omega)^2=0.2$ (continuous line) and 0 (broken line), and $\theta(x)$ for $4\epsilon_0^2\mathcal{N}/(\omega_0-\omega)^2=0.2$ according to choice A. $V_\uparrow(x)=-V_\downarrow(x)$.

V. SELF-CONSISTENT POTENTIAL FAR FROM RESONANCE

In this section we shall discuss the choice for the appropriate $\theta(x)$ in (2.1) when the detuning of the standing wave from the bare atomic Larmor frequency in large, i.e., for $2\epsilon_0\mathcal{N}^{1/2}<|\omega_0-\omega|$. We shall first argue qualitatively that in these conditions choice B is the appropriate one. For this we may rely on past experience and on the clear-cut limiting case $2\epsilon_0\mathcal{N}^{1/2}/|\omega_0-\omega|\to0$. In fact, in the latter limit (which we can think of as being attained for $\epsilon_0\to0$) we expect that the bare Hamiltonian coincides with the dressed Hamiltonian; con-

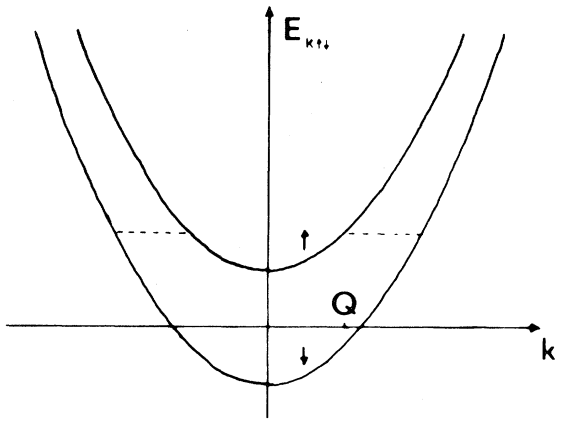

FIG. 7. Approximate eigenvalue spectrum of $\mathscr{H}_1$. $E_{k\uparrow\downarrow}=E(k,\mathcal{N},\uparrow\downarrow)-\omega(\mathcal{N}-\frac{1}{2})$. The points connected by the discontinuous segments of length Q correspond to eigenstates of $\mathscr{H}_1$ with the same energy of k differing by $\pm Q$.

sequently, there should not be any physical justification for the discontinuities of $V_{\uparrow\downarrow}(x)$ induced by choice A at points x_m and evident in Fig. 6(b). Moreover, the gentle slopes of $\theta(x)$ according to choice B for $2\epsilon_0\mathcal{N}^{1/2}/|\omega_0-\omega|>0$ but small [see Fig. 6(a)], imply small values of the matrix elements of $\mathscr{H}_2$ and $\mathscr{H}_3$, which depend on the derivatives of $\theta(x)$, as is obvious from (3.2). In contrast, the discontinuities in $\theta(x)$ introduced by choice A indicate large values of the matrix elements of $\mathscr{H}_2$ and $\mathscr{H}_3$ between the eigenstates of $\mathscr{H}_1$. We are thus led to conclude that for $2\epsilon_0\mathcal{N}^{1/2}<|\omega_0-\omega|$, choice B is the best and the associated potential $V_{\uparrow\downarrow}(x)$ shown in Fig. 6(a) is the most convenient starting point for a perturbation treatment of $\mathscr{H}_2$ and $\mathscr{H}_3$.

More quantitatively, we assume that R defined in (4.25) is large. Moreover, from (3.27) and for $2\epsilon_0\mathcal{N}^{1/2}<|\omega_0-\omega|$, we approximate

$$V_{\uparrow\downarrow}(x)\approx\pm\tfrac{1}{2}|\omega_0-\omega|\left[1+\frac{4\epsilon_0^2\mathcal{N}}{(\omega_0-\omega)}\frac{1}{8}(e^{2iQx}+e^{-2iQx}+2)\right]. \tag{5.1}$$

The effect of the periodic terms in (5.1) is to open gaps in the free particle spectrum of the atomic center of mass at points such as $k=Q$. These gaps, however, are very small, being of the order of $(2\epsilon_0\mathcal{N}^{1/2}/|\omega_0-\omega|)^2$, and we shall neglect them. Consequently, we further approximate (5.1) simply to a constant potential

$$V_{\uparrow\downarrow}(x)\approx\pm\tfrac{1}{2}|\omega_0-\omega| \tag{5.2}$$

and neglect the band structure of $\mathscr{H}_1$. Thus we label the eigenfunctions of $\mathscr{H}_1$, with $V_{\uparrow\downarrow}$ given by (4.2), as $|k,\mathcal{N},\uparrow\downarrow\rangle\equiv|k\rangle|\mathcal{N},\uparrow\downarrow\rangle$ with

$$\langle x|k\rangle=\frac{1}{\sqrt{L}}e^{ikx},\quad k=\frac{2\pi l}{L}\quad(l=0,\pm1,\pm2,\ldots), \tag{5.3}$$

where we have imposed periodic boundary conditions at points $0,L$. The corresponding eigenvalues are obviously

$$E(k,\mathcal{N},\uparrow\downarrow)=\omega(\mathcal{N}-\tfrac{1}{2})\pm\tfrac{1}{2}|\omega_0-\omega|+\frac{1}{2M}k^2 \tag{5.4}$$

and are represented in Fig. 7.

Coherently with the above approximations, and according to choice B, we take θ from (2.3) as

$$\theta\approx\frac{2\epsilon_0\mathcal{N}^{1/2}}{\omega_0-\omega}\cos Qx\ . \tag{5.5}$$

Elementary differentiation and integration lead to

$$\langle k|(2i\theta' p+\theta'')|k'\rangle\approx-\frac{\epsilon_0\mathcal{N}^{1/2}}{\omega_0-\omega}Q[(Q+2k')\delta_{k',k-Q}+(Q-2k')\delta_{k',k+Q}]\ . \tag{5.6}$$

Consequently, we obtain the matrix elements of $\mathscr{H}_2$ between the eigenstates of $\mathscr{H}_1$ as

$$\langle k,\mathcal{N},\downarrow|\mathscr{H}_2|k',\mathcal{N},\uparrow\rangle\approx-\frac{2\epsilon_0\mathcal{N}^{1/2}}{\omega_0-\omega}\frac{1}{8M}\{[k^2-(k-Q)^2]\delta_{k',k-Q}+[k^2-(k+Q)^2]\delta_{k',k+Q}\}\ , \tag{5.7}$$

while the matrix elements of $\mathscr{H}_3$, being proportional to θ'^2, are obviously of the order of $(2\epsilon_0\mathcal{N}^{1/2}/|\omega_0-\omega|)^2$ and must be neglected.

Equation (5.7) shows that $\mathscr{H}_2$ connects states of $\mathscr{H}_1$ with opposite pseudospins and subject to the selection rule $k-k'=Q$. For most of these states $\mathscr{H}_2$ can be treated by second-order perturbation theory, which yields the following shifts:

$$\Delta E(k,\mathcal{N},\uparrow\downarrow)\left[\frac{\epsilon_0^2\mathcal{N}}{(\omega_0-\omega)^2}\frac{1}{(4M)^2}\left[\frac{[k^2-(k-Q)^2]^2}{\pm|\omega_0-\omega|+k^2/2M-(k-Q)^2/2M}+\frac{[k^2-(k+Q)^2]^2}{\pm|\omega_0-\omega|+k^2/2M-(k+Q)^2/2M}\right]\right. . \tag{5.8}$$

Usually these terms should be neglected, being of the same order as θ'^2, except near where either of the energy denominators vanish. This happens for k near to

$$\begin{aligned} k_{0\uparrow} &= \mp\left[\frac{Q}{2}-\frac{M}{Q}|\omega_0-\omega|\right] \quad \text{(pseudospin}\uparrow\text{)} \\ k_{0\downarrow} &= \pm\left[\frac{Q}{2}+\frac{M}{Q}|\omega_0-\omega|\right] \quad \text{(pseudospin}\downarrow\text{)}. \end{aligned} \tag{5.9}$$

With the help of Fig. 7 and of (5.7), it easy to see that this implies real processes in which the dressed atom exchanges a photon with the standing-wave field to change both its internal state and its center-of-mass kinetic energy, the overall energy being conserved. Since (5.8) diverges, however, the effects of these processes on the eigenvalue spectrum of $\mathcal{H}_1$ must be evaluated exactly by solving secular equations of the form

$$\begin{vmatrix} E(k,\mathcal{N},\downarrow)-\lambda & \langle k,\mathcal{N},\downarrow|\mathcal{H}_2|k-Q,\mathcal{N},\uparrow\rangle \\ \langle k-Q,\mathcal{N},\uparrow|\mathcal{H}_2|k,\mathcal{N},\downarrow\rangle & E(k-Q,\mathcal{N},\uparrow)-\lambda \end{vmatrix} . \tag{5.10}$$

A straightforward calculation which uses (5.4), (5.7), and (5.9) yields, for $k=|k_{0\downarrow}|$, the result

$$\lambda_\pm = E(|k_{0\downarrow}|,\mathcal{N},\downarrow)\pm\epsilon_0\mathcal{N}^{1/2}/2 . \tag{5.11}$$

If we compare the relative shift $\lambda_+-\lambda_-$ induced by $\mathcal{H}_2$ with the splitting $|\omega_0-\omega|$ characteristic of the eigenvalue spectrum of $\mathcal{H}_1$, we obtain

$$\epsilon_0\mathcal{N}^{1/2} < |\omega_0-\omega| , \tag{5.12}$$

which may be interpreted as the condition for the validity of our approach, and consequently as the sufficient condition for the self-consistency of choice B for large detunings. We remark that (5.12) is less restrictive than $2\epsilon_0\mathcal{N}^{1/2}<|\omega_0-\omega|$, by which we have defined the domain of large detunings, and seems to indicate that choice B is self-consistent at least throughout all this domain.

IV. COMPARISON WITH PREVIOUS THEORIES

In this section we wish to compare our results with those previously obtained by other authors. The problem of representing by a suitable potential the effects of a standing electromagnetic wave on the dynamics of a two-level atom was taken up rather explicitly by Kazantsev and collaborators.[6–8] Using a semiclassical approach for the motion of atomic center of mass and the bare atom representation, he concluded[8] that the effective potential is of the form

$$V_{\uparrow\downarrow} = \begin{cases} \mp\epsilon_0\mathcal{N}^{1/2}\cos Qx & [(\omega_0-\omega)^2<2\epsilon_0\mathcal{N}^{1/2}Qv/\pi] \\ \pm\frac{1}{2}[(\omega_0-\omega)^2+4\epsilon_0\mathcal{N}\cos^2 Qx]^{1/2} & [(\omega_0-\omega)^2>2\epsilon_0\mathcal{N}^{1/2}Qv/\pi] \end{cases} \tag{6.1}$$

where we have expressed his results in our notation, and where v is the velocity of the atom. While the lower part of (6.1) coincides with the results of our choice B off resonance, we see that in the quasiclassical approach the discontinuities of choice A near resonance are entirely lost, since the upper part of (5.1) coincides with the exact resonance potential. Moreover the expression for the critical detuning which separates the two cases of (6.1) seems to differ both from our result (4.18) near resonance and from (5.12) off resonance. Here we shall show that the critical detuning in (6.1) can be obtained as an approximation from our off-resonance case of Sec. V. In fact, approximating θ as in (5.5) and us-

ing $p=mv$ with constant v in a semiclassical fashion, we obtain from (3.2)

$$\mathscr{H}_2=\frac{1}{4M}\frac{2\epsilon_0\mathscr{N}^{1/2}}{\omega_0-\omega}(2iQMv\sin Qx+Q^2\cos Qx)$$

$$\times\mathscr{N}^{-1/2}(\alpha S_+-\alpha^\dagger S_-)\,. \tag{6.2}$$

This operator may change the potential from $V_\uparrow$ to $V_\downarrow$ and vice versa along the classical trajectory of the dressed atom, particularly near points x_m (if $v\gg Q/M$), where $\mathscr{H}_2$ takes the form

$$\mathscr{H}_2(x_m)=(-1)^m i\frac{\epsilon_0\mathscr{N}^{1/2}}{\omega_0-\omega}Qv\mathscr{N}^{-1/2}(\alpha S_+-\alpha^\dagger S_-)\,. \tag{6.3}$$

As a glance at Fig. 6 will show, however, a change from $V_\uparrow$ to $V_\downarrow$ at any point x_m has the interesting result of transforming the potential from that of choice B to that of choice A; consequently, if the transition amplitude induced by (6.3) between states $|\mathscr{N},\uparrow\rangle$ and $|\mathscr{N},\downarrow\rangle$ is small with respect to the splitting $\sim|\omega_0-\omega|$ between these eigenstates of $\mathscr{H}_1$, we should expect that choice B is appropriate and that the self-consistent potential is that of Fig. 6(a). Otherwise the potential of choice A represented in Fig. 6(b) is a better approximation to the real situation. The condition for the validity of choice B is quantitatively expressed as

$$|\langle\mathscr{N},\uparrow|\mathscr{H}_2|\mathscr{N},\downarrow\rangle|=\frac{\epsilon_0\mathscr{N}^{1/2}}{\omega_0-\omega}Qv<|\omega_0-\omega|\,, \tag{6.4}$$

which coincides within a factor of $\pi/2$ with the Kazantsev expression for the critical detuning.[8] Thus we see that Kazantsev's result implies neglect of the fluctuation in the kinetic energy, and that the critical detunings turn out to be rather sensitive to this approximation.

We now compare our results with those of the exact Floquent-Lyapounov theory. From a qualitative point of view, we may now explain the physical origin of the doubling of the Brillouin zone of the system (when going from $\omega_0-\omega=0$ to $\omega_0-\omega\neq0$), which was obtained by Letokov and Minogin,[10,12] as follows. For $\omega_0=\omega$, the effective potential is simply cosinusoidal of period $2\pi/Q$ and $\mathscr{H}_2+\mathscr{H}_3=0$; consequently, the Brillouin zone is defined for $-Q/2<k\leq Q/2$, as is evident from (3.6). For $\omega_0-\omega\neq0$, but within the limit of choice A, the potential acquires the discontinuities evident in Fig. 2 and its period is still $2\pi/Q$; in an exact treatment, however, this symmetry is broken by $\mathscr{H}_2$ which induces transition to a final potential shifted over a distance $a/2=\pi/Q$ with respect to the initial potential, thereby introducing some doubly periodic features in the forces acting on the atom and enlarging the first Brillouin zone to $-Q>k\leq Q$. We remark that in view of our approximate treatment of $\mathscr{H}_2$ in choice A, we have found it natural not to change the amplitude of the first Brillouin zone. The doubling of the Brillouin zone in our treatment becomes evident for large detuning such that choice B is appropriate; in this case in fact the effective potentials are of period π/Q and of the same form as those represented in Figs. 3(a) or 6(a). We may conclude that our treatment has succeeded in relating the dimensions of the Brillouin zone to the form of the effective potential acting on the atomic center of mass. Another feature of the exact Floquet-Lyapounov theory whose physical origin is not clear in the Letokhov-Minogin treatment is the splitting of the bands. In our treatment this splitting is to be associated entirely to the action of $\mathscr{H}_2$ near resonance where choice A is valid, and to the combined action of $\mathscr{H}_2$ and of the detuning for $|\omega_0-\omega|>\epsilon_0\mathscr{N}^{1/2}$. $\mathscr{H}_2$ originates from the fact that the kinetic energy does not commute with the unitary operator T of (3.1) which performs a local dressing of the atom; consequently, we see that the appearance of $\mathscr{H}_2+\mathscr{H}_3$ is ultimately related to the impossibility of performing a local dressing without simultaneously changing the atomic velocity by an unpredicted amount, and that from a quantitative point of view the complementarity between momentum and the atomic dressing, which is impossible to eliminate, is entirely contained and represented in $\mathscr{H}_2+\mathscr{H}_3$. For $\omega_0=\omega$, $\theta(x)$ in T becomes a constant equal to $-\pi/2$, independent of the atomic coordinate, and the dressing can be performed exactly without perturbing the atomic momentum. We are thus led to the conclusion that the splitting of the bands near resonance is intimately related to the quantum-mechanical features of the atomic dynamics. As for a quantitative comparison of our splitting with that obtained by the Floquet-Lyapounov theory, we remark that it must be done on a numerical basis, since the closed analytical form of the results of the latter theory is too complicated. Moreover, Letokhov and Minogin have produced numerical examples only for the following values of the parameters[10,12]:

$$R=\frac{2\epsilon_0\mathcal{N}^{1/2}}{Q^2/2M}=13\ ,$$
$$\frac{\omega_0-\omega}{Q^2/2M}=\pm 0.4 \text{ and } R=10\ , \tag{6.5}$$
$$\frac{\omega_0-\omega}{Q^2/2M}=0.5\ .$$

Unfortunately all these examples fall out of the reach of our approximations, since on the one hand the relatively large values of R in (6.5) yield very restricted limits of validity of (4.29) for choice A, and on the other hand the relatively small value $|\omega_0-\omega|/\epsilon_0\mathcal{N}^{1/2}\approx 0.1$ makes choice B questionable because of (5.12). In spite of these limitations, however, it is possible to deduce from the dispersion curves of Letokhov and Minogin that the band splitting turns out to be of the order of $\epsilon_0\mathcal{N}^{1/2}$, which is of the same order as the band splitting of our choice B discussed in Sec. V; this is not unreasonable since the parameters in (6.5) correspond to situations nearer to choice B than to choice A. Finally, we wish to comment briefly on the localizability of cold atoms at particular points of the standing-wave field. As it is obvious from Fig. 2, near resonance our effective-potential approach immediately yields the antinodes of the standing wave as plausible sites for localization, while off resonance and within the domain of choice B, the nodes or the antinodes of the standing wave become preferred sites for excited and ground-state dressed atom, respectively.

VII. CONCLUSIONS

In summary, we have taken up the problem of a two-level atom in a standing-wave field with the aim of showing that the effects of this field on the atom can be represented by a suitable effective static potential. We have shown that a class of canonical transformations exists which formally eliminate the off-diagonal atom-field interaction from the Hamiltonian, dressing the atom by the standing-wave field. These canonical transformations, however, act also on the external degrees of freedom of the two-level atom, introducing new off-diagonal operators $\mathcal{H}_2$ and $\mathcal{H}_3$ in the kinetic energy of atomic center of mass. The member of this class of canonical transformations which is most suitable for the purpose of defining the effective potential is chosen in a self-consistent fashion as the one which, for a particular set of parameters (such as detuning and field amplitude) minimizes the matrix elements of $\mathcal{H}_2$ and $\mathcal{H}_3$ between the eigenstates of the rest $\mathcal{H}_1$ and the total Hamiltonian. This procedure yields, for each range of detunings $|\omega_0-\omega|\lesssim 2\epsilon_0\mathcal{N}^{1/2}$, $\mathcal{H}_1$ in the form of the Hamiltonian of a two-level atom in an effective pseudospin-dependent periodic potential $V_{\uparrow\downarrow}(x)$ which may be taken as representing in a first approximation (that is, neglecting $\mathcal{H}_2$ and $\mathcal{H}_3$) the effects of the standing-wave field on the atom. Roughly speaking, the features of $V_{\uparrow\downarrow}(x)$ as a function of the detuning can be described as follows.

(i) For $\omega_0=\omega$ the effective potential is of a pure cosine form and of period $a=2\pi/Q$ equal to that of the standing wave field, $V_\uparrow$ and $V_\downarrow$ being related by a simple shift over the distance $a/2$.

(ii) For $|\omega_0-\omega|<2\epsilon_0\mathcal{N}^{1/2}$ and small enough, the period of the potential is still a and $V_\uparrow$ and $V_\downarrow$ are simply related as in (i), but the self-consistent effective potential turns out to be periodically discontinuous.

(iii) For $|\omega_0-\omega|>2\epsilon_0\mathcal{N}^{1/2}$ the potential is periodic and continuous, but its periodicity is $a/2$; moreover $V_\uparrow$ and $V_\downarrow$ are different and not related to each other by a space translation. For each of the above ranges, approximate eigensolutions of $\mathcal{H}_1$ have been obtained which satisfy the Floquet theorem and which on resonance approximate the periodic solutions of the Mathieu equation. In particular, for $|\omega_0-\omega|<2\epsilon_0\mathcal{N}^{1/2}$ the tight-binding approximation has been used to study the low-energy solutions, which have been shown to consist of a set of bands for $V_\uparrow$ and of an identical set of bands for $V_\downarrow$, degenerate with the first; for $|\omega_0-\omega|>2\epsilon_0\mathcal{N}^{1/2}$ the free-atom approximation has been adopted as a reasonable starting point and has been shown to yield two free-energy spectra, one for each $V_{\uparrow\downarrow}$, displaced in energy from each other by the quantity $|\omega_0-\omega|$. All these eigensolutions of $\mathcal{H}_1$ are self-consistent in the sense discussed above. In a second approximation, we have shown that the effects of $\mathcal{H}_3$ on the self-consistent solutions of $\mathcal{H}_1$ are negligible in all the ranges of detuning studied, while the effects of $\mathcal{H}_2$ are the following.

(a) For $\omega_0=\omega$, $\mathcal{H}_2=0$ rigorously.

(b) For $|\omega_0-\omega|<2\epsilon_0\mathcal{N}^{1/2}$, $\mathcal{H}_2$ yields a splitting of the degenerate low-energy bands of $\mathcal{H}_1$ due to a modulation of the atomic velocity, which in turn is caused by the periodic change between $V_\uparrow$ and $V_\downarrow$ of the potential seen by the dressed atom.

(c) For $|\omega_0-\omega|>2\epsilon_0\mathcal{N}^{1/2}$, $\mathcal{H}_2$ may induce real processes which involve exchange of a photon with the field, change of the internal state of the dressed

atom, and change of its velocity, the total energy being conserved in each process; these processes turn out to be resonant in the neighborhood of particular values of k and cause anomalies in the free-atom dispersion relations of the order of $\epsilon_0 \mathcal{N}^{1/2}$.

The limit of validity of our procedure have been obtained in each range of detuning by requiring that the splittings and shifts induced by $\mathscr{H}_2$ be smaller than the typical energy differences of the $\mathscr{H}_1$ eigenvalue spectrum. For $|\omega_0-\omega| < 2\epsilon_0 \mathcal{N}^{1/2}$ this criterion gives different limits for different bands, opening the possibility that in this range of detuning some of the bands see an effective potential different from the others. On the other hand, for $|\omega_0-\omega| > 2\epsilon_0 \mathcal{N}^{1/2}$ the criterion has been shown to be satisfied for any energy of the quasifree atom. The above criteria for self-consistency of the different forms of the effective potential have been compared to that yielded by a semiclassical approach for the motion of the atomic center of mass, which we have obtained from our treatment as an approximation valid when the changes in the velocity of the dressed atom due to the effective potential can be neglected. Moreover, considerations of the results of the Floquet-Lyapounov exact theory in the limit of those of the present theory has been shown to yield a better understanding of the former, by relating the form of the eigenvalue distributions to the effective forces acting on the dressed atom and to the dynamical features of the atomic motion.

Finally, we take up briefly the question of the quantization of the electromagnetic field. It is interesting to point out that the self-consistency of our approach, up to Sec. III, is entirely independent of the commutative properties of the field operators α and $\alpha^\dagger$. This is also true in principle for the application of the tight-binding approximation of Sec. IV, although the practical limitations to the magnitude of the coupling constant make the validity of this approximation questionable for small photon numbers, since it may prove difficult to obtain $R > 1$ with small $\mathcal{N}$. Thus we may conclude that our results on the shape of the effective potential in the different ranges of detuning are valid in principle also for small intensities of the driving field, where the effects of field quantization are usually important. It is perhaps worth emphasizing that the discontinuities in the effective potential that we have found necessary to introduce near resonance are not due in fact to the field quantization, but to the quantization of the atomic center-of-mass motion, as we have already discussed.

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[1] A. Ashkin, Phys. Rev. Lett. 25, 1321 (1970); R. M. Hill, and T. F. Gallagher, Phys. Rev. A 12, 451 (1975); E. Arimondo, H. Lew, and T. Oka, Phys. Rev. Lett. 43, 753 (1979).

[2] A. Ashkin, Phys. Rev. Lett. 24, 156 (1970); 40, 729 (1978); J. P. Gordon and A. Ashkin, Phys. Rev. A 21, 1606 (1980).

[3] A. Yu. Pusep, Zh. Eksp. Teor. Fiz. 70, 851 (1976) [Sov. Phys.—JETP 43, 441 (1976)]; A. Yu. Pusep, A. B. Doktorov, and A. I. Burshtein, *ibid.* 72, 98 (1977) [*ibid.* 45, 52 (1977)]; V. G. Minogin, *ibid.* 79, 2044 (1980) [*ibid.* 52, 1032 (1980)]; T. K. Melik-Barkhudarov, Phys. Lett. A 82, 109 (1981); R. J. Cook, Phys. Rev. A 23, 1243 (1981).

[4] V. S. Letokhov, V. G. Minogin, and B. D. Pavlik, Zh. Eksp. Teor. Fiz. 72, 1328 (1977) [Sov. Phys.—JETP 45, 698 (1977)]; R. J. Cook, and A. F. Bernhardt, Phys. Rev. A 18, 2533 (1978); R. J. Cook, Phys. Rev. Lett. 44, 976 (1980); Phys. Rev. A 22, 1078 (1980); E. B. Gelman, D. F. Zaretskii, and V. V. Lomonosov, Opt. Spektrosk. 48, 451 (1980) [Opt. Spectrosc. (USSR) 48, 247 (1980)]; A. F. Bernhardt and B. W. Shore, Phys. Rev. A 23, 1290 (1981); E. Arimondo, A. Bambini, and S. Stenholm, Opt. Commun. 37, 103 (1981); Phys. Rev. A 24, 898 (1981).

[5] G. Compagno, J. S. Peng, and F. Persico, Phys. Lett. A88, 285 (1982).

[6] A. P. Kazantsev, Zh. Eksp. Teor. Fiz. 63, 1628 (1972) [Sov. Phys.—JETP 36, 861 (1973)]; 66, 1599 (1974) [39, 784 (1974)].

[7] A. P. Kazantsev, Zh. Eksp. Teor. Fiz. 67, 1660 (1974) [Sov. Phys.—JETP 40, 825 (1975)]; A. P. Botin, and A. P. Kazantsev, *ibid.* 68, 2075 (1975) [*ibid.* 41, 1038 (1976)]; A. P. Kazantsev, G. I. Surdutovich, and V. P.

Yakovlev, Pis'ma Zh. Teor. Fiz. 31, 542 (1980) [JETP Lett. 31, 509 (1980)].

[8]A. P. Kazantsev, Usp. Fiz. Nauk. 124, 113 (1978) [Sov. Phys.—Usp. 21, 58 (1978)].

[9]V. S. Letokhov and V. G. Minogin, Phys. Lett. A61, 370 (1977).

[10]V. S. Letokhov and V. G. Minogin, Zh. Eksp. Teor. Fiz. 74, 1318 (1978) [Sov. Phys.—JETP 47, 690 (1979)].

[11]V. G. Minogin, Opt. Commun. 37, 442 (1981); V. G. Minogin, V. S. Letokhov, and T. V. Zueva, *ibid.* 38, 225 (1981).

[12]V. S. Letokhov, V. G. Minogin, Phys. Rep. 73, 1 (1981).

[13]P. Carbonaro, G. Compagno, F. Persico, Phys. Lett. A73, 97 (1979); A76, 37 (1980); F. Persico, in *Modern Trends in the Theory of Condensed Matter,* edited by A. Pekalsky and J. Pryzstawa (Springer Berlin, 1980), pp. 571—597; G. Compagno, A. Panzerella, and F. Persico, Phys. Lett. A80, 125 (1980); G. Compagno and F. Persico, Phys. Rev. A 22, 2108 (1980); G. Compagno and F. Persico, Phys. Rev. A 25, 3138 (1982).

[14]J. C. Slater, Phys. Rev. 87, 807 (1952).

[15]G. Blauch, in *Handbook of Mathematical Functions,* edited by M. Abramowitz and I. A. Stegun (Dover, New York, 1965), pp. 721—750.

[16]N. W. Ashcroft, and N. D. Mermin, *Solid State Physics* (Holt, Rinehart, and Winston, New York, 1976), p. 176.

[17]U. W. Hochstrasser, in *Handbook of Mathematical Functions,* edited by M. Abramowitz and I. A. Stegun (Dover, New York, 1965), pp. 771—802.